Plenary I-A

The Role of Aerosols in the Transmission of COVID-19.

LINSEY MARR, *Virginia Tech*

There is growing evidence that aerosols are an important route of transmission of COVID-19. The virus that causes the disease, SARS-CoV-2, has been found in the air of hospital rooms and directly in the exhaled breath of patients, and certain superspreading events are best explained by aerosols. Transmission of infectious disease by aerosols is a highly interdisciplinary topic that draws upon epidemiology, virology, and especially aerosol science. Breathing, talking, coughing, and sneezing release respiratory droplets spanning a wide range of sizes. These may contain virus if a person is infected. Physically, virus-laden droplets are subject to the same transport and removal mechanisms as are airborne particles; we can apply fundamental principles about particle behavior to understand the dynamics of virus in the air. Evaporation of respiratory droplets leads to shrinkage and changes in chemical composition that may affect virus viability. Laboratory studies indicate that SARS-CoV-2 remains infectious in aerosols for many hours. While aerosol science informs our understanding of the transmission of COVID-19 and other respiratory infectious diseases, it also provides us with tools to mitigate transmission. Aerosol science explains why distancing, masks, and good ventilation can help reduce exposure to the virus.

Plenary I-B

Aerosols and Masks: Building Bridges from Aerosols Science to Clinical Infectious Disease Practice.

DONALD MILTON, *University of Maryland School of Public Health*

Respiratory viral infections in general can be transmitted via contact (direct and indirect), sprayborne drops from the mouth and nose, and aerosols composed of a wide range of droplet sizes. Medical literature frequently uses the terms respiratory droplets and aerosols – terminology that was established in the late 19th and early 20th centuries. The false dichotomy between droplets and aerosols produces confusion and miscommunication that hinders effective infection control. Dr. Milton will draw on respiratory physiology, aerosol and building science, aerobiology, exposure science, and industrial hygiene to provide a clear picture of transmission modes and their implications for understanding the data available on the modes of transmission for SARS-CoV-2 and the impact of universal masking.

Learning objectives:

Participants will be able to
1. Understand how the common medical use of the terms “respiratory droplets” and “aerosols” leads to confusion.
2. Describe the difference between an inhalable-nasopharyngeal, thoracic, and respirable aerosol and the implications of aerosol droplet size for infection transmission.
3. Understand the hierarchy of controls and the importance of engineering and source controls.

Plenary II

Nanoparticles from Engines: Then and Now. DAVID KITTELSON, *University of Minnesota*

The earliest measurements of engine exhaust size distributions involved manual collection and counting or weighing. Frey and Corn (1967) characterized particles collected from a small diesel engine with an electron microscope. They found them to be very small aggregates with geometric mean diameters ranging from 21 to 62 nm depending on engine load. Vuk et al. (1976) reviewed manual sizing methods focusing mainly on cascade impactors that had poor size resolution in the submicron size range, lumping all particles smaller than 600 nm into a single size bin. Such manual methods were associated with long collection and analysis times.

Whitby and Clark (1966) described the first automated, near real-time, instrument for sizing submicron particles. It sized particles by electrical mobility diameter in 12 size bins between 10 nm and 1 µm. Whitby et al., (1975) describe size distributions measured upwind and downwind of a California freeway in 1972. They found that nearly all the particles added by the roadway, weighted by surface area, were in the ultrafine range, This early on-road work laid the foundation for measurements of engine exhaust size distributions in controlled laboratory settings at the University of Minnesota. For many years the work focused on improving our understanding the influence engine design, operating conditions, and fuels on particle emissions. However, in the mid-1990s new interest in particle size emerged as a result of a study by the Health Effects Institute (Bagley et al., 1996). This work showed that some new diesel engine technologies reduced mass emissions, which were regulated, but increased number emissions, which were not. This focused attention on measurement of particles in the nucleation mode where most of the particle number, mainly nanoparticles smaller than 50 nm diameter, is found. Since then work all over the world has focused on measurement and regulation of engine generated nanoparticles, diesel, spark, and even aircraft gas turbine.

Critical issues associated with such measurements will be reviewed.

Plenary III: AEESP Lecture

The Clear Sky Bias in Atmospheric Chemistry. ANNMARIE CARLTON, *University of California, Irvine*

Liquid water is a critically important constituent of the troposphere. At any given time, more than half of Earth's surface is covered by visible clouds, and cloudiness changes in a changing climate. Aerosol-cloud interactions are critical to processes that govern air quality, radiative forcing and regional hydrological cycling. Yet, persistent uncertainties in these processes limit predictive skill of atmospheric models across scales. Clouds are primary drivers of vertical transport in the atmosphere, moving trace species from the polluted boundary layer to the Free Troposphere. Partitioning of water-soluble gases and their condensed phase chemistry generates particle mass aloft, such as sulfate, water-soluble organic carbon, and organosulfur compounds. Key uncertainties are related to the chemical nature of hygroscopic aerosol that become cloud condensation nuclei (CCN) and their interaction with organic species. Gas-to-droplet or gas-to-aqueous aerosol partitioning of organic compounds is affected by the intrinsic chemical properties of the organic species in addition to the pre-existing condensed phase. Environmentally relevant conditions for most atmospheric aerosol are non-ideal and chemical theory is incomplete. For example, salt identity and concentration, in addition to aerosol phase state, can dramatically affect organic gas miscibility for many compounds, in particular when ionic strength and salt molality are outside the bounds of limiting laws. The effects of inorganic salts on the fate and transport of organic species in the atmosphere are discussed.

Plenary IV

Air Quality in Spacecraft: What We Know about Aerosols in the International Space Station and What We Need to Know about Aerosols in Future Space Missions. MARIT MEYER, *NASA Glenn Research Center*

The International Space Station (ISS) gives a 6-member astronaut crew the ability to live and work in low Earth orbit. It is a unique indoor environment, which has served as both home and workplace to over 230 people since the year 2000. In this low gravity environment, smoke does not rise and cookie crumbs do not settle the way they do on Earth, causing aerosols to behave differently and pose unique hazards for crew members. In its existence, virtually the same volume of ISS air has been continuously conditioned and ‘revitalized,’ including the removal of particles by filtration. While gaseous constituents of ISS air are monitored meticulously, the indoor aerosols have only recently been prioritized by NASA. The quantities and types of ISS airborne debris have been investigated in two Aerosol Sampling Experiments. Results of the particle collection and implications for the air quality in future spacecraft will be presented. Further characterization follows in the next experiments, which will take the first real-time aerosol measurements for ISS air quality with a reference-quality instrument, followed by miniaturized instruments. This talk will show the progression of the NASA ‘technology roadmap’ for aerosol monitoring in spacecraft, which extends to longer duration exploration missions in the next decades. In particular, NASA’s Artemis Moon Mission in 2024, and the challenges of lunar dust aerosols will be presented.

Plenary V: Friedlander Lecture

Atmospheric Aerosol Chemistry: Climate and Air Quality. DOUGLAS WORSNOP, *Aerodyne Research, Inc.*

Despite much effort in the past decades, uncertainties in both climate impacts and health effects of atmospheric aerosols remain large. During the last twenty years, aerosol mass spectrometry (AMS) has shown that sub-micron aerosol chemical composition is roughly 50:50 inorganic and organic worldwide, with secondary highly oxidized organics dominating the latter. Parallel application of chemical ionization mass spectrometry (CIMS) has provided the first observation of molecular cluster ions involved in atmospheric nucleation, including detection of highly oxidized multifunctional (HOM) organics in the gas phase. These results will be discussed in the context of their impact on atmospheric aerosols, air quality and climate; from the boreal forest to Chinese megacities.

1AC.1

Global Distribution of the Phase State and Mixing Times within Secondary Organic Aerosol Particles in the Troposphere Based on Room-Temperature Viscosity Measurements. ADRIAN MACLEAN, Ying Li, Natalie R. Smith, Giuseppe Crescenzo, Anusha P.S. Hettiyadura, Kyla Siemens, Celia Faiola, Alexander Laskin, Sergey Nizkorodov, Manabu Shiraiwa, Allan Bertram, *University of British Columbia*

Information on the phase state of secondary organic aerosol (SOA) and the mixing time of water in SOA are critical for predicting when SOA can act as ice nuclei in the atmosphere. As well, information on the mixing times of organics in SOA are important for predicting SOA growth, evaporation, and reactivity. Using meteorological fields and laboratory viscosity data, we estimated the phase state and mixing times of organics and water in biogenic and anthropogenic SOA in the troposphere. Based on the laboratory viscosity data, biogenic and anthropogenic SOA are in a glassy state in the upper free troposphere. Mixing times of water are often > 1 h at altitudes > 10 km. Mixing times of organics are often > 1 h at altitudes > 7 km, suggesting the particles are not in equilibrium with the surrounding environment in the upper free troposphere. The results obtained using our methodology are consistent with the results from Shiraiwa et al. (Nature Communications, 2017) using a different approach and further illustrate the importance of the glass state and slow mixing times of water and organic molecules in the upper part of the free troposphere.

1AC.2

Secondary Organic Aerosol Volatility on Mixed Anthropogenic and Biogenic Precursor Systems.
ARISTEIDIS VOLIOTIS, Yu Wang, Yunqi Shao, Mao Du, Thomas Bannan, Rami Alfarra, Gordon McFiggans, *University of Manchester*

Secondary organic aerosols (SOA) are ubiquitous in the atmosphere and contribute a large fraction of the total aerosol mass with substantial impacts on climate (Jimenez et al., 2009; Kanakidou et al., 2005). Aerosol volatility is linked with the partitioning of their components between the gas and the particle phase, defining their transformation pathways into the atmosphere and eventually, their physical and chemical properties (Ehn et al., 2014). Over the last decades, smog chamber studies have proposed several mechanisms through which gas to particle partitioning is governed (Hallquist et al., 2009). Nevertheless, the vast majority of these studies are focused on single-component precursors.

Recent evidence has showed that upon mixtures of atmospheric vapours, the potential of aerosol formation is governed by the mechanistic interactions between the products of the oxidised precursors (McFiggans et al., 2019). These results demonstrate the deficit in our knowledge regarding the aerosol behaviour in such conditions.

This study is exploring the volatility of SOA formed from the photo-oxidation of mixtures of characteristic biogenic and anthropogenic volatile organic precursors, in an atmospheric simulation chamber. Furthermore, our analysis is framed by detailed gas and particle phase chemical composition measurements and the effect of the various chemical processes on the volatility is investigated.
The experiments were representative of “daytime” photo-oxidation and conducted at the University of Manchester Aerosol Chamber (MAC) facilities. Two types of experiments conducted: (a) single precursor and (b) mixture experiments. All the experiments conducted under low NOx conditions (VOC/NOx ~6±2), moderate RH and temperature conditions (~50±5% and 25±2 oC, respectively), under the presence of ammonium sulfate seed (~53±12 μg m-3).

A scanning mobility particle sizer and a high-resolution time of flight aerosol mass spectrometer were sampling downstream of a thermal denuder (TD), operating at temperatures ranging from 25 to 90 oC. To obtain SOA volatility distributions, the resulted mass fraction remaining (MFR) in each step was used under the approach of Karnezi et al (2014). Furthermore, near-real time gas and particle molecular composition was measured by employing the Filter Inlet for Gas and Aerosols coupled to an Iodine high-resolution time of flight chemical ionisation mass spectrometer (FIGAERO-CIMS).

The results that will be presented provide new and additional information on SOA volatility, clearly illustrating the effect of mixing on SOA volatility. The combination of TD and FIGAERO techniques has the potential to substantially contribute to an improved understanding of the processes influencing the phase partitioning of the organic components.

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1AC.3

Mass Accommodation and Gas-Particle Partitioning of Semivolatile Compounds in Organic Aerosols: Diffusivity, Viscosity, and Penetration Depth Dependence. MANABU SHIRAIWA, Ulrich Pöschl, *University of California, Irvine*

Mass accommodation is an essential process for gas-particle partitioning of semi-volatile organic compounds into organic aerosols. The mass accommodation coefficient is commonly used to represent a probability of a molecule collided to the surface to be incorporated into the particle phase. It is often applied, however, without specifying if and how deep a molecule has to penetrate beneath the surface to have entered the condensed phase (adsorption vs. absorption). While this aspect may usually not be critical for liquid particles with rapid surface-bulk exchange, it can be critical to distinguish and resolve the kinetics of accommodation at the surface, transfer across the gas-particle interface, and further transport into the particle bulk for viscous semisolid or glassy solid particles. In this study, we suggest a novel concept of penetration-depth-dependent mass accommodation coefficient, which is a function of surface accommodation coefficient, volatility, bulk diffusivity, and particle-phase reaction rate coefficient. Its application in traditional Fuchs-Sutugin gas-phase diffusion model yields consistent results with detailed kinetic multilayer modeling for partitioning of secondary organic aerosols (SOA). We reveal that for highly viscous particles mass accommodation coefficient of low-volatile compounds would remain unity, but it can be reduced by several orders of magnitude for semivolatile compounds which need to be properly accounted to accurately simulate kinetics of particle growth. These results challenge traditional approach of SOA models and provide a practical method to properly account for effects of viscosity on SOA processes in regional and global air quality models.

1AE.1

Green Heart Louisville: Community-Level Assessment of Exposure to Air Pollution. PRADEEP S. PRATHIBHA, Eben Cross, Richard Strehl, Ray Yeager, Aruni Bhatnagar, Jay R. Turner, *Washington University in St. Louis*

Green Heart Louisville (greenheartlouisville.com) is a prospective cohort study examining linkages between urban vegetation and cardiovascular health, an association potentially mediated by the effect of vegetation on local air quality. We monitor long-term air quality and greenness in a 12 km^2 study area in Louisville, KY, in tandem with a clinical study assessing cardiovascular function and risk factors in area residents. A 2.5 km^2 contiguous section serves as the intervention area where mature vegetation is installed beginning in Fall 2019; the remaining area serves as the control.

We monitor high time-resolution ambient particulate pollution through (1) periodic $PM_{2.5}$ measurements (1min) using PurpleAir and Alphasense OPCN2 particulate monitors—the latter mounted in QuantAQ air quality nodes—at four fixed locations and (2) recurring ultrafine particle (UFP) number concentrations (1s) on a mobile-platform. Log-transformed daily mean $PM_{2.5}$ mass concentrations from collocated PurpleAir and OPCN2 sensors are well-correlated ($R=0.72$, $p \ll 0.001$), but the mean of ratios (OPC/PA, 0.19 ± 0.10) of absolute $PM_{2.5}$ reveals large bias. Contemporaneous $PM_{2.5}$ from QuantAQ nodes are highly correlated ($0.77<r<0.83$) at locations with varying proximities to an interstate highway, an international airport, and commercial/industrial facilities.

Mobile-platform UFP measurements show strong dependence on wind direction: for winds parallel to an interstate highway with a 10ft sound wall, near-road (10-50m) concentrations remain at background levels during rush hour traffic conditions; under crosswinds, however, 3-5-fold elevated concentrations extend 750m downwind of the sound wall even at night. These measurements show that air pollutants have distinct and persistent spatiotemporal patterns within the study domain. Future work will integrate advanced GIS techniques like hyperlocal landuse regression models to estimate residential-level exposure to air pollution before and after planting to inform the clinical study.

1AE.2

First Measurements of PM2.5 in Kinshasa, Democratic Republic of Congo (DRC). CELESTE MCFARLANE, V. Faye McNeill, Daniel Westervelt, *Columbia University*

With an estimated annual count of 780,000 premature deaths linked to air pollution in Africa, there is a great need for improved air pollution monitoring efforts to motivate the policy changes necessary to improve health outcomes. Kinshasa, DRC is a megacity with over 11 million inhabitants and no reference grade air pollution monitors, leading to much concern for air quality. Recently, a few reference grade monitors have been deployed elsewhere in Africa, including Kampala, Uganda. Reference grade air quality monitors can serve as an important basis for the correction and calibration of low cost sensors (LCS) for air quality monitoring. While LCS offer a path to remedy the lack of air pollution data in Africa, they are affected by environmental factors such as temperature and humidity, leaving a need for a correction factor to establish high quality data.

We present the first ever in-field calibration of LCS against reference grade monitors in Kampala, Uganda. A Purple Air $PM_{2.5}$ monitor was colocated next to the Kampala US Embassy BAM-1020 in August 2019. Raw Purple Air data is strongly correlated with BAM ($r = 0.94$), but has a mean absolute error of approximately 12 µg/m^3. Two calibration models, multiple linear regression and a random forest machine learning approach show that the mean absolute error decreased to less than 0.01 from 12 µg/m^3 with the correlation improved to $r = 0.96$. We then apply the colocated in-field correction factors to four Purple Air sensors in Kinshasa, DRC and one in neighboring Brazzaville, collecting data from as far back as April 2018. This results in a high quality sensor network data set. Data shows peaks from June-September, when rain is infrequent, with a trend of decreasing peak size every calendar year (approx. 80 µg/m^3 in 2018, 55 µg/m3 in 2019 and 38 µg/m^3 in 2020) . Regionally averaged diurnal trends show a peak of approximately 48 µg/m^3 at 6 pm GMT (7 PM WAT). Comparing data from the COVID lockdown period of 2020 to that of 2019 shows a reduction in $PM_{2.5}$ concentrations from 45 µg/m^3 in April of 2019 to approximately 10 µg/m^3 in April of 2020. All of the pre-COVID values are well above the US EPA national air quality annual mean standard for $PM_{2.5}$ of 12 µg/m3 , suggesting a need for air quality policy reform in Kinshasa, DRC.

1AE.3

Source-Resolved Primary Organic Aerosol Exposure Estimates in the United States. Provat Saha, Ellis Shipley Robinson, Wenwen Zhang, Steven Hankey, Julian Marshall, ALLEN ROBINSON, Albert A. Presto, *Carnegie Mellon University*

Primary organic aerosol (POA) has a significant contribution to fine particulate matter concentration at urban scales. High-resolution aerosol mass spectrometer (HR-AMS) data and Positive Matrix Factorization analysis offer source-resolved speciation of organic aerosol, which has been extensively applied in atmospheric field studies. We bring this technique in exposure research. We develop traffic and cooking POA exposure estimates through highly spatially resolved HR-AMS mobile sampling in three North American cities (Oakland, Pittsburgh, Baltimore) and empirical land-use regression modeling. As expected, we find both cooking and traffic POA concentrations vary substantially within and between cities. Within-city spatial variabilities are (4-6x) greater than between-city spatial variabilities (2x). Surprisingly, cooking POA concentration is higher than traffic POA concentration in each city. In land-use regression model development, traffic-related land-use variables (road density, transportation land use) explain the spatial variably of traffic POA, and cooking related variables (restaurant density, commercial land use) explain the spatial variability of cooking POA. External validation of model estimates against data from different atmospheric field studies across the US shows good agreement. This indicates the extrapolation of models over wider geographic areas is possible. We apply our models to predict national concentration surfaces of cooking and traffic POA in the US at the census block level. We use these estimates to assess the POA exposure inequality by race, income, and region.

1AP.1

Particle Size Distribution Dynamics Can Help Constrain the Phase State of Secondary Organic Aerosol. CHARLES HE, Ali Akherati, Theodora Nah, Jeffrey R. Pierce, Rahul Zaveri, Christopher Cappa, Lauren A. Garofalo, Nga Lee Ng, Delphine K. Farmer, Shantanu Jathar, *Colorado State University*

Particle phase state is an important property of atmospheric aerosols that has implications for the formation, evolution, and gas/particle partitioning of secondary organic aerosol (SOA). Yet, the phase state of SOA and its relation to the VOC precursor, SOA molecular composition, and environmental variables remain largely uncertain. In this work, we use a size-resolved chemistry and microphysics model (i.e., SOM-TOMAS), updated to include an explicit treatment of particle phase state, to constrain the bulk diffusion coefficient (D_b) of SOA produced from alpha-pinene ozonolysis. By leveraging laboratory experiments performed in the absence of a seed and under dry conditions, we find that the D_b for SOA can be constrained ($\sim 4\times10^{-19}$ m^2 s^{-1} in these experiments) by simultaneously reproducing the time-varying SOA mass concentration, O:C ratio, and, most importantly, the evolution of the number size distribution. The D_b could not be constrained with the seeded experiments because the model-predicted evolution of the particle size distribution was nearly identical over a large range of D_b values (10^{-16} to 10^{-23} m^2 s^{-1}) due to the SOA coating thickness being relatively thin and similar across all seed diameters. An updated version of our model that used the model-predicted SOA composition to calculate the glass transition temperature, viscosity, and, ultimately, D_b ($\sim 10^{-19}$ m^2 s^{-1}) of the SOA was able to reproduce the measurements when we also included rapid oligomer formation that accounted for more than half of the SOA mass. Our work highlights the potential of a size-resolved SOA model to constrain the particle phase state of SOA by leveraging historical measurements of the evolution of the particle size distribution.

1AP.2

Diurnal and Seasonal Variations of Secondary Organic Aerosol Phase State over the Continent US Simulated in CMAQ.

YING LI, Annmarie Carlton, Kirk Baker, Manabu Shiraiwa, *University of California, Irvine*

Secondary organic aerosol (SOA) accounts for a substantial portion of atmospheric particulate matter. Accurate descriptions of formation and evolution of SOA remain a grand challenge in air quality models in which SOA particles have often been assumed to be homogeneous and well-mixed liquids and the semi-volatile oxidation products rapidly establish a gas-particle equilibrium partitioning. Recent laboratory experiments and atmospheric measurements, however, have demonstrated that SOA can occur in amorphous solid or semi-solid phase states, which may result in kinetic limitations in gas-particle partitioning. A phase transition between amorphous solid and semi-solid state occurs at glass transition temperature (T_g), which can be predicted based on organic molecular composition (Shiraiwa et al., 2017; Li et al., 2020). In this study we simulate T_g and SOA phase state over the contiguous US in 2016 using the Community Multiscale Air Quality (CMAQ) model to investigate potential locations where thermodynamic gas-particle partitioning should be more thoroughly evaluated. Simulations show that T_g and SOA viscosity are higher in the west than the eastern US which is due to higher mass fractions of accretion products and lower relative humidity in the western US. SOA viscosity is predicted to be higher in the daytime than the nighttime, and higher in Spring than other seasons. The diurnal and seasonal variations in SOA viscosity are substantially smaller than the difference between the viscosity in the western and eastern US. Vertical profiles show that SOA occur mainly as semi-solid and solid in the middle and upper troposphere, consistent with our previous global simulations (Shiraiwa et al., 2017).

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1AP.3

The Effect of Rotation and Preferred Orientation on Particle Mobility in the Free Molecular Regime.

CARLOS LARRIBA-ANDALUZ, Viraj Gandhi, *IUPUI*

A recently developed MonteCarlo algorithm, IMoS 2, explores the drift-diffusion of an ion which is subject to an arbitrary field in a modeled real gas. See Figure 1 where the ion is in a buffer gas and subject to an electric field. The electric field accelerates the ion producing gas-ion collisions.

The ion can freely rotate and its orientation, angular velocity and drift velocity are a function of the gas-ion collisions, the reduced mass, the strength of the field over concentration(E/N), and the position of the charges within the ion. The position of the charges may provide a dipole moment that will be taken into account. It is the effect of the collisions and the particle orientation together with the electric field which now establishes the equilibrium drift velocity, preferred orientation, if any, and angular velocity. This equilibrium drift velocity, together with non-linearized theory, establishes the relation between field and mobility which in turn yields the true mobility of the ion.

The mobility calculator has been tested with different sets of isotopomers, (Iodo-TMT molecules) and isotopologues (arginine molecule). The mobility of Iodo-TMT and arginine ions was measured in Nitrogen and Helium using the Structure for Lossless Ion Manipulations (SLIM) platform which allows resolutions of 200-500. Small deviations were observed for both arginine and TMT ions suggesting that the effect of angular momentum and moments of inertia is sufficient to separate two entities in the gas phase. The results of IMoS 2 prove, for the first time, that an ion with identical structure and mass may be separable using electrical/ion mobility through shifts in angular momentum and moments of inertia alone.

1CA.1

Changes in Light Absorption Driven by Two Different Oxidation Processes on Atmospheric Tar Balls from Wildfires in Western United States. BENJAMIN SUMLIN, Nishit Shetty, Andrew Lambe, Edward Fortner, Andrew Lambe, Rajan K. Chakrabarty, *Washington University in St. Louis*

Carbonaceous aerosol interacts with sunlight to drive radiative forcing by scattering and absorbing incoming sunlight. Carbonaceous aerosol is broadly categorized as either black carbon (BC), otherwise known as soot or elemental carbon, and organic carbon (OC). Organic carbon aerosol was once thought to be purely scattering; however, we now understand that a class of organic carbon aerosol known as tar balls strongly absorbs sunlight, particularly in the short visible and near-UV wavelengths, contributing positively to Earth's radiation balance. Furthermore, there is a growing body of evidence that the light absorption characteristics of these aerosol are impacted by atmospheric processing, including oxidation reactions. A new multiwavelength photoacoustic spectrometer, developed in the Complex Aerosol Systems Research Laboratory at Washington University in St. Louis, was installed on board the Aerodyne Mobile Laboratory during FIREX-AQ. It measured light scattering and absorption by aerosol at four wavelengths (405, 488, 561, and 637 nm) from several wildfires in the western United States, both from ambient air and after these aerosols were subjected to two different oxidation processes using an Aerodyne Potential Aerosol Mass oxidation flow reactor. Daylight-driven oxidation was mimicked by exposing tar balls to varying quantities of OH radical, while nighttime processes were mimicked using NO3. We present a comparison of the effects on light absorption of these two processes in context of previous laboratory findings.

1CA.2

Examination of Brown Carbon Absorption from Wildfires in the Western U.S. during the WE-CAN Study. AMY P. SULLIVAN, Rudra Pokhrel, Yingjie Shen, Shane Murphy, Darin Toohey, Teresa Campos, Jakob Lindaas, Emily Fischer, Jeffrey Collett, *Colorado State University*

Brown carbon (BrC) can potentially be a significant contributor to the visible light absorption budget. However, the contribution of particulate BrC to light absorption as well as the sources of BrC are not well understood. One major source of BrC is thought to be biomass burning. Therefore, as part of the WE-CAN (Western Wildfire Experiment for Cloud Chemistry, Aerosol Absorption and Nitrogen) Study we collected BrC absorption data from aboard the C-130 aircraft as it flew through smoke from wildfires occurring in the Western U.S. in July-August 2018. BrC absorption measurements were obtained by two techniques. The first coupled a Particle-into-Liquid Sampler (PILS) with a Liquid Waveguide Capillary Cell and a Total Organic Carbon analyzer for near real-time measurements of BrC absorption and WSOC (water-soluble organic carbon). The second employed a custom-built Photoacoustic Aerosol Absorption Spectrometer (PAS) to measure total absorption at red and blue wavelengths and then calculate black carbon and BrC absorption. Airborne results from these measurements for a number of different wildfires will be presented. A high correlation was found between WSOC and BrC absorption for wildfire smoke. It was also observed that the fraction of the BrC absorption in wildfire smoke due to water-soluble species was ~45%. When using calculated particle mass concentrations, provided by UHSAS (Ultra-High-Sensitivity Aerosol Spectrometer) measurements, to account for the non-water-soluble fraction of BrC absorption, good closure was found between the absorption determined by the PAS and PILS measurements when accounting for the differences in particle vs. bulk solution absorption. In addition, the relationship between the BrC absorption and known smoke markers will be examined. How parameters such as aging and fire dynamics might play a role on the BrC absorption from wildfires will also be discussed.

1CA.3

Light Absorbing Properties of Biomass Burning-influenced Organic Aerosols in Southeast Asia.

NETHMI KASTHURIARACHCHI, Laura-Helena Rivellini, Alex Lee, *National University of Singapore*

Biomass burning (BB) used for agriculture and forest management in Southeast Asia have been responsible for severe haze that have generated light absorbing aerosols that heat up the upper troposphere by up to 20 Wm^{-2} (Ge et al., 2014). The widespread peatlands in this region usually undergo smoldering conditions below surface levels at low temperatures for prolonged periods with occasional surface flaring, which is different to the burning conditions of surface vegetation.

In this work, we use a soot particle aerosol mass spectrometer (SP-AMS) to identify the sources of organic aerosols (OA) during two BB-influenced periods in Singapore, a highly urbanized country in Southeast Asia where influence from transboundary smoke together with local urban emissions and atmospheric processing of BB-influenced aerosols during transport results in a complex mixture of OA. Together with absorption measurements from a seven-wavelength aethalometer, we quantify the absorption properties of both primary and secondary OA (POA and SOA) influenced by BB. We find that for the first period, which was influenced by relatively fresh BB, a small fraction of strongly absorbing BBOA were responsible for a majority of the light absorption by OA while another BBOA factor had very weak light absorbing properties. Haze, influenced by transboundary smoke, governed the second BB-influenced period where the BBOA factors were more oxygenated and less light absorbing than the fresh BB observed in the previous campaign, likely due to photobleaching that may have occurred during transport. A SOA factor, influenced by both local chemistry and atmospheric processing of BB emissions, had significant light absorbing properties highlighting the importance of the impact of BB on the absorptivity of SOA. This is the first field study to quantify absorption properties of different types of POA and SOA influenced by BB in Southeast Asia.

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1ID.1

Measurements of Patient-Generated SARS-CoV-2 Aerosols and Surface Contamination at the University of Nebraska Medical Center.

JOSHUA SANTARPIA, St. Patrick Reid, Danielle Rivera, Vicki Herrera, Shanna Ratnesar-Shumate, Kevin Crown, Nicholas Markin, Steven Lisco, St. Patrick Reid, Jane Morwitzer, Paul Denton, Jacob Martens, Ying Fang, Michael Callahan, Jana Broadhurst, Hanna Creager, Conoan Nicholas, David Brett-Major, Elizabeth Schnaubelt, James Lawler, John Lowe, *University of Nebraska Medical Center*

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) originated in Wuhan, China, and the resulting disease, COVID-19, is an ongoing global pandemic. Initial uncertainty around the role of aerosols in transmission led to shifting guidance from worldwide public health organizations. We began environmental surveys around patients beginning with those transferred from the Diamond Princess cruise ship, and continues with patients in isolation care. In these studies, we have collected both aerosol and surface samples with both severely ill and less symptomatic individuals, during various stages of illness. We have used rRT-PCR analysis to identify the presence of SARS-CoV-2 in the samples, and have performed cell culture to determine viral infectivity. Aerosol collections initially focused on high-volume sampling (50 Lpm) and later focused on size-segregated samples and measurements of aerosol distributions. Cell culture proved difficult, particularly with initial samples, but infectious virus was identified in several samples. Ongoing work is attempting to understand the viral shedding rate of infected patients and the characteristics of viral aerosol shed by patients throughout the course of disease. These studies produced the first observations of infectious SARS-CoV-2 from environmental samples. Therefore, these studies, in context with other studies, suggest the importance of the airborne transmission route, and further indicate the breathing and vocalization may be important to the production of viral aerosols, providing potential explanation for reported asymptomatic and presymptomatic transmission events and highlight the importance of airborne isolation precautions in hospital care and the importance of implementing effective measures against aerosol transmission in public health.

1ID.2

Collection of SARS-CoV-2 Virus from the Air in a University Student Health Care Center and Analyses of its Viral Genomic Sequence. John Lednicky, SRIPRIYA NANNU SHANKAR, Maha Adel El Badry, Julia C. Gibson, MD Mahbubul Alam, Caroline J Stephenson, Arantzazu Eiguren Fernandez, John Glenn Morris, Carla Nartuhi Mavian, Marco Salemi, James R Clugston, Chang-Yu Wu, *University of Florida*

Tracking the progression of COVID-19 worldwide can be achieved by identifying mutations within the genomic sequence of SARS-CoV-2 that occur as a function of time. Currently, such efforts rely on genomic sequencing of SARS-CoV-2 in patient specimens (direct sequencing) or of virus isolated from patient specimens in cell cultures. We conducted a pilot air sampling study at a clinic within a university student health care center in late March, 2020, and detected the virus RNA (vRNA) with an estimated concentration of 0.87 virus genomes/L of air. Attempts were made to isolate the virus in cell cultures to determine whether the virus detected was viable (‘live’). Virus-induced cytopathic effects (CPE) were observed within two days post-inoculation of Vero E6 cells with collection media from air samples; however, rRT-PCR tests for SARS-CoV-2 vRNA from cell culture were negative. Instead, three other fast-growing human respiratory viruses were isolated and subsequently identified (Human coronavirus OC43, and Influenza A H1N1 and H3N2 viruses), illustrating the challenge in isolating SARS-CoV-2 when multiple viruses are present in a test sample. The complete SARS-CoV-2 genomic sequence was determined by Sanger sequencing of vRNA extracted from the aerosol sample and deposited as SARS-CoV-2/ENV/USA/UF-3/2020 in GenBank (accession no. MT324684.1). Maximum likelihood (ML) phylogenetic tree analysis revealed that this virus’ genome exactly matches (100% identity) a SARS-CoV-2 genome previously described in Georgia, USA. Results of this study illustrate the feasibility of tracking progression of the COVID-19 pandemic using environmental aerosol samples instead of human specimens. Collection of a positive sample from a distance 3 m away from the nearest patient traffic implies the virus was in an aerosol.

1ID.3

Comparison of the Performance of Personal Biological Aerosol Samplers for SARS-CoV-2. SHANNA RATNESAR-SHUMATE, Gregory Williams, Brian Holland, Jordan Bohannon, Melissa Krause, Brian Green, Denise Freeburger, Paul Dabisch, *DHS NBACC*

To understand and mitigate the potential risk of person-to-person aerosol transmission of SARS-CoV-2, characterization of the viral load near or around infected individuals is critical. Multiple types of aerosol sampling devices have been employed in recent studies to measure the amount of virus present around infected humans and animals and in exhaled breath. Aerosol sampling devices employ multiple capture mechanisms such as impingement, filtration or impaction of bioaerosols into or onto a substrate for subsequent assay and quantification. Depending on the biological organism being studied, the type of device used for sampling may cause inactivation and thus prevent detection of infectious aerosol. In this study, the biological sampling efficiencies of the SKC Biosampler, AGI-4, Midget Impinger, Sioutas Impactor, NIOSH BC251 sampler, gelatin and Teflon filters were evaluated and assayed to measure relative concentrations of infectious virus and RNA copies per liter of air. Results demonstrating that RNA copies per liter of air do not consistently correlate with infectious viral titers under different environmental conditions will be presented along with general recommendations for interpreting current data on the SARS-CoV-2 viral loads in air samples and guidance for future studies.

This work was supported by the DHS Science and Technology Directorate (under agreement number HSHQDC-15-C-00064) awarded to Battelle National Biodefense Institute for the management and operation of the National Biodefense Analysis and Countermeasures Center, a Federally Funded Research and Development Center.

1RA.1

Persistent Influence of Biomass Burning Aerosols during Clean Air Conditions in the Western United States.

RYAN FARLEY, Noah Bernays, Daniel Jaffe, Qi Zhang, *University of California, Davis*

Biomass burning (BB) is an important source of primary and secondary air pollutants, and biomass burning aerosols can directly influence regional and global air quality and climate. The aging of these aerosols and impacts on the remote background is still poorly understood. In this study, we deployed a high-resolution time-of-flight soot particle aerosol mass spectrometer (SP-AMS) coupled with a thermodenuder at the Mt. Bachelor Observatory (MBO) in Oregon to characterize the chemical composition and properties of wildfire-influenced aerosols during the summer of 2019 (Aug. 1 – Sept. 8). MBO is a high altitude site (~2800m a.s.l.) which has previously been used to examine long-range transport and BB plumes. Relatively low submicron aerosol concentrations (PM_1) were seen (2.2±1.9 $\mu g/sm^3$) compared to previous years, with the mass dominated by organic species (82.1%). Through positive matrix factorization analysis, an oxidized BB organic aerosol (BBOA) was found to comprise 18% of OA mass on average, and above 50% during plume events. This BBOA factor shows a high O/C (0.65), low volatility and a strong correlation with $C_2H_4O_2^+$ (m/z = 60.021), an SP-AMS BB tracer ion. Five biomass burning plumes were analyzed with transport times estimated to vary from ~10 hours to >10 days. The more processed biomass burning plumes consist of a higher fraction of the CO_2^+ ion to the total organic signal (f_{44}), and a lower fraction of the $C_2H_4O_2^+$ ion (f_{60}). The more aged plumes show lower volatility, and an increase in the peak mass-based size distribution from 400nm to 700nm, suggesting more pronounced aqueous phase processing. This work suggests that BB emissions significantly affect aerosol extinction and atmospheric chemistry in remote locations, with the chemical and physical properties varying depending on atmospheric processing.

1RA.2

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 the 2018 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 nearby desert areas. 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 the internal composition of individual particles. This allowed us to provide quantitative description of the particles’ mixing states. Our findings reveal extensive coating of particle dust components and biomass burning particles with secondary organic material, which affects the aerosol optical properties and present quantitative metrics for practical speciation of aerosol in models.

1RA.3

Relationships between Supermicrometer Sea Salt Aerosol and Marine Boundary Layer Conditions: Insights from Repeated Identical Flight Patterns.

JOSEPH SCHLOSSER, Hossein Dadashazar, Eva-Lou Edwards, Ali Mardi, Gouri Prabhakar, Connor Stahl, Haflidi Jonsson, Armin Sorooshian, *University of Arizona*

The MONterey Aerosol Research Campaign (MONARC) in May–June 2019 featured 14 repeated identical flights off the California coast over the open ocean at the same time each flight day.

The objective of this study is to use MONARC data along with machine learning analysis to evaluate relationships between both supermicrometer sea salt aerosol number (N>1) and volume (V>1) concentrations and wind speed, wind direction, sea surface temperature (SST), ambient temperature (Tamb), turbulent kinetic energy (TKE), relative humidity (RH), marine boundary layer (MBL) depth, and drizzle rate. Selected findings from this study include the following: (i) Near surface (1 and V>1 concentration ranges were 0.1–4.6 cm−3 and 0.3–28.2 µm3 cm−3, respectively; (ii) four meteorological regimes were identified during MONARC with each resulting in different N>1 and V>1 concentrations and also varying horizontal and vertical profiles; (iii) the relative predictive strength of the MBL properties varies depending on predicting N>1 or V>1, with MBL depth being more highly ranked for predicting N>1 and with TKE being higher for predicting V>1; (iv) MBL depths >400 m ((higher) N>1 and V>1 concentrations; (v) enhanced drizzle rates coincide with reduced N>1 and V>1 concentrations; (vi) N>1 and V>1 concentrations exhibit an overall negative relationship with SST and RH and an overall positive relationship with Tamb; and (vii) wind speed and direction were relatively weak predictors of N>1 and V>1.

2AC.1

Photodegradation of Secondary Organic Aerosols by Long Term Exposure to Solar Actinic Radiation.

VAHE BABOOMIAN, Yiran Gu, Sergey Nizkorodov, *University of California, Irvine*

The photochemical aging of secondary organic aerosols (SOA) are crucial to understand the climate and health-related properties of particulate matter, but these photochemical processes are not well understood. We measured the photodegradation rates of SOA by condensed phase photochemical reactions over long time periods of multiple days of ultraviolet exposure. The photodegradation rates of various SOA types were quantified using a quartz crystal microbalance. We observed that 254 nm irradiation degraded SOA almost entirely after 24 h. In contrast, 305 nm irradiation led to initially high mass loss rates (corresponding to 1-5 % fractional mass loss per hour) but slowed down after 24 h of irradiation with a photorecalcitrant fraction of SOA degrading much slower (< 1% fractional mass loss per hour). The mass loss rates were observed to increase at higher relative humidity due to increased diffusivity. Long term changes in chemical composition were observed using a high-resolution electrospray ionization mass spectrometer and suggests a more complex mixture of species remain after degradation. The compounds in the degraded samples had on average lower H:C and higher O:C compared to the compounds in fresh SOA. These experiments confirm that condensed phase photochemical processes are an important SOA aging mechanism during long range transport.

2AC.2

Aqueous Photochemistry of Synthesized Pinene-Derived Carboxylic Acids and Dimer Esters.

CHRISTOPHER KENSETH, Yuanlong Huang, Nathan Dalleska, John Seinfeld, *California Institute of Technology*

Atmospheric aqueous phases (i.e., cloud, fog, and aerosol liquid water) constitute important reaction media for (photo)chemical processing of water-soluble compounds in secondary organic aerosol (SOA). Monoterpenes ($C_{10}H_{16}$), emitted in large quantities from terrestrial vegetation (~150 Tg y^{-1}), represent a dominant source of SOA globally. Multifunctional carboxylic acids and dimer esters have been identified as significant components of both laboratory-derived and ambient monoterpene SOA, and are expected to be sufficiently water soluble to undergo aqueous-phase processing. Due to a lack of authentic standards, however, aqueous-phase studies of such compounds have been limited, almost exclusively, to commercial terpenoic acids (e.g., *cis*-pinonic acid). Here, we investigate the aqueous-phase photooxidation (kinetics, products, and mechanisms) of six recently synthesized, enantiopure, pinene-derived carboxylic acid and dimer ester homologues, at cloudwater-relevant concentrations, using liquid chromatography/negative electrospray ionization mass spectrometry [LC/(−)ESI-MS] together with MS/MS analysis and H/D exchange. Characterization of the OH reactivity of the carboxylic acids and dimer esters, which respectively differ only in the identity of the terminal functional group (i.e., ketone vs. carboxylic acid vs. alcohol), affords detailed insight into the dependence of aqueous-phase photochemical processing on both molecular size and functionality, as well as evaluation of structure-activity relationships (SARs) for aqueous-phase OH oxidation of monoterpene SOA constituents.

2AC.3

Synthesis and Hydrolysis of Atmospherically Relevant Monoterpene Organic Nitrates.

YUCHEN WANG, Masayuki Takeuchi, Tianchang Xu, Amanda J Schwartz, Ivan Piletic, Stefan France, Nga Lee Ng, *Georgia Institute of Technology*

Partition of gas phase organic nitrates (ON) to aerosols and subsequent hydrolysis has been identified as an important loss approach for ON species. Considering the different hydrolysis lifetimes, ONs may act as a permanent sink or temporary reservoir of NO_x, which further impact NO_x recycling, O_3 formation, and SOA formation. However, the hydrolysis mechanisms and the major factors controlling the hydrolysis lifetime are not fully understood. To systematically investigate ON hydrolysis, we synthesized six monoterpene hydroxy nitrates and two ketone nitrates based on two unified synthetic strategies. In situ nuclear magnetic resonance and high-resolution time-of-flight chemical-ionization mass spectrometer (HR-ToF-CIMS) coupled with the filter inlet for gases and aerosols (FIGAERO) were utilized for determining the hydrolysis rate constants for these synthetic standards. We observed that the hydrolysis lifetimes are in the range of 13 mins to 10.1 h for allylic primary ON and tertiary ON but there is no depletion for secondary ON for seven days in neutral condition. The ON hydrolysis was hypothesized to proceed via an acid catalyzed S_N1 mechanism through carbocation intermediate. In our detection, the number of alkyl substitutions, functional groups in adjacent position of nitrooxy group, and carbon skeleton are proposed to be three important factors controlling hydrolysis rates. The degraded products were identified by liquid chromatography-Orbitrap mass spectrometry (LC-Orbitrap MS) and enthalpies were calculated by density-functional theory (DFT). These findings provide new insights into ON hydrolysis mechanism, assessment of ON as NO_x reservoirs/sinks, and fate of atmospheric ON.

2AE.1

Trends in Inter- and Intra-Urban Ultrafine Particle Concentrations in North America: Exposure Implications.

ALBERT PRESTO, Provat Saha, Allen Robinson, *Carnegie Mellon University*

The climatology of ultrafine particles (UFP; particles smaller than 100 nm) has been extensively studied for their ability to grow into cloud condensation nuclei and thereby impact Earth's climate. Human exposures to UFPs are also of concern because these particles, which are not directly regulated in the U.S., may have distinct health effects from exposure to PM2.5 mass. However, less is known about temporal and spatial trends in UFPs and how these trends impact exposure. This talk will address several exposure-relevant questions about UFP: (1) What are typical concentrations? (2) What are the long-term temporal trends? (3) What are inter- and intra-urban spatial patterns? (4) What are the major UFP sources, and how do they drive observed spatial patterns? (5) What are contributions of primary and secondary UFPs to human exposure? (6) Can existing monitoring data be used to estimate national-scale exposures for use in epidemiology?

We will answer these questions by synthesizing a combination of new/unpublished data and results from the literature. These data include long-term (>1 year) measurements in eight cities along with mobile sampling data collected in three cities (Baltimore, Oakland, and Pittsburgh). Since UFPs share many common sources with primary PM2.5 and secondary PM2.5 precursors, concentrations of both UFP and PM2.5 have fallen by ~35% over the past 15 years. UFP exhibit large spatial variability; concentrations vary by a factor of 2-3 within cities, and mean concentrations vary by about a factor of two across cities. A major driver of both the long-term temporal trends and the intra-city spatial patterns are emissions from vehicles. The importance of vehicular emissions highlights that in urban areas, UFP are dominated by primary emissions rather than secondary particles.

2AE.2

In-Car Measurements of Traffic-Related Air Pollutants during Car Commuting. CHEOL H. JEONG, Taylor Edwards, Carson Clark, Alison Traub, Dana Umbrio, Greg J. Evans, *SOCAAR, University of Toronto*

Traffic-related air pollution (TRAP) has been linked to adverse health outcomes and known to have strong temporal and spatial variabilities. In most urban areas, in-car environments for daily car commuters represent one of the more important contributors to daily TRAP exposure. The exposure to TRAP may induce oxidative stress by stimulating cells to produce excessive reactive oxygen species (ROS). Air pollution exposure in this microenvironments needs to be better characterized to assess any resulting production of ROS and to mitigate in-car exposure to TRAP.

Continuous and integrated measurements of TRAP were carried out inside an electric vehicle during morning and evening rush hours on weekdays in summer, fall, winter, and spring in 2019-2020. The In-Car AiR pollution Exposure study (I-CARE) was conducted over 140 commutes between suburbs and downtown Toronto with both highway and local road routes composed of heavy-traffic roads and quiet residential streets. The in-car measurements of gas and particle-phase air pollutants on roadways included nitrogen oxides (NO_x), carbon monoxide (CO), carbon dioxide (CO_2), particulate matter (PM2.5), ultrafine particles (UFP), black carbon (BC), and traffic-related trace metals. In this study, continuous concentrations of these gases and PM2.5 were measured by a portable sensor array (AirSENCE), while real-time UFP and BC were measured by a DiSCmini (Matter Aerosol) and MicroAeth (AE51, AethLabs), respectively. In-car trace metals were determined by analyzing integrated filter samples. In addition to the in-car sampling, outside concentrations of UFP and BC were determined simultaneously while driving. All routes and vehicle speeds were recorded by a GPS receiver and a dashcam.

The in-vehicle exposure to TRAP was assessed under various ventilation modes (open vs. closed), road types, cabin filters, and seasons. In order to estimate the production of ROS of in-car PM2.5, filters extracts were analyzed for oxidative potential (OP), the ability of PM2.5 to deplete antioxidants such as ascorbic acid and glutathione. In-car exposure to TRAP in the open mode was approximately double the ambient level in the downtown area. Substantial exposure reduction was achieved in the closed mode. It was found that OP in the open mode was approximately 8 times higher than that in the closed mode. However, excessive CO_2 accumulation was observed in the closed mode. Various seasonal mitigation strategies by locations and time intervals were explored to reduce in-car TRAP exposure without the issue of excessive CO_2 accumulation.

2AE.3

High-Resolution Cumulative Exposure Assessment of Traffic-Related Air Pollution with Different Google Navigation Route Options. MINMENG TANG, Deb Niemeier, *University of California, Davis*

In this paper, we calculate exposure concentrations of traffic-related air pollutants for different traffic modes in the urban environment. We simulate 5,000 trips in Oakland California, US, and calculate the exposure concentrations of nitric oxide (NO), nitrogen dioxide (NO2), and black carbon (BC) using high-resolution sensors measured air pollution concentration data. These data were collected by Aclima and Google. For each bicycle, transit, and vehicle trip simulation, we calculate the average concentrations and the cumulative exposure of all three pollutants. The cumulative exposure is calculated as the total mass of pollutants being inhaled within the trip. Our results show that cumulative exposure is a more useful metric to assess travel pollutant exposure than average concentration, which is typical in the literature. For all three traffic modes, the average concentrations of each trip are not significantly different. But due to the trip duration and route variations for different traffic modes and the inhalation rates, the cumulative exposure of different traffic modes varies dramatically. Cumulative exposure for those in vehicles tends to be lowest, as well as having the lowest average per meter and per minute exposure based on all simulated trips. Bicyclists and public transit users tend to experience higher cumulative exposures because of the increased inhalation rate and the longer trip duration, respectively. Last but not least, our study shows that total trip duration is more important than total trip distance for air pollution exposure; the shortest duration routes also tend to produce less air pollution exposure than the shortest distance route.

2AP.1

Primary Ion Diffusion Charging and Particle Wall Loss in Smog Chamber Experiments. NASER MAHFOUZ, Neil Donahue, *Carnegie Mellon University*

We investigate the effect of primary ion diffusion charging on particle wall loss in Teflon smog chamber experiments. Primary ion losses are balanced between wall deposition and diffusion charging to larger particles; further, the particle charge distribution evolves toward a chamber-specific charge steady state, different from the so-called “neutralizer steady state” attained inside laboratory neutralizers. This chamber charge steady state depends on the particle size distribution, and the timescale to reach it is often hours. Applying conditions typical of chamber experiments, we conclude that primary ions play an important role in particle wall loss and should be taken into consideration when interpreting experiments.

2AP.2

Inter-comparison of Particle Wall Loss Among UCR Chambers and Caltech Chamber. CHEN LE, Don Collins, David R. Cocker III, *University of California, Riverside*

Understanding particle wall loss mechanisms is critical in environmental chamber studies because accurate wall loss corrections minimize uncertainty in measured aerosol yield. The driving forces of particle wall loss are Brownian motion, gravitational settling and the Electrostatic effect (*McMurry and Rader, 2007*). Supported by a general comparison of reported particle wall loss patterns from several laboratories (*McMurry and Rader, 2007; Nah et al., 2017; Charan et al., 2018; UC Davis, personal communication*), it is found that chambers from different research groups have varied particle wall loss patterns as a function of particle size. The Electrostatic effect among the chambers is believed to vary significantly due to different physical chamber designs leading to sometimes extreme variations in the size-dependent wall-loss behaviors observed.

This study evaluates the particle wall loss characteristics in three typical types of chambers: i) CE-CERT’s collapsible chamber (EPA chamber) which holds a constant pressure, ii) Caltech’s suspended chamber with minimal volume change and iii) CE-CERT’s naturally suspending chamber (Mez chamber) where neither pressure nor volume is controlled. Separate wall-loss characterization experiments were conducted injecting monodisperse or poly-disperse ammonium sulfate particles and monitoring their size dependent concentration decay over several hours. Losses due to the electrostatic effect were observed to be greater in the CE-CERT EPA chamber than in the Caltech chamber. These findings are further supported by comparing the Caltech chamber with the CE-CERT Mez chamber, which has less contact with external materials and is, therefore, expected to have a reduced source of static charge. The acquired size-dependent wall loss pattern for the CE-CERT EPA chamber was applied to historical data, which was originally treated using an observed average particle size independent loss rate from each experiment, to evaluate the sensitivity from different wall-loss correction methods. Evaluation of the chamber and particle dynamics increases our understanding of differences observed between facilities. Mitigation strategies for particle wall loss within environmental chambers will be suggested.

2AP.3

Influence of Particle Size, Concentration and Drying Conditions on Colloidal Droplet Drying Kinetics and Dry Microparticle Morphology. JUSTICE ARCHER, Jim Walker, Jonathan P. Reid, *University of Bristol*

The drying of aerocolloidal suspensions in aerosol droplets provides particles that are fundamental building blocks in many industrial applications including sprays in pharmaceuticals, inhaled drug delivery, cosmetics, ceramics and many more. 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 drying process.

In this work, we will present measurements of drying kinetics of colloidal droplets composed of polystyrene beads of varying sizes and concentrations to explore how these colloidal droplet composition affects evaporation rates and the particle formation processes under different drying conditions -temperature and relative humidity based on single droplet drying experiments. Additionally, we will show scanning electron microscopy (SEM) images of dried aggregates of polystyrene beads from droplet chain experiments that demonstrate how control over initial colloidal droplet composition can be used to influence the dry particle morphology for a range of Péclet numbers. Using single droplet drying experiment and the droplet chain technique, we aim to provide a comprehensive experimental study resulting in improved understanding of the influence of droplet composition, concentration, drying conditions and the interaction mechanisms involved in dry microparticle morphology development, that are particularly encountered in spray-drying processes.

2CA.1

Evolution of Black Carbon Coatings in Biomass Burning Plumes during FIREX-AQ. BRADEN MEDIAVILLA, Joseph Katich, Joshua P. Schwarz, Glenn Diskin, Richard Moore, Elizabeth Wiggins, Donald Blake, Barbara Barletta, Nicola Blake, Simone Meinardi, Anne Perring, *Colgate University*

Uncertainties regarding the physical and optical properties of black carbon (BC) emissions, and their evolution in time, influence our ability to appropriately predict BC's atmospheric lifetime and its radiative effect. Here we present the variability and evolution of BC-core mass median diameter and average coating thickness with fuel type and burn conditions for fires sampled during the Boise phase of FIREX-AQ. In nearly all cases, substantial growth is observed in coating thickness over time while the BC-core mass median diameter shows no clear trend. Coagulation rates, calculated based on bulk aerosol number concentrations and size distributions, are too small to explain these observations. When considering condensational growth, two regimes emerge: denser plumes show significant and rapid coating thickness growth in the absence of photochemistry while more dilute plumes show moderate, yet still notable, growth with increasing photochemical age. These two regimes are readily differentiated by examination of CO2 integrated over plume transects. The observed trends can be used to parameterize BC emissions from biomass burning sources for improved BC mixing state predictions.

2CA.2

Imaginary Refractive Index Comparison of Water- and Methanol-soluble Brown Carbon Aerosol from western US Wildfires.

Pai Liu, NISHIT SHETTY, Benjamin Sumlin, Yutong Liang, Allen Goldstein, Rajan K. Chakrabarty, *Washington University in St. Louis*

Brown Carbon (BrC) aerosols absorb light at near-ultraviolet wavelengths and therefore contribute positively to Earth’s radiation balance. An accurate characterization of the complex refractive index (????=????+????????) for BrC aerosols is fundamental to a better estimation of their radiative forcing in climate models. The wavelength-dependent imaginary part of the refractive index ????, albeit being scrutinized via many laboratory studies over the past decade, remains highly uncertain when it comes to the real-world BrC emissions from large-scale biomass combustions, such as wildfires. Here we report the full absorption spectra of BrC aerosol samples taken from the Nethker fire during the FIREX-AQ campaign that took place between Aug 9th and Aug 16th, 2019. The filter collected BrC samples were dissolved into methanol and ultrapure water extractants via sonication with a 45 minutes duration. The solution-phase absorption spectra of the methanol and water extracts were measured with a spectrophotometer operated with incident wavelength (????) ranging between 300 and 800 nm. Subsequently, values of ????(????) within the complete visible range were determined with estimated BrC concentration in both extractants per the extraction efficiency values reported in previous publications. Our results show average ????BrC, Water≈ 0.076 and ????BrC, MeOH≈ 0.088 at 400 nm (respectively for the BrC extracted into water and methanol), beyond which the values of ????BrC, Water and ????BrC, MeOH are seen to converge on an identical curve, until ???? exceeds ca. 475 nm. These experimentally determined ????(????) spectra will next be integrated into radiative transfer models, towards an evaluation of their broader implications.

2CA.3

Submicron Soot Microphysical and Chemical Signatures from Detonations of High Explosive Composites in Controlled Atmospheres.

ALLISON AIKEN, Rachel Huber, Andrew Schmalzer, Mark Boggs, James D. Lee, Kyle Gorkowski, Manvendra Dubey, *Los Alamos National Lab*

Carbonaceous particles are lofted and transported long distances in the atmosphere that can impact climate and human health at local, regional and global scales. Submicron particles containing soot are formed during detonation of high explosives. Chemical and microphysical properties of ambient soot particles depend on fuel and source conditions as shown for biomass burning and fossil fuel combustion that have been studied for decades. In contrast, analogous dynamic aerosol processes of explosions and high fluence fires have been less studied. Here, we compare detonation soot aerosol physical, optical and chemical properties with biomass burning and fossil fuel emission sources in the lab and field. Carbonaceous signatures such as the presence of fullerenes and polycyclic aromatic hydrocarbons are compared with more common ambient and laboratory-generated soot surrogates. Offline analysis of inorganics and metals validate SP-AMS trace-metal detection and our interpretation of water uptake properties.

We utilize sensitive and selective ambient aerosol techniques to identify soot from two well-known high explosive composites (1) Comp-B: trinitrotoluene (TNT) and 1,3,5-Trinitro-1,3,5-triazinane (RDX) and (2) PBX 9501: 1,3,5,7-Tetranitro-1,3,5,7-tetrazoctane (HMX). Results from the Soot Particle Aerosol Mass Spectrometer (SP-AMS), Single Particle Soot Photometer (SP2), Scanning Mobility Particle Sizer (SMPS), Three-wavelength Photoacoustic Soot Spectrometer (PASS-3) and a custom RH-controlled Cavity-Attenuated Phase Shift-Single Scattering Albedo PM monitor (H-CAPS-PMSSA) at 450 nm are presented.

The soot sampled had small mobility diameters (< 100 nm) and unique optical and chemical signatures depending on the explosive composite composition, detonation atmosphere (e.g., Argon, air) and pressure. Single Scattering Albedos (SSA) from 0.3 to 0.8 and Absorption Angstrom Exponents (AAE) from 0.5 to 2.0 were measured across 405 to 870 nm wavelengths and were found to depend on the explosive composite composition and detonation conditions.

2ID.1

Quantitative Aerobiologic Analysis of an Influenza Human Challenge-Transmission Trial.

P. JACOB BUENO DE MESQUITA, Noakes Catherine, Donald Milton, *University of Maryland School of Public Health*

Despite evidence that airborne transmission contributes to influenza and other respiratory infection epidemics or pandemics, limited knowledge of the infectiousness of human cases hinders pandemic preparedness. We used airborne viral source strength and indoor CO2 monitoring from the largest human influenza challenge-transmission trial (EMIT: Evaluating Modes of Influenza Transmission, ClinicalTrials.gov number NCT01710111) to compute an airborne infectious dose generation rate q=0.11 (95% CI 0.088, 0.12)/h and calculate the quantity of airborne virus per infectious dose =1.4E+5 RNA copies/quantum (95% CI 9.9E+4, 1.8E+5). We then compared these calculated values to available data on influenza airborne infectious dose from several previous studies, and applied the values to dormitory room environments to predict probability of transmission between roommates. Transmission risk from typical, moderately to severely symptomatic influenza cases is dramatically decreased by exposure reduction via increasing indoor air ventilation. The minority of cases who shed the most virus (i.e., supershedders) may pose great risk even in well-ventilated spaces. Our modelling method and estimated infectiousness provide a groundwork for a) epidemiologic studies of respiratory infection (including SARS-CoV-2) transmission in non-experimental settings and b) evaluation of the extent to which airborne exposure control strategies could limit transmission risk.

2ID.2

Evidence of Transmission of SARS-CoV-2 in Exhaled Breath Aerosols of Experimentally-Infected Nonhuman Primates.

CHAD ROY, *Tulane University*

The zoonotic emergence of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has resulted in a historic global pandemic that has markedly impacted planetary disease morbidity and mortality. Transmission of the virus via direct inhalation of exhaled breath aerosols (EBA) from an infected host has been perceived as an opaque exposure pathway relative to more prominent modalities such as large droplet transfer. We demonstrate that SARS-CoV-2 is effectively transmitted in EBA in experimentally-infected nonhuman primates (NHP). Collection of EBA in two species (Macaca mulatta and Chlorocebus aethiops) of SARS-CoV-2-infected animals showed significant, temporal increase of total particle production correlative and timed to the development of viral titers in the lung and nasal mucosa. EBA distributions skewed smaller (<3 µm) as a function of increase of total particles and peaked at the height of post-infection viral titer in experimentally-infected animals. These results clearly demonstrate that SARS-CoV-2 can effectively transmit in the smaller fraction of EBA at a particle size consistent with longer-term environmental transport and associated respirability potential.

2ID.3

Comparison of Different Methods for Respiratory Exposure to COVID-19 and Impact on Subsequent Disease and Virus Shedding in Animal Models.

Katherine O'Malley, Dominique Barbeau, Emily Olsen, Mengying Xia, Jeneveve Lundy, Shamkumar Nambulli, Cynthia McMillen, Natasha Tilston-Lunel, Emily Cottle, Theron Gilliland, Anita McElroy, Amy Hartman, William Klimstra, Paul Duprex, DOUGLAS REED, *University of Pittsburgh*

In late 2019, a novel coronavirus, SARS-CoV-2, emerged in Wuhan, China and has rapidly spread across the planet. In most people the virus causes a mild respiratory disease with fever and a dry cough the most commonly reported symptoms. However, fifteen percent may require hospitalization and an estimated one percent die from the disease, dubbed COVID-19. Severity fluctuates by region, patient age, and co-morbidities. Transmission appears to be by contact, droplet, and aerosol. We report here our efforts to develop animal models to support research into COVID-19. Hamsters, ferrets, and African green monkeys (AGM) were exposed to SARS-CoV-2 by mucosal inoculation (intranasal, oral, and/or intratracheal inoculation) or small-particle aerosol. Clinical signs of disease (weight loss, fever, respiratory disease) in all species were mild but were typically greater after mucosal inoculation than aerosol exposure. It should be noted that doses were 100-fold higher for mucosal inoculation compared to aerosol exposures. Despite the lower doses for aerosol exposure, virus shedding was equivalent to mucosal inoculation both in terms of peak and duration of shedding by all routes examined (nasal, oral, and rectal). These results suggest that dose and upper respiratory deposition are important for disease caused by SARS-CoV-2 but surprisingly do not affect virus shedding.

2RA.1

Organic Composition of Aerosol Particles over the Southern Ocean by STXM-NEXAFS. LYNN RUSSELL, Georges Saliba, Kevin Sanchez, Cynthia Twohy, Greg Roberts, Savannah Lewis, Jeramy Dedrick, Christina McCluskey, Kathryn Moore, Paul DeMott, Cynthia Twohy, *Scripps Institution of Oceanography*

The OM fraction of the submicron marine aerosol has been linked to cloud properties. Very few measurements exist of the organic composition and contribution to cloud condensation nuclei (CCN) over the Southern Ocean. Airborne and shipboard samples of particles, cloud residuals, and ice nucleating particles were collected to measure organic composition during the Southern Ocean Clouds, Radiation, Aerosol Transport Experimental Study (SOCRATES) by scanning transmission X-ray microscope (STXM) with near edge X-ray absorption fine structure (NEXAFS) for particles 0.25–1.75 µm diameter. Organic functional groups from STXM-NEXAFS microscopy indicate that the majority of particles between 0.25 and 1.75 µm diameter with detectable organic components were consistent with marine organic signatures associated with sea spray particles. Specifically, 73 out of the 96 particles analyzed by STXM-NEXAFS were consistent with sea spray organic components with and without a salt core. These particles were characterized by absorption in the alkyl, carbonyl, carboxylic carbonyl, carbonate, and potassium regions. Scanning transmission electron microscopy with energy dispersive X-ray spectroscopy (STEM-EDS) analysis of a subset of the particles analyzed with STXM-NEXAFS confirmed the sea spray origin for the majority of the particles between 0.25 – 1.75 µm diameter sampled over the Southern Ocean. Ice nucleating particles sampled by immersion freezing <-27°C were also largely consistent with sea salt and sea spray organic functional groups, although 2 of 33 particles were consistent with long-range transport of particles from continental sources.

2RA.2

Characterization of Rural vs. Urban PM2.5 in the Indo-Gangetic Plain.

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The Indo-Gangetic Plain (IGP) experiences severe air pollution, with typical annual-average fine particulate matter ($PM_{2.5}$) concentrations in the range 75 – 150 µg m^{-3}, leading to average life expectancy for nearly a billion people to be shortened by approximately two years. Air pollution policies often emphasize city-by-city management, yet air pollution in the IGP is a regional challenge, and in-situ observations of rural air quality are limited. Here, we present initial results from a pilot study to characterize rural vs. urban air pollution gradients in North India, based on a stratified sampling scheme designed to cover a broad range of conditions from villages to towns to megacities.

Our experimental approach employs a carefully maintained network of lower-cost $PM_{2.5}$ sensors (Purple Air [PA] II, each encompassing two Plantower PMS5003 nephelometers), calibrated on the basis of multiple beta-attenuation reference $PM_{2.5}$ monitors (MetOne BAM-1022) and hourly-average measurements. During two mass colocation events in urban Bangalore (South India) and rural Hamirpur (IGP), we observed that PA sensors produced highly reproducible results with low unit-to-unit variability. The PA sensors estimated BAM-reported $PM_{2.5}$ with $R^2 > 0.8$ and normalized root-mean-squared error (NRMSE) of 20-30%, for concentration ranging from 5 to 150 µg m^{-3}.

We deployed PA sensors in a clustered pattern to characterize within-settlement variability along a gradient from remote rural to highly urban conditions in eastern Uttar Pradesh. We observed mass concentration of $PM_{2.5}$ ranged from 8.5 to 560 with an average of 82.7 µg m^{-3} in Varanasi city (population ~1.2 million) whereas Mai village (population ~5200) observed a concentration range from 9.1 to 512.7 µg m^{-3} with an average of 105.2 µg m-^{3}. Overall, we found that $PM_{2.5}$ concentrations in our pilot sample of villages and small towns were often similar to or higher than the nearest large city. These initial results suggest that additional observations in rural settings may provide valuable new information about the sources, dynamics, and consequences of $PM_{2.5}$ across this region.

2RA.3

Variability in the Composition and Chemical Impacts of Biogenic Volatile Organic Compounds in the Southeastern U.S.

DEBORAH MCGLYNN, Sally Pusede, Gabriel Isaacman-VanWertz, *Virginia Tech*

Despite their significant contribution to organic aerosol, there are few long-term year-round measurements of speciated, BVOC composition. These measurements are critical, as BVOC emissions vary widely due to ecosystem composition and environmental factors, and different BVOCs widely in their reaction rates with atmospheric oxidants and aerosol yields. To address this gap, hourly measurements of chemically resolved biogenic volatile organic compounds (BVOCs) are being collected at a research tower outside of Charlottesville, VA in a mixed forest representative of the Southeastern U.S. The measurements are taken using a custom-built, field-deployable gas chromatograph (GC) - flame ionization detector (FID) capable of measuring concentrations of individual BVOCs from all major terpenoid classes: isoprene (C_5H_8), monoterpenes ($C_{10}H_{16}$), and sesquiterpenes ($C_{15}H_{24}$). Measurements began in summer 2019 and are planned to be taken continuously over the next three years in conjunction with a number of other ecological and meteorological parameters. We observe not only changes in the magnitude of BVOC concentrations, as expected, but also changes to the composition of the BVOC mixture which affects the average reactivity and aerosol yield of emissions. This work will focus on the temporal variability in BVOC composition, and discussion of the variable importance of individual species in terms of their impacts on local and regional chemistry.

3AC.1

Volatility Distributions and Solubility of Monoterpene-derived Organic Nitrates. MASAYUKI TAKEUCHI, Yuchen Wang, Gamze Eris, Nga Lee Ng, *Georgia Institute of Technology*

Organic nitrates (ON) in the atmosphere contribute to a major fraction of the oxidized reactive nitrogen (NOy) budget; however, their complex interaction in the cycling of NOy via the formation, evolution, and decay remains largely unelucidated. Key parameters to understand the dynamics of this NOy cycling include volatility distribution and solubility because these two properties affect gas/particle partitioning of ON and subsequent chemical pathways and physical processes. Monoterpenes are a large source of atmospheric gaseous and particulate ON and serve as good candidates to investigate the partitioning behaviors. In this study, we perform a series of chamber experiments to estimate volatility distributions of bulk ON formed from hydroxyl and nitrate radical oxidation of α-pinene and β-pinene. To estimate volatility distributions, four independent methods are employed: yield-based approach using a High Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS) and a Scanning Mobility Particle Sizer (SMPS), thermogram-based approach, molecular formulae approach, and partitioning 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). We do not observe a good agreement in the ON mass concentration between HR-ToF-AMS and FIGAERO-HR-ToF-I-CIMS, pointing towards the critical needs to understand potential causes of such discrepancy. Solubility is studied by investigating partitioning behaviors of synthesized, atmospherically relevant hydroxyl nitrates in the presence of deliquesced ammonium sulfate aerosols. Our results regarding ON volatility and solubility values would provide fundamental constraints in chemical transport models and help better understand the role of ON in NOx cycling, ozone and SOA formation.

3AC.2

Formation and Chemical Evolution of Organic Nitrates during Oxidation of Volatile Organic Compounds. QING YE, Abigail Koss, Manjula Canagaratna, Alexander Zaytsev, Jordan Krechmer, Martin Breitenlechner, Kevin Nihill, Christopher Lim, James Rowe, Joseph Roscioli, Frank Keutsch, Jesse Kroll, *MIT*

Organic nitrates are understood to comprise a large fraction of total reactive oxidized nitrogen in the atmosphere and are important contributors to aerosol mass. However, our understanding of the chemical fate of organic nitrates during atmospheric processing remains incomplete. In this work, we study the formation and multigenerational aging of organic nitrates from VOC oxidation in chamber experiments. Organic nitrates were formed via oxidizing alpha-pinene and toluene by OH radicals under high NOx condition. A suite of state-of-the-art mass spectrometric instruments, including several chemical ionization mass spectrometers with different ionization schemes and an aerosol mass spectrometer, was deployed to capture a variety of organic nitrate species. Our multi-mass spectrometer technique provides unique insight into the evolution of both individual organic nitrate species and ensemble properties including volatility, carbon number and carbon oxidation state of the chemical system. In addition, we investigated whether aging of organic nitrates will result in renoxification that significantly affects the NOx budget.

3AC.3

Gas and Particle-phase Highly Oxygenated Organic Molecules and Organic Nitrates from Chlorine-Initiated Photo-Oxidation of α-Pinene. CATHERINE MASOUD, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Measurements have shown that Cl can substantially affect particulate matter formation; yet, Cl-initiated SOA formation has not been studied in detail. In this work, we focus on Cl-initiated photo-oxidation of α-pinene leading to the formation of highly oxygenated organic molecules (HOMs) and organic nitrates in the vapor and particle phases.

Using a Filter Inlet for Gases and Aerosol mounted onto a Chemical Ionization Mass Spectrometer (FIGAERO-CIMS) operated in Iodide-mode, we identify and quantify HOMs in the gas and particle phases, which include chlorinated and nitrated HOMs. We report for the first time the gas- and particle-phase yields of HOMs from the α-pinene + Cl reaction under different experimental conditions, including different NOx levels, temperature, and precursor concentrations. (Previous work has focused on HOM yields in the vapor-phase alone.) We observe combined (vapor + particle phase) HOM monomer yields exceeding 5%, with particle-phase HOM yields up to six times higher than vapor-phase HOM yields. These high yields underscore the importance of HOM in the formation of organic aerosol.

We measure particulate organic nitrates (pONs) that are formed from different experimental conditions using an Aerosol Chemical Speciation Monitor (ACSM) and FIGAERO-CIMS. We use the FIGAERO-CIMS and a thermodenuder in tandem with the ACSM to explore the volatility of pONs formed. Data from both instruments are consistent with the particulate organic nitrates having higher vapor pressure than other oxygenated organics. We also compare the chemical composition of gas- and particle-phase products formed from the reactions of α-pinene + Cl versus α-pinene + OH under low and high NOx conditions.

3AE.1

Characterizing Infiltration and Indoor Contribution of PM2.5 Based on Volunteer-generated Monitoring Data at Large Spatial and Temporal Scales. JIANZHAO BI, Lance Wallace, Jeremy A. Sarnat, Yang Liu, *Emory University*

Personal $PM_{2.5}$ exposure may deviate from ambient levels due to differential infiltration and contribution of indoor sources. It is important to quantify infiltration factors (F_{inf}) and the contribution of indoor sources. Research in this area has been historically limited in space and time due to the high labor and capital costs of deploying and maintaining collocated indoor/outdoor monitors. Recently, the growth of volunteer-generated $PM_{2.5}$ data provides an unprecedented opportunity to characterize F_{inf} and indoor contribution at large spatial and temporal scales. In this study, 94 volunteer-maintained PurpleAir indoor/outdoor $PM_{2.5}$ monitor pairs with ~1.1 million hourly measurements were identified within 500 m from each other during a 20-month period (November 2018 to June 2020) in California. A data-driven method was developed based on local polynomial regression to estimate site-specific F_{inf} with an assumption that indoor sources were negligible when outdoor levels were sufficiently high (the highest 20 outdoor measurements for each site). The estimated F_{inf} had a mean of 0.25 (25th, 75th percentiles = [0.13, 0.32]) with a mean standard error of 0.05, the scale of which generally agreed with those reported in previous studies. A seasonal analysis (dry and wet seasons) showed no significant difference in F_{inf} across seasons probably because the seasonal changes were mild in California. The F_{inf} estimates were also similar for different building types (homes or buildings). By applying the F_{inf} estimates, we found the indoor-generated $PM_{2.5}$ contributed an average of 50% (25th, 75th percentiles = [35%, 65%]) of the total indoor levels. We further identified outdoor level thresholds for individual sites above which the indoor sources were not substantial for personal exposure assessment. This is the first time the indoor contribution for multiple sites monitored over thousands of hours were characterized at a large spatial scale.

3AE.2

Mongolia PM2.5 Ambient Air Quality and Children's Indoor Exposures at School. ZHIYAO LI, Munkhbayar Buyan, Rufus Edwards, Alex Heikens, Jay R. Turner, *Washington University in St. Louis*

Mongolia's population centers experience poor wintertime air quality because the cold climate drives strong ground-level inversions and pervasive solid fuels use for distributed residential space heating. Ulaanbaatar (UB, pop. ~1.5MM) has robust air monitoring but measurements outside of UB are sparse. Project objectives include using low-cost sensors (LCS) to quantify $PM_{2.5}$ spatiotemporal variability outdoors in Bayankhongor (BKH, pop.~30K) and assess children's $PM_{2.5}$ exposures in kindergartens in both UB and BKH.

Pilot studies commenced in Nov. 2019 to inform the Feb. 2020 deployment of larger-scale indoor and outdoor LCS networks. One site in BKH consists of three units each of five LCS types collocated with a US EPA Federal Equivalent Method beta attenuation monitor (BAM) to evaluate LCS accuracy, precision, and ruggedness. For the period Nov. through Feb. 2020, three of the five LCS types exhibited high data capture and high correlation with the BAM for temperatures as low as -30°C and hourly $PM_{2.5}$ ranging ~10-300 $\mu g/m^3$ (5^{th}-95^{th} percentiles). These device types were biased high by 25-40% with a discernible temperature-dependent bias. The pilot study continues through 2020 to evaluate seasonal patterns in the LCS-to-BAM relationships.

Children's exposures at school are estimated through kindergarten measurements which also assess, to the extent practicable, the efficacy of interventions such as air purifiers and mechanical ventilation. This indoor pilot study includes two BKH and four UB locations. Each site has one device each of five LCS types (with three of each device at one of two locations), and one device outdoors. Indoor $PM_{2.5}$ and indoor/outdoor $PM_{2.5}$ temporal profiles are observed to vary by kindergarten location and type of intervention.

The presentation will summarize results from the pilot studies and the first half-year of full network operation.

3AE.3

Problems at Home: Comparing Health Risks of Indoor and Outdoor Emissions during the HOMEChem Campaign. ANNA HODSHIRE, Matson A. Pothier, Erin K. Boedicker, Delphine K. Farmer, *Colorado State University*

Although humans spend ~90% of their lives indoors, air quality standards are focused on outdoor, ambient particulate matter concentrations and composition. The 2018 HOMEChem (House Observations of Microbial and Environmental Chemistry) field campaign consisted of realistic cooking, cleaning, and house-opening activities within a test house. HOMEChem demonstrated that these events had variable aerosol compositions, and that the indoor aerosol concentrations during events such as cooking can exceed United States ambient air quality standards. Not all aerosol are created equally: recent studies have shown that variable particle compositions may have nonlinear health impacts with increasing particle concentrations. For example, regional analysis in Canada indicates that black carbon and nitrate have a larger influence on cardiovascular outcomes than components such as dust and sulfate. Particle composition also influences the oxidative potential of aerosol (another marker for aerosol toxicity), with metals and organic species recently implicated as strong drivers of oxidative potential. As well, recent work indicates the health effects of particulate matter may be modified by O_3 and NO_2, and these oxidant profiles indoors often do not follow outdoor profiles. Here, we examine particle composition and concentrations along with oxidant gas concentrations during HOMEChem as observed during cooking, cleaning, house-opening, and unoccupied time periods to determine how changing composition may influence particle toxicity during different events. We further compare indoor trends in aerosol composition and concentrations and oxidant gas concentrations with ambient trends to provide a broad overview of the relevance of indoor air quality to the epidemiology community.

3AP.1

Tuning Nanoparticle Aggregation with Externally Applied Magnetic Field Strength.

PRITHWISH BISWAS, Pankaj Ghildiyal, George Mulholland, Michael Zachariah, *University of California, Riverside*

Assemblies of metal nanoparticles occurring during aerosol routes of synthesis often limits their applications. Due to weak inter particle Hamaker type interaction forces, fast Brownian motion limits the aggregation of metal nanoparticles, a phenomenon, popularly known as diffusion limited cluster aggregation (DLCA). Nanoparticle aggregates formed by DLCA has a universal fractal dimension of ~1.8, which is undesirable, as this type of aggregation greatly reduce the effective surface area. However, in the case of magnetic nanoparticles, an external magnetic field can be used to tune the fractal dimension of the aggregates formed. The presence of a magnetic field induces attractive interaction forces between two magnetic particles only along the direction of the magnetic field, whereas repulsive interaction forces are induced along all other directions. A canonical ensemble Monte Carlo simulation has been performed for a system of spherical particles interacting with each other through a directional magnetic potential, to study the effect of the directional magnetic field in tuning the aggregate shape. The pair distribution function between the particles and the radius of gyration of the aggregates have been evaluated to estimate the fractal dimensions, both of which follow a scaling law with the aggregate size. It has been observed that the fractal dimensions of the aggregates decreases with the increase in the strength of potential and reaches a saturation at ~1.17. The particles also show a tendency to get aligned along the direction of the magnetic field forming linear chain aggregates, as the strength of the magnetic field is increased. These linear aggregates are desirable in making high density composites for various applications and the strength of the magnetic field required for this transition in the shape of the aggregates is practically achievable. Hence, this study will be useful in designing nanoparticle synthesis procedures with controlled aggregation.

3AP.2

Heat Transfer in Nanometer Scale Aerosol Particles.

Huan Yang, CHRISTOPHER J. HOGAN, *University of Minnesota*

Aerosol particles are usually considered to be in thermal equilibrium with their surroundings. However, subsequent to condensation, coagulation, and evaporation events, particles, particularly those in the 1 nm size range, can be appreciably hotter (condensation, coagulation) or colder (evaporation) than the surrounding gaseous medium because of exchange between potential and thermal energy brought about by these processes. Collisions with surrounding gas, i.e. conduction, typically bring the particle back to thermal equilibrium; however, this re-equilibration process is often either ignored (assumed instantaneous) in models of nanometer scale particle growth, or assumed to occur at a rate described by complete thermal-accommodation collision models. Here, we utilize molecular dynamics simulations in conjunction with a collision rate theoretical framework to examine the heat transfer rate in the free molecular regime to gold and copper nanoclusters in Helium, Hydrogen, Argon, and diatomic nitrogen gas. We show that the traditionally invoked thermal accommodation coefficient, i.e. a coefficient place in front of the net diffuse heat transfer rate to account for non-accommodated collisions, does not follow from collision rate theory, as the incoming energy from gas molecules (during impingement) is exactly calculable and requires no such correction. Instead, we introduce a thermal reemission coefficient, parameterizing the energy carried away by a gas molecule after collision with a particle in comparison to its expected energy based upon a fully-accommodating collision model. Bounds are easily placed on the thermal reemission coefficient by the fact that heat transfer must occur from the hotter to the colder system (e.g. from a hotter particle to a colder gas). We find that the thermal reemission coefficient is rather insensitive to particle size in the investigated size range, but that it is strongly dependent upon the mass of gas atoms/molecules impinging relative to the masses of the atoms in the particle. For the lightest gases examined, the thermal reemission coefficient adopts a value extremely close to the zero-heat transfer limit, suggesting that in light gases, heat transfer in the free molecular regime occurs extremely slowly to nanoclusters and in a system where nanoclusters form and grow, the assumption of instantaneous thermal equilibrium may not be fully justified. We do not find agreement with the fully accommodating model under any conditions where the temperature difference between the gas and particle is large.

3AP.3

An Experimentally Validated Model of Diffusion Charging of Arbitrary Shaped Aerosol Particles. LI LI, Ranganathan Gopalakrishnan, *The University of Memphis*

Experimental studies have shown that particle shape strongly influences the diffusion charging of aerosol particles exposed to low energy (~0.03 keV) bipolar/unipolar ions. It is expected that the highly non-spherical particles such as aggregates with low fractal dimension or cylinders with very high length to diameter ratios may acquire more charges than a spherical particle of the same mobility diameter – the most commonly used size metric for aerosol nanoparticles. This aspect warrants the need for an accurate model to predict the charge distribution of non-spherical particles. This work presents a Langevin dynamics (LD)-based approach to describe the collision kernel between a charged/neutral arbitrary shaped particle and an unlike/oppositely charged ion. The diffusion charging model including Coulombic and image potential interactions published by Li et al. (J. Aerosol Sci. 140: 105481) for spherical particles is generalized for arbitrary shapes following the approach suggested by Gopalakrishnan et al. (J. Aerosol Sci. 64: 60-80) using LD simulations of aggregate-ion collisions for attractive Coulomb-image potential interactions. This extended model for collisions between unlike charged particle-ion (bipolar charging) and the model for like charged particle-ion (unipolar charging) put forward by Gopalakrishnan et al. (J. Aerosol Sci. 64: 60-80) are validated by comparing against measured bipolar charge distributions from prior experimental work. Comparison to the data for fractal aggregates reported by Matti (Aerosol Sci. Tech. 42(4): 247-254) and Xiao et al. (Aerosol Sci. Tech. 46(7): 794-803) reveal that the LD-based models predict within overall 30% without any systematic bias. In the case of linear chain aggregates reported by Wen et al. (J. Aerosol Sci. 15(2): 103-122), the mean charge on each particle estimated by model is found to be in good agreement with the measurements. The comparison with experimental results supports the use of LD-based diffusion charging models to predict the bipolar and unipolar charge distribution of arbitrary shaped particles for a wide range of particle size, and gas temperature, pressure.

We thank The University of Memphis High Performance Computing Cluster for providing computational resources to carry out this research. Funding for this work was provided by US National Science Foundation (NSF) PHY Grant Award Number 1903432 under the Directorate of Mathematical & Physical Sciences.

3CA.1

Determination of the Refractive Index of Carbon Black Engulfed by Ammonium Sulfate from Effective Medium Approximations. JAMES RADNEY, Christopher Zangmeister, *National Institute of Standards and Technology*

Calculation of aerosol optical properties in radiative transfer models requires accurate knowledge of the size distribution, number density, mixing state, hygroscopicity and complex refractive index (RI) of the input particles. These input particle types can take many forms, but are often split into sulfate, black carbon, organic carbon and mineral dust. While the optical properties of external mixtures of these components can be easily calculated, internal mixtures pose challenges and an effective refractive index (RI_{eff}) of the mixed particle must be determined; often using an effective medium approximation (EMA). The chosen EMA can vary depending upon whether the particles are homogeneously or heterogeneously mixed. Here, we investigate whether, for well-characterized core-shell particles under well-controlled laboratory conditions, the refractive index of the absorbing core (an aged black carbon mimic, CB) could be isolated from the ammonium sulfate shell using optical measurements of absorption and extinction by photoacoustic and cavity ring-down spectroscopy, respectively. Refractive index retrievals of size- and mass-selected particles were performed as a function of CB mass fraction to determine the RI_{eff} and we observe that the real (n) and imaginary (k) components are composition dependent; $n_{eff} = (1.47 \pm 0.01) + (0.21 \pm 0.07)w_{CB}$ and $k_{eff} = (0.76 \pm 0.07)w_{CB}$. Various EMAs (volume fractions, average dielectric, Maxwell-Garnett and Bruggeman) are then tested to retrieve the RI of the CB core (RI_{CB}). We find that the retrieved RI_{CB} is EMA dependent, but the calculated optical properties always agree with the measured data to better than 5 %. In addition, the calculated values are less sensitive to RICB of and the choice of EMA than they are to the assumed refractive index of the ammonium sulfate shell.

3CA.2

Estimation of the Mass Absorption Cross Section of Atmospheric Black Carbon using Regression and Machine Learning Approaches. HANYANG LI, Andrew May, *The Ohio State University*

Mass absorption cross section of black carbon (MAC_{BC}) describes the absorptive coefficient per unit mass of black carbon and is thus an essential parameter to estimate the radiative forcing of black carbon. In the atmosphere, due to the complex physicochemical properties and different mixing states of BC, the values of MAC_{BC} have been observed to vary from 2.3 to 18 m^2 g^{-1} at different wavelengths. Many studies have sought to estimate MAC_{BC} from a theoretical perspective, but these studies require the knowledge of aerosol complex refractive indices, mixing state, and morphology, which are difficult and/ or labor-intensive to measure. This work attempts to investigate the alternative data-driven approaches (including multivariate regressions, support vector machine, and neural networks) in estimating MAC_{BC} for aerosols from various environments.

Our model utilizes multi-wavelength absorption and scattering coefficients as well as aerosol size distribution as input variables to estimate MAC_{BC} at 870 nm. The model has been applied to two field campaigns, the Two-Column Aerosol Project (TCAP) and the Cloud, Aerosol and Complex Terrain Interactions (CACTI) project, as well as biomass burning emissions collected during the Fire Influence on Regional to Global Environments Experiment (FIREX) laboratory campaign.

We assessed the applicability of the proposed approaches in estimating MAC_{BC} using statistical metrics (e.g., coefficient of determination (R^2), fractional error, and fractional bias) and visual comparisons against different aerosol properties (e.g., aerosol compositions and Absorption Ångström Exponent). Overall, the approaches used in this study can estimate MAC_{BC} appropriately, but the prediction performance varies across approaches and atmospheric environments (for example, R^2 ranges from 0.45 to 0.80 for the training and test datasets, and from 0.15 to 0.50 for the independent validation datasets). Ultimately, the data-driven approaches presented in this work provide a new insight to estimate MAC_{BC} with high accuracy.

3CA.3

Refractive Index of Black Carbon (BC) and Brown Carbon (BrC) Particles with True Monodisperse Selection. DAWEI HU, Rami Alfarra, Kate Szpek, Justin Langridge, Chenjie Yu, Michael Cotterell, Claire Belcher, Ian Rule, Yunqi Shao, Aristeidis Voliotis, Zixia Liu, Dantong Liu, Jim Haywood, Hugh Coe, James Allan, *University of Manchester*

The refractive index (RI) of black carbon (BC) and brown carbon (BrC) are important parameters to consider when predicting their radiative forcing in the atmosphere. Previous studies have used a differential mobility analyzer (DMA) to select mono-disperse BC/BrC particles to derive its RI according to a Mie model, which introduces large uncertainties associated with multiple charging. During the Soot Aerodynamic Size Selection for Optical properties (SASSO) project, we coupled a charging-free Cambustion Aerodynamic Aerosol Classifier (AAC) with the Met Office Extinction, Scattering and Absorption of Light for Airborne Aerosol Research (EXSCALABAR) system, delivering a high-resolution, multi-wavelength extinction and absorption measurements with truly mono-disperse cuts. Different types of light absorbing carbon were studied, including BC from catalytically stripped diesel exhaust and controlled flaming wood combustion. BrC was also investigated in the form of organic matter from wood burning (pyrolysis and smoldering) and ‘brown’ SOA produced in a chamber. Finally, coated particles were also investigated to test the accuracy of different mixing models used in optical treatments. The data generated from this study will be used to inform climate models, such as HadGEM at the UK Hadley Centre.

3ID.1

Survival of Viruses in Droplets as a Function of Relative Humidity, pH, and Salt, Protein, and Surfactant Concentrations. Kaisen Lin, Chase Schulte, LINSEY MARR, *Virginia Tech*

Successful transmission of certain infectious diseases requires that pathogens survive (i.e., remain infectious) in the environment, outside the host. The survival of viruses in droplets is known to depend on their chemical composition. However, the effect of individual components of the droplet solution on the viability of viruses has not been extensively explored. We investigated the effects of salt, protein, surfactant, and pH on the viability of viruses in stationary droplets at 20%, 50%, and 80% relative humidity (RH). Results showed that the viability of MS2, a non-enveloped virus, was generally higher than that of Φ6, an enveloped virus, in droplets after 1 hour. Both RH and the chemical composition of droplets greatly influenced virus viability. In general, RH and pH had the largest effects on viability. Consistent with our previous work, virus viability tended to be lowest at intermediate to high RH. The survival of MS2 was similar in droplets with different initial pH values, but the viability of Φ6 was significantly reduced in acidic and basic droplets compared to neutral ones. The presence of bovine serum albumin (BSA), a protein derived from cows, protected both MS2 and Φ6 in droplets. The effects of sodium chloride and the surfactant sodium dodecyl sulfate were variable by RH level and virus type. The results demonstrate that the viability of viruses is determined by the chemical composition of carrier droplets, environmental factors, and possibly changes in the spatial distribution of viruses in droplets. These findings emphasize the importance of understanding the chemical composition of carrier droplets in order to predict the persistence of viruses contained in them and provide insight into infectious disease transmission.

3ID.2

Survival of SARS-CoV-2 in the Aerosol Phase Across a Broad Range of Temperature (5 to 40 oC), Relative Humidity (<5 to >90%) and Time (<5 seconds to >24 Hours). ALLEN E. HADDRELL, Henry Oswin, Tristan Cogan, Jamie Mann, Jonathan P. Reid, *University of Bristol*

The rapid spread of COVID-19 across the globe in 2020 has led to hundreds of thousands of deaths worldwide and brought considerable harm to the global economy. The major mechanisms by which the SARS-CoV-2 virus is spread from one individual to another is critical in the development of effective public health guidelines (e.g. consider the debate over social distancing, 2m or 1m?). Thus, detailed measurements of how environmental conditions effect the length of time SARS-CoV-2 remains infectious while suspended in the aerosol phase is key in limiting the virus's spread.

A next generation device to study the longevity of infectious species directly in the aerosol phase, termed CELEBS (Controlled Electrodynamic Levitation and Extraction of Bioaerosol onto a Substrate), has been recently reported.(1) Among the novel features of CELEBS include the complete control over the chemical and biological composition of the bioaerosol droplet, and highly resolved aerosolization time periods. In this study, the longevity of SARS-CoV-2 was directly measured in the aerosol phase using a CELEBS across a broad range of temperatures (<5 to >35 oC), relative humidities (<5 to >90%) and time periods (<5 seconds to >24 hours). Furthermore, the effect of longevity as a function of particle composition (e.g. growth media, artificial saliva) was explored.

[1] Otero Fernandez, M., Thomas, R., Garton, N., Hudson, A., Haddrell, A., Reid, J. (2019). Assessing the Airborne Survival of Bacteria in Populations of Aerosol Droplets with a Novel Technology. Journal of the Royal Society Interface, 16(150), [20180779].

3ID.3

Effects of Environmental Conditions, Suspension Liquid, and Particle Size on SARS-CoV-2 Persistence in Aerosols.

MICHAEL SCHUIT, Shanna Ratnesar-Shumate, Jason Yolitz, Gregory Williams, Wade Weaver, Brian Green, David Miller, Melissa Krause, Katie Beck, Stewart Wood, Brian Holland, Jordan Bohannon, Denise Freeburger, Idris Hooper, Michael Hevey, Paul Dabisch, *DHS NBACC*

Aerosol transmission has been implicated in the spread of SARS-CoV-2 by both epidemiological and direct sampling studies. However, the potential for aerosol transmission in specific scenarios is affected by a variety of factors, including the susceptibility of the virus to inactivation by environmental parameters. To better understand the potential for SARS-CoV-2 aerosol transmission in different settings, our laboratory conducted a series of studies in two environmentally-controlled rotating drum aerosol chambers to determine the effects of temperature, relative humidity, and simulated sunlight on SARS-CoV-2 decay in aerosols. Aerosols were generated from suspensions of virus in either culture medium, simulated saliva, or simulated respiratory tract lining fluid, with target mass median aerodynamic diameters of either two or four microns to assess the effects of suspension liquid and particle size on the virus's susceptibility to environmental parameters. Temperature, simulated sunlight, and humidity all influenced SARS-CoV-2 infectivity, although simulated sunlight had the largest effect. Small differences in responses to environmental parameters were observed between suspension liquids and particle sizes, though general trends were similar. Overall, decay rates ranged from near zero in darkness at 10°C to approximately 40%/min in full intensity simulated sunlight at 20% RH and 40°C. These results can be used to better understand the potential of SARS-CoV-2 to transmit by the aerosol route and to inform risk mitigation strategies in both indoor and outdoor settings.

3RA.1

Dynamical Downscaling of a Global Chemistry-Climate Model to Study the Influence of Climate Change and Variability on Mid-21st Century PM2.5 in the Continental US.

SURENDRA KUNWAR, Jared Bowden, George Milly, Previdi Michael, Arlene Fiore, Jason West, *University of North Carolina at Chapel Hill*

Anthropogenically induced climate change and associated feedbacks from natural emissions (biogenic VOCs, wildfires) have the potential to alter air quality in the coming decades, but noise from climate variability can confound the climate change signal. Here, we aim to quantify the impacts of climate change and variability on US $PM_{2.5}$ levels at fine spatial resolution, by statistically combining probability distributions from multi-year global model ensembles with dynamical downscaling over the continental US.

We use a 3-member ensemble of simulations varying only in initial conditions from the GFDL-CM3 global chemistry-climate model for the period 2006-2100 under the RCP8.5 scenario. The GFDL-CM3 simulations fix aerosol and O_3 precursor emissions at 2005 levels to isolate the impact of climate change on air quality. Empirical Orthogonal Function analysis of the simulations identifies eastern US regions that vary coherently, from which we carefully select four present (2006-2020) and four future (2050-2060) years that include several high and medium annual mean $PM_{2.5}$ levels in each region.

We dynamically downscale the GFDL-CM3 meteorology and chemistry to 12-km with the regional models WRF and CMAQ for the selected years. The 3-member GFDL-CM3 model simulations (at 2^o spatial resolution) from 2006 to 2060 provide a broader context for the downscaled CMAQ simulations. Additionally, another global model NCAR CESM (12-member ensemble, 1^o spatial resolution) run under the same future scenario as GFDL-CM3 also contributes to the context and statistics. From the downscaled CMAQ simulations, we construct mean annual $PM_{2.5}$ probability distributions for the present and the future in individual 12 km grid cells using distributions from the global models. Finally, we examine the differences in fine scale mean annual $PM_{2.5}$ distributions between the present and the future to quantify the effects of climate change and climate variability on $PM_{2.5}$.

3RA.2

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

Accurately modeling aerosol dynamics is required to obtain an understanding of the ambient size distribution, 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 processes with a network of ground-based size distribution measurements. The CTM utilized here is GEOS-Chem TOMAS driven by GEOS meteorological fields. 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 novel inverse method previously developed for a box model. This method transforms the full size distribution into three aerosol properties, 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 measurement station. We utilize measurements from 13 stations in Western Europe, of which seven stations are used as a training dataset to constrain the three uncertain processes and six stations are used as a testing dataset.

Applying the inverse method reduces bias in the training dataset for the three aerosol properties. For particle number concentration between 3 and 6 nm, the model-measurement bias decreases by over a factor of two and the correlation improves. The constrained nucleation rate is, on average, scaled down during local noon from the rate predicted by GEOS-Chem TOMAS.

3RA.3

Effect of a Forest Canopy on the Spatial Distribution of Windborne Dust Concentration during a Dust Storm. BORIS KRASOVITOV, Andrew Fominykh, Avi Levy, Itzhak Katra, *Ben-Gurion University of the Negev, Israel*

Numerous studies show that exposure to fine dust particles transported in the atmospheric surface layer during dust storms increases the risk of exacerbation of various bronchopulmonary and allergic diseases in humans. Forest canopy may absorb atmospheric particulate matter (PM) and reduce air pollution. This study investigated the impact of forest canopy on the spatial distribution of PM_{10} concentration following dust events in a region that is subjected to frequent dust storms. The developed model considers the interaction between the open area on the windward side of the forest, forest structure, and forest aerodynamics. The two-dimensional model is based on the application of theory of turbulent diffusion in the forest canopy in conjunction with model of dust particles deposition on vegetation elements. The leaf area density (LAD) distribution with height as well as dust particle size distribution are taken into account. The initial wind velocity profiles on the windward side of the forest, used in the simulations were fitted from data obtained in field measurements in the studied region. The resulted dust transport in the forest canopy was validated by comparison of theoretical results with empirical data. PM concentration measurements were conducted during dust-storm days and non-dust (clean) days inside a pine forest located in Northern Negev in Israel using portable real-time dust monitoring devices. Particle size distribution (PSD) was derived by laser particle sizer. Numerical calculations performed using the developed model showed that in high-level dust storms, PM_{10} concentrations in an urban environment that is located at the leeward side of the forest are reduced by 34%. Our model results of the atmospheric PM distribution show fairly good agreement with the data of the field measurements.

4AC.1

Anthropogenic Influences on Amazonian Organic Aerosol: A Molecular-Level Analysis. EMILY BARNES, Lindsay Yee, Gabriel Isaacman-VanWertz, Rebecca Wernis, Nathan Kreisberg, Robert Weber, Scot T. Martin, Brett Palm, Weiwei Hu, Pedro Campuzano-Jost, Douglas Day, Jose-Luis Jimenez, Paulo Artaxo, Allen Goldstein, *University of California, Berkeley*

The formation processes of secondary organic aerosols (SOA) in remote, biogenically dominated regions such as the Amazon are as yet incompletely understood and characterized. While the majority of SOA mass in such areas is understood to result from the oxidation of biogenic volatile organic compounds (BVOCs) including isoprene, monoterpenes, and sesquiterpenes, the processes by which anthropogenic emissions, biomass burning activities, and climatological conditions influence oxidation pathways and aerosol yields remain obscure. By changing the concentrations and classes of atmospheric oxidants present, anthropogenic emission plumes can significantly alter the yield and characteristics of biogenic SOA formed. In this work, we analyze a series of quartz fiber filters collected during the wet and dry season intensive operating periods (IOP's) of the 2014/5 GoAmazon field campaign at a semi-remote site in central Amazonia. These filters were analyzed using thermal desorption two-dimensional gas chromatography coupled with high resolution time-of-flight mass spectrometry. Hundreds of compounds were separated and resolved from each sample. From 11 samples representing a wide range of Amazonian conditions, 1,484 unique compounds were identified and compiled into a custom mass spectral library. These compounds were traced through ~3 week periods of each IOP with 12 hour resolution in the wet season and 4 hour resolution in the dry season. Compounds without authentic standards or published mass spectra are categorized through a variety of techniques including mass spectral similarities to known compounds, identification in filters from laboratory oxidation experiments, and time series correlation with known tracers of specific sources and oxidant-influenced reaction pathways. Relevant source categories include biomass burning derived OA, isoprene OA, monoterpene OA, and sesquiterpene OA. The relative abundances of individual tracer compounds and total contributions of the various categories under varying degrees of anthropogenic influence are compared and contrasted to probe the processes by which anthropogenic emissions alter biogenic SOA.

4AC.2

Solvent-modulated Effects on the Physical Properties of Secondary Organic Aerosol Mimicking Solutions. Emmaline Longnecker, Rebecca Miller, Lucy Metz, Tracy Rompich, ANDREW BERKE, *Smith College*

The kinetics of light-absorbing compounds and physical properties of secondary organic aerosol mimicking solutions are substantively affected by the surrounding solvent environment. We have found that alcohols perturb this chemical system in species- and concentration-dependent ways. Our present work explores the role that alcohol solutes have on organization, and physical properties, within the solvent using a technique we developed. We freeze tubes of ammonium sulfate-based solvent and then monitor stratification using infrared spectroscopy (ATR-IR). We find that the sign of the octanol-water partitioning coefficient of the added solute controls whether the resultant solution will stratify or not. We then add components of the chemical system and show how this solvent environment can help explain previous kinetics results.

4AC.3

Vibrational Modes of 2-Methyltetrol Sulfates from Raman and Infrared Spectroscopy.

ALISON FANKHAUSER, Ziying Lei, Kimberly Daley, Yao Xiao, Andrew Ault, *University of Michigan*

Vibrational modes of the isoprene oxidation product 2-methyltetrol sulfates (2MTS) were spectroscopically probed using Raman and infrared (IR) spectroscopies, supported with density functional theory. Experimental Raman and attenuated total reflectance-Fourier transform IR spectra collected for aqueous 2MTS at pH 3 agreed with the calculated deprotonated 2MTS spectra better than those of protonated 2MTS. Vibrational modes identified for ν($RO\text{-}SO3^-$) include Raman- and IR-active 1035 cm^{-1} and 1059 cm^{-1} as well as IR-active 1192 cm^{-1} and 1237 cm^{-1}. Comparing the Raman spectra for 2MTS across a range of acidities (pH = 0 – 10) suggest that organosulfates will be in their deprotonated form in atmospheric particles. Markers identified for $RO\text{-}SO3^-$ were in good agreement amongst various IR techniques, including first of its kind optical-photothermal infrared (O-PTIR) and atomic force microscopy-PTIR spectroscopies, and can be used to analyze future chamber and field data for the presence of 2MTS.

4AC.4

Simulating Wall-free Aromatic Secondary Organic Aerosol Formation via Multiphase Reactions in the Presence of Electrolytic Inorganic Aerosol.

SANGHEE HAN, Myoseon Jang, Chufan Zhou, *University of Florida*

The impact of the Teflon reactor wall on aromatic secondary organic aerosol (SOA) formation are explicitly simulated by using the Unified Partitioning Aerosol Phase Reaction (UNIPAR) model integrated with the gas-wall partitioning (GWP) model. The formation of oxygenated semivolatile organic compounds (SVOCs) from the photooxidation of ten different aromatic hydrocarbons is simulated by using an explicit gas-kinetic mechanism (MCM v3.3.1). In the model, SVOC's GWP and gas-particle partitioning onto preexisting particulate matter are kinetically processed with the absorption and desorption kinetics. The UNIPAR model simulates aerosol growth via the oligomerization of reactive SVOCs in both organic phase and aqueous reactions containing electrolytic inorganic salts. For the GWP model, GWP coefficient and the deposition rate constant of SVOCs are predicted by using a quantitative structure activity relationship (QSAR) employing SVOCs' physicochemical descriptors. This GWP model is then incorporated with the UNIPAR model in the DSMACC-KPP platform and simulated SOA chamber data. The UNIPAR-GWP model simulates SOA data obtained using UF-APHOR chamber varying NOx levels, humidity, temperature, and seed conditions. In the absence of aqueous reactions, the underestimation of SOA due to GWP is significant raging 25% and 65% at the high NOx levels (HC ppbC/NOx ppb =3). In the presence of wet-inorganic seed, the impact of GWP on SOA was much small owing to rapid reactions of organic species in the aqueous phase.

4AC.5

Heterogeneous Oxidation of Benzo[a]pyrene: Kinetics, Products and Toxicity. AMY HRDINA, James Rowe, Simran Kaushal, Bevin Engelward, Jesse Kroll, *MIT*

Polycyclic aromatic hydrocarbons (PAHs) are a class of chemical pollutants formed by incomplete combustion. PAHs are known carcinogens and mutagens; while atmospheric oxidation will degrade PAHs, it may also lead to the formation of toxic secondary products, modulating their health impacts in important but poorly understood ways. To better understand the rates and product of these degradation reactions, laboratory studies were conducted on the heterogeneous oxidation of particle-phase benzo[a]pyrene (BaP). BaP-coated ammonium sulfate aerosol particles were exposed to two common atmospheric oxidants, ozone (O_3) and OH, in an environmental chamber. Reaction products and kinetics were investigated by measuring the evolving particle-phase composition with an Aerosol Mass Spectrometer (AMS). The reaction rate is described in terms of the uptake coefficient, the fraction of oxidant-particle collisions that lead to reaction; measured uptake coefficients of O_3 and OH suggests atmospheric lifetimes of surface-bound BaP on the order of several hours, within the (very wide) range of previously reported values. The major products, observed by online AMS and offline liquid chromatography mass spectrometry (LCMS, operated in positive electrospray ionization mode), in both reaction systems include BaP-dione isomers ($C_{20}H_{12}O_2$), 4-oxabenzo[d,e,f]chrysene-5-one ($C_{19}H_{10}O_2$), and BaP epoxide or diol ($C_{20}H_{12}O$). The reaction with OH formed a higher yield of oxygenated compounds than the reaction with O_3, suggesting OH reacts with both first- and second-generation products. However, such species account for only ~50% of the particulate products, with a large fraction of product species still unidentified. Preliminary toxicity studies of BaP coated aerosol particles were conducted using the high-throughput ‘CometChip’ assay to quantify DNA damage upon exposure to fresh versus oxidized BaP-coated aerosol particles.

4AC.6

Comparison of Chemical Characteristics of PM2.5 Haze Events in Beijing, China and Gwangju, Korea. JIHO JANG, Haebum Lee, Minhan Park, Nohhyeon Kwak, Ilhwa Seo, Dahye Oh, Min-Suk Bae, Kyoung-Soon Jang, Yujue Wang, Min Hu, Kihong Park, *Gwangju Institute of Science and Technology*

To better understand the characteristics of $PM_{2.5}$ haze events in Beijing, China, and Gwangju, Korea, simultaneous measurements of chemical composition (ions, elements, organic carbon (OC), elemental carbon (EC), and organic compounds) of fine particles were performed during the 2018-2020 winter. In this study, the $PM_{2.5}$ haze event day was defined when the daily average $PM_{2.5}$ mass concentration was more than the top 10% values or higher than 100 $\mu g/m^3$ (Beijing, China) or 50 $\mu g/m^3$ (Gwangju, Korea). During the total 82 days measurement period, 9 days of $PM_{2.5}$ haze events occurred in the Beijing site and were classified into five cases. In the Gwangju site, a total of 13 days of $PM_{2.5}$ haze events occurred, which could be classified into two cases. Chemical composition data suggests that $PM_{2.5}$ haze events in Beijing were possibly caused by a combination of multiple primary combustion emissions (e.g. biomass burning, coal combustion, and vehicle exhaust), secondary aerosol formation under low wind speed conditions or crustal dust under high wind speed. During the $PM_{2.5}$ haze events in Gwangju, the combination of secondary formation of inorganic and organic aerosols and biomass burning contributed to the fine particle which significantly increased under low wind speed conditions. During the $PM_{2.5}$ haze event, K^+/EC and WSOC/OC increase in Beijing site, and OC/EC and WSOC/OC increase in Gwangju site. Increase of secondary aerosol components (e.g. sulfate, nitrate, ammonium, organic acids) in fine particle was observed as a significant cause of the $PM_{2.5}$ haze events in both sites, while primary combustion sources and crustal dust components contributed more to $PM_{2.5}$ haze events in Beijing site than in Gwangju site.

4AC.7

The Effects of Ammonium on the Atmospheric Aging of 3-Oxodicarboxylic Acids. ALEXANDRA KLODT, Jorge Fernandez, Michael Olsen, Sergey Nizkorodov, *University of California, Irvine*

3-oxocarboxylic acids are observed less often in field-collected SOA than in laboratory-generated SOA. This can be explained by 3-oxocarboxylic acids' ability to undergo a decarboxylation reaction. These molecules are often water soluble, and exist in aerosols alongside hygroscopic salts, such as ammonium sulfate. This work studied the effects ammonium can have on the decarboxylation reaction of a representative 3-oxocarboxylic acid, oxaloacetic acid (OAA). The decarboxylation of OAA to pyruvic acid was monitored using UV-vis spectroscopy, and pseudo-first order rate constants were calculated for 1 mM OAA solutions containing varying concentrations of ammonium sulfate, ammonium bisulfate, ammonium chloride, and acidified sodium sulfate (to make the pH more comparable to the ammonium sulfate condition). OAA's decarboxylation reaction was determined to be catalyzed by ammonium over a broad range of conditions found in the atmosphere. In weakly acidic solutions, pH's near 3 to 4, increasing ammonium concentrations linearly increased the calculated rate constant until 2.7 M ammonium, after which additional ammonium had no further effect. However, at pH's less than 2, the decarboxylation reaction was much slower, even in the presence of ammonium. Based on these results, 3-oxocarboxylic acids will have lifetimes near 5 hours in cloud/fog water, between 1 and 5 hours in aerosols which have been neutralized by ammonia, and nearly 40 hours in highly acidic particles, even if they are partly neutralized by ammonia.

4AC.8

pH-Dependence of the OH-Reactivity of Organic Acids in the Aqueous Phase. JESSICA LIMA AMORIM, Keifer Klimchuk, Florence Williams, Ran Zhao, *University of Alberta*

Studies from the past decade have identified cloudwater as an important reaction media for many organic compounds in the atmosphere. In aqueous-phase environments, organic molecules are subjected to a wide range of conditions that can affect their chemical processing and lifetimes in the atmosphere. Of these conditions, acidity is particularly important, as acid-base chemistry is a unique nature of aqueous-phase processing. Yet, the impact of solution pH on the OH-reactivity of many organic acids important to SOA formation remains unknown. A major challenge in studying the aqueous-phase processing of SOA-relevant compounds is a lack of compounds commercially available, which is limited to a few monoterpene-derived compounds. The goal of this study is to improve our fundamental understanding of the pH dependence of the aqueous-phase oxidation of organic acids by hydroxyl radicals (OH). Using (-)ESI-LC/MS, we investigated the second-order reaction rate coefficients (kIIOH) of organic acids relevant to α-pinene SOA at uncontrolled pH, pH 2 and 10. We compared the kIIOH values of pinic acid (PA), cis-pinonic acid (CPA) and limononic acid (LA) - organic acids with large aliphatic chains (C9-10) - with formic acid (FA, C1). Here, PA was synthesized and its photochemistry was investigated for the first time. In addition to PA, CPA, LA and FA we extended our study to other organic acids present in the water-soluble fraction of α-pinene SOA. The results obtained by our study indicate that the kIIOH of formic acid, the smallest organic acid, is highly pH dependent, while PA and many other organic acids arising from α-pinene are not. These findings could help simplify model parameters needed for cloudwater chemistry models.

4AC.9

Formation of Reactive Oxygen Species in Heated Cooking Oil Fumes and Real Cooking Emissions. LU LU, Vanessa Yan Zi Ng, Zheng Hao Melvyn Tan, Yue Qian Tan, Wei Jie Seow, Alex Lee, *National University of Singapore*

Numerous studies have reported that the risk of lung cancer in people who never smoke is significantly associated with the exposure to cooking emissions, which is one of the major particulate sources in both indoor and outdoor environments. Studies have reported that cooking organic aerosols have the potential to generate reactive oxygen species (ROS, e.g., organic peroxides). The major component emitted from cooking is fatty acids with different degrees of unsaturation. Those unsaturated fatty acids have been shown to generate ROS through an oxidation process in the atmosphere, which may damage cell DNA and proteins and eventually lead to lung cancer.

In this study, we quantified water-soluble fraction of particle-bound ROS on per carbon basis (WS-ROS/C) using a 2’,7’-dichlorofluorescin (DCFH) fluorescence probe from cooking emissions in Singapore hawker centres, which are statistically higher than those observed in office spaces, lab-generated secondary organic aerosols, and diesel engine emissions. In particular, stir frying, a popular Chinese cooking style, can generate more WS-ROS/C than other cooking styles, such as deep frying, steaming and boiling. To evaluate what we observed from real cooking emissions, we investigated the formation of WS-ROS in fresh and aged lab-generated heated cooking oil fumes. The WS-ROS/C of fresh heated oil emissions is in the lower range of the real cooking emissions. In general, the WS-ROS/C increased continuously along with 3-days aging experiments, depending on ozone exposure levels and degree of unsaturation of cooking oils. Our observations indicate that the enhancement of WS-ROS/C in organic particles generated by poly- and mono-unsaturated fatty acids dominant cooking oils are more sensitive to low (~5 ppb) and high (~100 ppb) ozone concentrations under dark condition, respectively. Dark ozonolysis of real cooking emissions were also investigated in order to better understand ROS formation potential of cooking-related emissions in typical urban environments.

4AC.10

Humidity Dependence of the Condensational Growth Rate of Secondary Organic Aerosol Particles. YIMING QIN, Jinghao Zhai, Paul Ohno, Jianhuai Ye, Yuemei Han, Pengfei Liu, Rahul Zaveri, Scot T. Martin, *Harvard University*

The condensational growth rate of the secondary organic aerosol (SOA) particles has a profound impact on the health and climate perturbation of atmospheric particles. This growth rate is typically represented in atmospheric models with a fixed value, regardless of the relative humidity (RH), even though the actual RH in the atmosphere varies widely with the location, season, and time. Whether and how RH affects the growth rate of atmospheric particles remains unclear. The study herein investigates the humidity dependence from 0% to 75% RH of the condensational growth of SOA particles derived from α-pinene ozonolysis in a continuously mixed flow reactor. A repeating pattern of the rapid growth of nanoparticles to larger particles of several hundred nm was observed even the total particle number concentration. A notable and monotonous increase of the particle area growth rate, from 1.1 ± 0.6 to 4.6 ± 0.4 nm2 s-1, were observed for a shift in RH from 0% to 75%. Aerosol mass spectrometer analysis shows that changes in chemical composition do not appear to explain the changes in the growth rate. However, mass transfer kinetic model (Model for Simulating Aerosol Interactions and Chemistry, MOSAIC) simulation shows that changes in the diffusivity inside the particle and the surface mass accommodation coefficients can reproduce the RH-dependent growth phenomena. The findings presented herein highlight the need to incorporate physical properties of atmospheric particles in probing and modeling the continuous size evolution of the particles at varying environmental conditions, which is expected to significantly influence the lifetime and potential health and climate impacts of atmospheric particles.

4AC.11

Frequency-Dependent Humidity Response in Ultraviscous and Gel Particles.

CRAIG SHELDON, Chelsea Price, Ryan Davis, James F. Davies, *University of California, Riverside*

The amount of water within an aerosol particle, determined by the relative humidity (RH), affects many aspects of an its characteristics. At low RH, the physical state of an aerosol can be crystalline, amorphous, or a combination of the two, such as in a gel, depending on the composition of the particle. These states are associated with slow diffusive mass transport, with implication for equilibration times and chemical reaction rates.

This research explores the relaxation times of various mixtures of inorganic and organic components of liquid particles exposed to changes in RH. For particles that form ultraviscous states, it is expected that the relaxation time will increase continuously with decreasing RH as diffusion rate decreases. However, if the particle experiences a phase change, to a gel state for example, relaxation time may change in a non-continuous manner. In a gel state, water transport will become restricted by slow percolation through pores within the particle, increasing the relaxation time. In this work we measure the response of levitated particles to RH oscillations (±2.5%) in a linear quadrupole electrodynamic balance to explore the relaxation time of these particles over a full range of RH. The response time following gel formation will be a function of both diffusive mass transport and percolation and detailed analysis may provide insight into the microstructure of the gel.

4AC.12

Long-term Aging of Secondary Organic Aerosols Derived from Monoterpenes in the Presence of Water Vapor and Liquid Water.

CYNTHIA WONG, Daniel Vite, Sergey Nizkorodov, *University of California, Irvine*

Secondary organic aerosols (SOA) can have a long lifetime in the atmosphere where they are exposed to different forms of water, including water vapor, aerosol liquid water, and cloud and fog droplets. In these environments, they can undergo a variety of chemical processes (i.e. hydrolysis) leading to changes in chemical composition. Previous studies have mainly focused on short term aging or hydrolysis of model organic compounds. This study investigates the stability of SOA compounds over longer time scales of days using SOA compounds from the ozonolysis of monoterpenes and exposing them to the different forms of aging scenarios where hydrolysis is likely. SOA samples were generated in an oxidative flow reactor and then impacted onto a foil substrate. Samples were then aged by exposure of water vapor for a couple of weeks or in an aqueous solution for several days and analyzed using direct infusion electrospray mass spectrometry (ESI-MS). Some of the MS scans were recorded in high-resolution mode permitting accurate formula assignments of the products. The results from the mass spectral analysis suggest that SOA compounds derived from the ozonolysis of monoterpenes were stable with respect to uncatalyzed hydrolysis for a period of up to two weeks. This demonstrates that hydrolysis is not likely to be a leading aging mechanism of SOA in humid environments. Aging by OH oxidation, acid-catalyzed aqueous reactions, and direct photochemistry occurs at faster rates than uncatalyzed hydrolysis.

4AC.13

Simulation of Monoterpene SOA Formation via Multiphase Reactions of Lumping Species Generated from Explicit Gas Mechanisms. ZECHEN YU, Myoseon Jang, Tianyu Zhang, Azad Madhu, Sanghee Han, *University of Florida*

Monoterpene Secondary Organic Aerosol (SOA) is simulated using the Unified Partitioning Aerosol Phase Reaction (UNIPAR) model coupled with the near-explicit gas kinetics including MCM V3.3.1 and the proxy radical autoxidation mechanisms under varying aerosol acidity, NO_x levels, temperature, and relative humidity. The UNIPAR model predicts SOA formation via multiphase partitioning (gas phase, organic phase, and inorganic phase) and in-particle chemistry of the lumping species, which are classified based on volatility and aerosol phase reactivity. The model streamlines three SOA formation pathways including partitioning of gaseous oxidized products onto both the organic phase and inorganic aqueous phase; oligomerization in organic phase; and aqueous phase reactions (i.e., acid-catalyzed oligomerization and organosulfate formation). The simulation is demonstrated for three different monoterpene SOA data (α-pinene, β-pinene and d-limonene) under various experimental conditions using a large outdoor photochemical smog chamber (UF-APHOR). Terpene SOA growth is significantly accelerated in aqueous phase anchored in acidic seed but much weak with neutral seed because terpene products are hydrophobic and weakly soluble in aqueous phase. The model underestimates the production of polar functional groups, such as -OH, -COOH, and $-ONO_2$, compared to the compositions measured using Fourier Transform Infrared spectral data. Under the current emission trends in which SO_2 and NO_x have been decreasing, our simulation results suggests that the reduction of sulfate could be a more efficient way to reduce SOA mass than the reduction of NO_x in the urban environments.

4AC.14

Heterogeneous Hydroxyl Radical Oxidation of Isoprene Epoxydiol (IEPOX)-Derived Secondary Organic Aerosol: Identification of Highly Oxygenated Products by HILIC/ESI-HR-QTOFMS. N. CAZIMIR ARMSTRONG, Yuzhi Chen, Tianqu Cui, Yue Zhang, Jin Yan, Zhenfa Zhang, Barbara Turpin, Man Nin Chan, Andrew Ault, Avram Gold, Jason Surratt, *UNC Chapel Hill*

Acid-driven multiphase chemistry of isoprene-derived epoxydiols (IEPOX) substantially contributes to secondary organic aerosol (SOA) formation. However, atmospheric chemical sinks of freshly-generated IEPOX-derived SOA remain unclear, and thus, are not considered in atmospheric chemistry models. We systematically examined the heterogeneous oxidation of authentic IEPOX-derived SOA particles by gas-phase hydroxyl radicals (OH) and its role as one potential atmospheric sink for IEPOX-derived SOA. Chemical changes in smog chamber-generated IEPOX-derived SOA were assessed after 1 and 4 hours of gas-phase OH exposure (10^7-10^8 molecules cm_{-3}) using hydrophilic interaction liquid chromatography coupled to electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (HILIC/ESI-HR-QTOFMS), an optimal protocol for characterization of highly-oxygenated and sulfur-containing organic compounds. HILIC/ESI-HR-QTOFMS has been previously demonstrated by our group to chromatographically resolve IEPOX-derived SOA constituents. Tentative structures and formation mechanisms are proposed here for previously measured IEPOX-derived ambient fine particulate matter ($PM_{2.5}$) constituents whose chemical sources were until now uncertain; this work focuses on atmospherically-relevant SOA constituents formed from the heterogeneous OH oxidation of the most abundant constituents of freshly-generated IEPOX-derived SOA, including 2-methyltetrols, 2-methyltetrol sulfates, and 2-methyltetrol sulfate dimers. Products with structures and formation mechanisms proposed here include ions at mass-to-charge ratios (*m/z*) 133 ($C_5H_9O_4^-$), 139 ($C_2H_3O_5S^-$), 149 ($C_5H_9O_5^-$), 195 ($C_5H_7O_6S^-$), 211 ($C_5H_7O_7S^-$), 213 ($C_5H_9O_7S^-$), 229 ($C_5H_9O_8S^-$), 243 ($C_6H_{11}O_8S^-$), and 273 ($C_7H_{13}O_9S^-$). We propose that subsequent to H abstraction by OH these compounds are formed predominantly via Russell reactions, Bennett-Summers reactions, and β-scission of alkoxy radicals. Understanding the formation mechanisms and structures of these atmospherically relevant SOA constituents will make it possible to quantify them, investigate reaction kinetics, and study their climate-specific properties such as ice nucleation efficiency.

4AC.15

SOA Formation in Mixed Oxidant (OH + Cl) Environments.

NIRVAN BHATTACHARYYA, Mrinali Modi, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Chlorine radicals are part of a complex oxidant mixture in the troposphere. Cl both competes with and produces hydroxyl radicals during oxidation of volatile organic compounds (VOCs). Here we study secondary organic aerosol (SOA) formation from mixed oxidant (Cl + OH) chemistry, using m-xylene as a model VOC. Mixed oxidant environments can be generated several ways, and chemical box modeling showed that $ClNO_2$ experiments form similar amounts of Cl and OH oxidized m-xylene. Environmental chamber experiments were conducted using Cl_2, $ClNO_2$, and H_2O_2 as radical sources for Cl, Cl + OH, and OH oxidation experiments. SOA composition assessed using an iodide mode, chemical ionization mass spectrometer (I^- FIGAERO-CIMS) showed clear differences based on radical source. Organochloride formation was observed in Cl experiments, indicating that Cl oxidized later-generation products since Cl + xylene oxidation occurs via hydrogen abstraction, not chlorine addition. SOA formed from $ClNO_2$ and H_2O_2 radical sources had a smaller average carbon number and was more highly oxidized than SOA formed in Cl_2 experiments. SOA yields from the Aerosol Chemical Speciation Monitor (ACSM) were higher for experiments without NO_X. The dynamics of these mixed radicals on SOA formation and composition may have a significant impact on outdoor air.

4AC.17

Inorganic Sulfur Species Formation upon Heterogeneous OH Oxidation of Organosulfates: Methyl Sulfate.

Kai Chung Kwong, Yao Ge, Hon Yin Poon, Rongshuang Xu, Jian Zhen Yu, MAN NIN CHAN, *The Chinese University of Hong Kong*

Increasing evidence has revealed that sulfur in atmospheric particles can exist in its organic form, namely, organosulfur compounds. Organosulfates are characterized by the sulfate ester functional group and are one of the most important classes of organosulfur compounds detected in atmospheric particles. Organosulfates are generally thought to be chemically stable in the atmosphere. In this work, we show that methyl sulfate, the smallest organosulfate, can be oxidized heterogeneously by gas-phase OH radicals. A significant amount of inorganic sulfur (i.e. bisulfate and sulfate ions) is formed at a reasonable rate upon oxidation. To date, a variety of organosulfates with significant concentrations has been detected in atmospheric particles. These results suggest the importance of a sulfur conversion between its organic and inorganic forms in atmospheric particles or cloud droplets.

4AC.18

Heterogeneous Hydroxyl Radical Oxidation of Isoprene Epoxydiol-Derived Methyltetrol Sulfates: Plausible Formation Mechanisms of Previously Unexplained Organosulfates in Ambient Fine Aerosols. YUZHI CHEN, Yue Zhang, Andrew Lambe, Rongshuang Xu, Ziying Lei, Nicole Olson, Zhenfa Zhang, Tessa Szalkowski, Tianqu Cui, William Vizuete, Avram Gold, Barbara Turpin, Andrew Ault, Man Nin Chan, Jason Surratt, *UNC-Chapel Hill*

Methyltetrol sulfates are unique tracers for secondary organic aerosol (SOA) formed from acid-driven multiphase chemistry of isoprene epoxydiols. Ambient measurements demonstrate that methyltetrol sulfates are the single most abundant SOA tracer, up to 13% of organic carbon (OC) mass and up to 80 % of organosulfate (OS) mass, in PM2.5 collected from the Southeast US and Amazon rainforest. Thanks to recent developments in liquid chromatography rendering excellent separations of OSs, 2-methyltetrol sulfate diastereomers (2-MTSs) have been identified as the dominant isomers of methyltetrol sulfates, but their atmospheric sinks remain unknown. We investigated the oxidative aging of authentic 2-MTS aerosols by gas-phase hydroxyl radical (•OH) at a relative humidity of 61 ± 1 % using an oxidation flow reactor. The effective rate constant for this heterogeneous reaction was determined as 4.9 ± 0.6 × 10−13 cm3 molecule−1 s−1, corresponding to an atmospheric lifetime of 16 ± 2 days (assuming •OH concentration of 1.5 × 106 molecule cm−3). Chemical changes to 2-MTSs were monitored by hydrophilic interaction liquid chromatography interfaced to electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (HILIC/ESI-HR-QTOFMS). Previously unknown OSs detected in atmospheric $PM_{2.5}$ at mass-to-charge ratios (m/z) 139 ($C_2H_3O_5S^-$), 155 ($C_2H_3O_6S^-$), 169 ($C_3H_5O_6S^-$), 171 ($C_3H_7O_6S^-$), 185 ($C_3H_5O_6S^-$), 199 ($C_4H_7O_7S^-$), 211 ($C_5H_7O_7S^-$), 213 ($C_5H_9O_7S^-$), 227 ($C_5H_7O_8S^-$), 229 ($C_5H_9O_8S^-$) and 231 ($C_5H_{11}O_8S^-$) were observed as oxidation products of 2-MTSs and plausible reaction mechanisms were proposed. This work highlights that heterogeneous •OH oxidation could be a competitive sink for particulate 2-MTSs and a source of more oxygenated/functionalized OSs detected in atmospheric $PM_{2.5}$, likely modifying air quality- and climate-relevant aerosol physicochemical properties of SOA containing 2-MTSs. Heterogeneous oxidation chemistry is currently lacking and should be considered in large-scale models to better understand the transformation and abundance of atmospheric particulate OSs.

4AC.19

Atmospheric Particle Composition at Different Altitude via Tethered Balloon System. SWARUP CHINA, Nurun Nahar Lata, Fan Mei, Darielle Dexheimer, Kuo-Pin Tseng, Zihua Zhu, Rhenton Brimberry, Noah Wilson, *Pacific Northwest National Laboratory*

The radiative forcing of the ambient aerosol is strongly influenced by the vertical distribution of aerosols. The estimation of the indirect effect of aerosol also has a significant uncertainty due to the spatial variation of the aerosol, especially at the cloud base. The unmanned systems have gained significant interest in atmospheric science, which could minimize the error, risk and cost in environmental research. Deployment of an unmanned aerial system such as ARM’s tethered balloon system can provide important information about the vertical profile of aerosol with longer temporal coverage. In this study, the tethered balloon system was deployed at the Southern Great Plains (SGP; DOE ARM mega site), Oklahoma, and Oliktok Point, Alaska (OLI site) collecting aerosol particles at different boundary layers. Particle samples were collected using a 4-stage cascade impactor. Particle samples were collected from different air-masses, from clean condition to polluted biomass burning plume. The morphology and chemical composition of individual particles were analyzed via multi-modal micro-spectroscopy techniques such as computer-controlled scanning electron microscopy with energy dispersive X-ray spectroscopy, transmission electron microscopy, scanning transmission X-ray microscopy, time-of-flight secondary ion mass spectrometry and Raman spectroscopy. Single particle composition results show the clear difference in aerosol compositions at various altitudes. Our analysis shows a considerably increase in sulfates at higher altitude than ground level. In general, we observed substantial amount of dust particles at higher altitude, suggesting the importance of supermicron size particles and their potential to influence atmospheric ice nucleation in mixed-phase clouds. We also observed super micron size carbonaceous particles at 800m altitude during a biomass burning event. The research can benefit in understanding the short-range, long-range transportation of atmospheric particles and vertical profile of atmospheric particle composition. The experiments performed via unmanned system could provide a long-term observation in atmospheric science efficiently and economically.

4AC.20

Aqueous-phase Secondary Organic Aerosol Formation: Laboratory Simulations and Field Observations in China.

XINLEI GE, Zhaolian Ye, *Nanjing University of Information Science & Technology*

Secondary organic aerosol formation in atmospheric aqueous phases (cloud/fog droplets or wet aerosols) (aqSOA) has been recognized as a possible and significant pathway that can help reconcile the discrepancies between observed and modelled PM properties. However, the efficient precursors, formation mechanisms, mass yields and properties of aqSOA are still less clear. In this presentation, we will present both laboratory experimental results and field observations regarding aqSOA. First, we studied the aqSOA formation originated from a series of biomass burning emitted organic compounds mimicking the atmospheric cloudy/foggy conditions. Reaction rates, formation yields, light absorption properties as well as the chemical compositions of the aqSOA formed from oxidation by various oxidants were investigated. Secondly, we investigated aqueous oxidation of a few species that belong to the intermediate volatility organic compounds (IVOCs), and demonstrate aqueous processing of IVOC can be a significant source of SOA as well as light-absorbing organics (Brown Carbon, BrC). At last, we analyzed the measurement data obtained by Aerodyne high resolution aerosol mass spectrometers in Chinese megacities including Beijing and Nanjing, and explored the relationships of different organic aerosol factors resolved by positive matrix factorization with the relative humidity and photochemical activities, etc. Field evidence of aqSOA, its chemical characteristics, controlling factors, etc., will be discussed.

4AC.22

SOA Production from Chlorine Radical Oxidation of Alkanes: Effects of Structural Branching, NOx, and Relative Humidity. LEIF JAHN, Dongyu S. Wang, Surya Venkatesh Dhulipala, Felipe Cardoso Saldaña, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Atmospheric chlorine radicals (Cl) have recently been observed in a variety of continental as well as coastal regions at concentrations significant for the formation of secondary organic aerosol (SOA). Experiments have shown that Cl oxidizes most VOC precursors more rapidly than hydroxyl (OH) radicals and that Cl-oxidation often results in higher SOA yields. This effect is especially pronounced for alkanes, however comparatively little is known about the mechanism and products of the reactions of chlorine radicals with alkanes of different structures. We investigated the Cl-oxidation of a series of C10 hydrocarbon precursors with linear (n-decane), branched (2-methylnonane and 3,3-dimethyloctane), and branched cyclic (butylcyclohexane) structures through laboratory smog chamber experiments utilizing an iodide-adduct chemical ionization mass spectrometer (I- CIMS) with a filter inlet for gases and aerosols (FIGAERO) and an aerosol chemical speciation monitor (ACSM). Experiments were performed with or without added NOx and at low (<5%) or medium (40-50%) relative humidity. Under all examined conditions SOA production decreased on the order butylcyclohexane > n-decane > 2-methylnonane > 3,3-dimethyloctane. Lower SOA production observed for branched hydrocarbons is consistent with increased fragmentation to higher volatility molecules and was observed through early-generation gas-phase fragmentation products. Patterns in fragmentation products of the branched alkanes also suggest that chlorine radicals are able to abstract primary hydrogen atoms, confirming prior theory; this likely contributes to increased SOA production. More SOA was produced under low-NOx conditions, while experiments under low and medium RH conditions produced comparable amounts of SOA but some differences in particle-phase composition were observed. Further details on the products and mechanisms contributing to these trends will also be discussed.

4AC.24

Single Particle Analysis to Study Heterogeneous Oxidative Aging of Aerosols.

RAVLEEN KAUR KOHLI, James F. Davies, *University of California, Riverside*

Aerosols are a major component of Earth's atmosphere and affect the formation and optical properties of clouds, absorb and scatter solar radiation, provide surfaces on which chemistry can occur, and adversely impact air quality and human health. The composition of atmospheric aerosol particles comprises of a wide range of organic compounds. Due to aerosols' incredible composition along with supporting conditions in the atmosphere, their properties and composition continuously transform as a result of various physical processes (evaporation/condensation) and chemical reactions (in/on particles).

A major area of focus in present day atmospheric research is to understand and predict how aerosol particles evolve in the atmosphere due to various heterogeneous oxidation processes, involving ozone (O_3) and radicals such as OH· and NO_3·. This has led to extensive explorations of their physical and chemical properties through the development of various single particle and ensemble measurement techniques. While these individual techniques have been developed to independently measure specific properties, there remains a need to allow a complete physicochemical characterization of an aerosol sample for developing the connection between its physical properties with evolving composition.

In this work we discuss the development of an experimental platform that couples a **linear quadrupole electrodynamic balance (LQ-EDB) with paper spray mass spectrometry (PS-MS)** to precisely measure the physicochemical properties of levitated aerosol particles. This technique allows us to simulate heterogeneous reactions happening in atmosphere, such as ozonolysis and OH-initiated oxidation, on single levitated particles and precisely measure their physical and optical properties as a function of their evolving composition with extent of reaction. Preliminary measurements on model aerosol samples demonstrate that the LQ-EDB-PS-MS technique is an effective tool for real-time qualitative and quantitative analysis of complex aerosol particles undergoing chemical transformations.

4AC.25

Investigating the July 1st/2nd 2018, Pollution Event at Whiteface Mountain with Box Modeling and WRF-Chem.

CHRISTOPHER LAWRENCE, Mary Barth, Sara Lance, Paul Casson, Dan Kelting, Elizabeth Yerger, *University at Albany, SUNY*

Organic matter is an important constituent of aerosols, comprising 20-90% of aerosol mass. However, despite considerable research, the formation and composition of organic aerosol remain highly uncertain, mainly due to uncertainties related to secondary organic aerosols (SOA), formed from the oxidation of volatile organic compounds (VOCs) into less volatile compounds. The controlling factors for the composition and chemical aging of these VOCs are complicated and can be difficult to predict due to limited observational data, often requiring modeling to investigate. During July 1st/2nd 2018, a pollution event was identified by measurements of cloud water composition and air quality at the summit of Whiteface Mountain in Upstate New York. This pollution event was characterized by high concentrations of water soluble organic carbon, organic acids such as formic and acetic acids, and ammonium. To investigate this event and potentially important SOA precursor gases for this site, a combination of WRF-Chem and the chemical box model BOXMOX were used. WRF-Chem was used to create air-mass trajectories providing input data for BOXMOX which was run along the trajectory. Two chemical mechanisms were used within BOXMOX: the Model for Ozone and Related Chemical Tracers (MOZART) T1 mechanism, comprised of 151 gas-phase species and 352 reactions, and the Master Chemical Mechanism (MCM) 3.3.1., comprised of 143 VOC species and nearly 17,000 reactions. The formation and removal of important SOA gases such as glyoxal, methylglyoxal, formic acid, and acetic acid are compared between the two mechanisms to highlight the importance of reactions that may not be captured in WRF-Chem and MOZART-T1. Due to the similarity of their gas phase chemical mechanisms, outputs from both WRF-Chem and BOXMOX using the MOZART T1 scheme are also compared to investigate the importance of aerosol and aqueous chemistry on SOA precursors.

4AC.26

Atmospheric Reactivity of Brake Wear Particulate Matter: Implications for Predicting and Improving Air Quality.

LAURA MATCHETT, Kristyna Stix, Maya Abou-Ghanem, Sarah Styler, *University of Alberta*

Atmospheric particulate matter (PM) is a concern for human health, visibility, and climate. In urban environments, vehicular traffic emits large quantities of PM through either exhaust (engine combustion) or non-exhaust (brake, tire, and road abrasion) processes. Due to regulations and technological improvements surrounding exhaust emissions, non-exhaust emissions are becoming the dominant contributor to traffic PM. One of the largest sources of non-exhaust emissions is brake wear. Although studies have examined its emission, size, chemical composition, and toxicity, virtually nothing is known regarding its atmospheric reactivity. One measure of reactivity is the extent to which brake wear interacts with pollutant gases, which could alter both the concentration of the gas and the properties (*e.g.* toxicity) of the PM. In this study, we used a coated-wall flow tube apparatus to determine uptake coefficients for ozone, an important urban pollutant, at the surface of three types of brake wear (ceramic, semi-metallic, and organic) under both dark and light conditions. We find that all types are very reactive with ozone in the dark and that their reactivity increases in the presence of light, which may reflect photocatalytic contributions from metal oxides and light-absorbing organic species found in brake wear. The uptake coefficients for the three types of brake wear differ, which may reflect the significant differences seen in their composition. To elucidate which components of brake wear may be contributing to the observed reactivity, we also investigated the uptake of ozone by some of the main components in our samples: phenolic resin, graphite, iron powder, and iron oxide. Although the uptake coefficients for these brake wear types differ, they are within one order of magnitude; this has the potential to simplify the implementation of this chemistry into atmospheric models, leading to a better understanding of urban air quality.

4AC.27

Detailed Comparisons of Results From Comprehensive Chamber Studies and Explicit Chemical Mechanisms.

JOSHUA MOSS, Abigail Koss, Alexander Zaytsev, Martin Breitenlechner, Jordan Krechmer, Kevin Nihill, Jonathan Franklin, Christopher Lim, James Rowe, Joshua L. Cox, Joshua Shutter, Manjula Canagaratna, Brian Lerner, Douglas Worsnop, Richard Valorso, Marie Camredon, Bernard Aumont, Frank Keutsch, Jesse Kroll, *MIT*

Chamber experiments with mass spectrometric measurements and chemical mechanistic models have greatly contributed to our community’s knowledge of SOA and VOC oxidation. However, both measurements and mechanisms have inherent limitations: mass spectra typically can not provide detailed molecular structures or deconvolute overlapping signals of constitutional isomers, and mechanisms must be validated against experimental data and are hindered by uncertainties in our understanding of the chemistry. Herein we explore how coupled measurement-mechanism analyses enable us to use the strengths of one approach to improve the other. Chamber studies were performed with a suite of instruments including a PTR-MS (Proton Transfer Reaction Mass Spectrometer), a CIMS (Chemical Ionization Mass Spectrometer), and an AMS (Aerosol Mass Spectrometer) to measure the vast majority of secondary organic compounds, and mechanisms were generated using GECKO-A (the Generator of Explicit Chemical Kinetics of Organics in the Atmosphere). GECKO-A uses structure-activity relationships (SARs) to predict reaction products and rates if they are not already explicitly known, and these SARs may be modified to affect classes of reactions (e.g. alkoxy radical decomposition) throughout the entire mechanism. The n-butane oxidation system was chosen for this study because its chemistry is well-characterized and it produces relatively few major products which are all measured by PTR-MS. Results show strong agreement between GECKO-A’s mechanism and the chamber data. Furthermore, this analysis elucidated PTR-MS ion chemistry including losses of water, nitrate, and PAN functional groups which has implications for interpreting mass spectra of functionalized species (including organonitrogen species). Analysis of more complex systems including 1,2,4-trimethylbenzene allow for further examination of SOA ensemble properties, phase partitioning, and interpretation of mass spectra. The combined results of these analyses suggest that they can serve as a template for future studies to yield new insights into SOA systems while simultaneously improving our ability to interpret chamber data and construct detailed mechanisms.

4AC.28

Quantification of Organic Aerosol Evaporation Rates in Aircraft Inlets and Instruments. DEMETRIOS PAGONIS, Benjamin A. Nault, Pedro Campuzano-Jost, Hongyu Guo, Jason Schroder, Douglas Day, Jose-Luis Jimenez, *University of Colorado-Boulder*

The semivolatile character of part of the organic aerosol (OA) can lead to aerosol evaporation in sampling systems. This can be especially important during aircraft measurements, where there is often significant warming of the air upon entering the inlet system in the cabin. We have carried out quantitative airborne measurements of aerosol evaporation rates using an Aerodyne Aerosol Mass Spectrometer (AMS), and a thermodenuder. These measurements were carried out aboard the NASA DC-8 aircraft during the KORUS-AQ and FIREX-AQ studies, and aboard the NSF/NCAR C-130 during the WINTER study. During those studies the temperature difference between ambient air and the OFR ranged from 10–30 K, and the OA mass fraction remaining (MFR) ranged from 0.68–0.83. We analyze these results using an established kinetic model of aerosol evaporation, and published volatility basis sets. The model reproduces the OA evaporation within 15% error across the three studies, and thus provides unique information on ambient aerosol volatility aloft. We perform case studies of OA evaporation inside inlets where charcoal denuders are used to remove VOCs, which are applicable to the extractive electrospray ionization mass spectrometry (EESI) measurements made during FIREX-AQ. For the EESI inlet (residence time was 1.6 s, charcoal denuder) we estimate significant evaporative loss inside the inlet (MFR > 0.7). AMS inlet residence times are sufficiently short to minimize OA evaporation (MFR > 0.99 KORUS-AQ and WINTER; MFR > 0.95 FIREX-AQ). Finally, we explore the evaporative losses when black conductive tubing (which acts as a denuder) is used in an inlet.

4AC.29

Investigation of Brown Carbon Formation in Cloud Droplets and Ambient Particles Undergoing Drying. VIKRAM PRATAP, Michael Battaglia Jr., Amy Christiansen, Annmarie Carlton, Christopher Hennigan, *University of Maryland, Baltimore County*

Recent laboratory studies have reported the formation of light-absorbing organic carbon compounds (brown carbon, BrC) in aqueous particles undergoing drying. Atmospheric particles undergo humidification-drying cycles and most clouds are not precipitating, which implies particle and cloud droplet drying could potentially be an important source of BrC globally. In this work, we investigated BrC formation in ambient particles sampled during the summertime in Baltimore, Maryland. In the second part of the project, we investigated drying induced BrC formation in aerosolized cloud water collected at Whiteface Mountain (WFM), Wilmington, NY. Ambient particles as well as cloud droplets did not show evidence of drying induced BrC formation. Ambient particles appear to have BrC precursor (for example, glyoxal and methylglyoxal) levels lower by 2-5 orders of magnitude in comparison to the concentrations used in laboratory experiments where drying induced BrC formation has been observed. In the cloud water samples, the BrC precursor level was likely depleted during the regional transport of air masses reaching WFM. The implications of this work on the atmospheric budget of BrC are discussed.

4AC.30

Organic Fraction of the <0.15 µm Diameter Aerosol Particles over the Southern Ocean. GEORGES SALIBA, Kevin Sanchez, Savannah Lewis, Lynn Russell, Cynthia Twohy, Greg Roberts, *Scripps Institution of Oceanography*

Aerosol particles smaller than 0.15 µm in diameter can be cloud condensation nuclei (CCN) active at supersaturations typical of marine stratocumulus clouds depending on their chemical composition. However, little is known about the composition and contribution to CCN of organic mass (OM) for particles over the Southern Ocean marine boundary layer. Airborne measurements of aerosol number and mass size distributions, chemical composition using scanning transmission electron microscopy with energy dispersive X-ray spectroscopy (STEM-EDS), and CCN spectra during the Southern Ocean Clouds, Radiation, Aerosol Transport Experimental Study (SOCRATES) provide a comparison of organic contributions. Here, we estimate the organic fraction of the <0.15 µm particles indirectly by comparing CCN spectra to particle size distributions. STEM-derived composition of particles smaller than 0.15 µm diameter was consistent with a larger fraction of sulfate and sodium-based sea spray particles with OM components accounting for less than 2% of analyzed particles. Particles <0.15 µm diameter had kappa values of 0.2 – 0.5, indicating the substantial presence of OM at these sizes. These inferred organic components are found mostly at sizes below STEM range. The OM fraction estimated from comparing the size distribution and supersaturation spectra varied from <10% to 70% for particles <0.15 µm in diameter. This variable OM fraction accounted for <0.1 µg/m3 mass concentrations of particles smaller than 0.15 µm diameter but may play a role at cloud supersaturations greater than 0.3%.

4AC.31

Molecular Characterization of Brown Carbon Produced from the OH/NOx Photo-oxidation of Naphthalene. KYLA SIEMENS, Ana Morales, Anusha P.S. Hettiyadura, Quanfu He, Chunlin Li, Yinon Rudich, Alexander Laskin, *Purdue University*

Brown carbon (BrC) has been identified as a class of secondary organic aerosol (SOA) constituents with substantial light-absorption in the visible light range that influences regional visibility and radiative forcing of the climate. In this study, we investigate the chemical composition of BrC formed during the photo-oxidation of naphthalene, a polyaromatic hydrocarbon emitted during fossil fuel combustion, in the presence of OH and NO_x ($NO + NO_2$). We provide molecular insights to the effect of atmospheric ageing on optical properties of the BrC components of this system. We employ high performance liquid chromatography equipped with a photodiode array detector and a high-resolution mass spectrometer (HPLC-PDA-HRMS) to determine the chemical composition of naphthalene-derived SOA and its BrC constituents formed in the presence of NOx. Results of this work reveal the buildup of highly absorbing nitro-aromatic chromophores formed in high NO_x environments, and the extent of their degradation during processes of atmospheric ageing. This research contributes to the development of high performance and high-resolution techniques for the structural elucidation of strongly absorbing organic aerosol, specifically BrC chromophores. This project also contributes to a predictive understanding of the processes and conditions that form BrC from anthropogenic aromatic hydrocarbons.

4AC.32

Simulation of the Impact of Particle Phase State on SOA Formation from the Photooxidation of Isoprene and Beta-pinene Cocktail in the Presence of Electrolytic Salts.

ZECHEN YU, Myoseon Jang, *University of Florida*

In the presence of the inorganic salts, the formation of secondary organic aerosol (SOA) can be influenced by a particle phase state: liquid-liquid phase separation (LLPS) and homogeneous aerosol phase (HAP). The particle phase state is not only dynamic under the ambient environment where humidity are dynamically changing, but it also changes with SOA’s polarity and hygroscopicity of inorganic salts. In this study, the model approach to determine aerosol phase state will be discussed and the impacts of aerosol phase state on SOA production will also be evaluated. For the determination of aerosol phase state, the phase separation relative humidity (SRH) between organic and inorganic phase is predicted using a polynomial equation, which is obtained by fitting SOA physicochemical parameters (i.e., organic to carbon (O:C) ratio, molecular weight, and hydrogen-bonding ability) and inorganic salt compositions to SRH data. Both literature data and the measured data in this study using an optical microscopy are used for the derivation of SRH predictive equation. The SRH prediction is then implemented into the Unified Partitioning Aerosol Phase Reaction (UNIPAR) model to predict SOA via multiphase reactions of hydrocarbons. The UNIPAR model coupled with aerosol phase state prediction is demonstrated by simulating SOA formation from the photooxidation of the blend of isoprene and β-pinene at different ratios under varying seed conditions to yield SOA varying at O:C ratios and salts compositions. Isoprene SOA typically grows in HAP and β-pinene SOA in LLPS. We also demonstrate the difference between the prediction of SOA mass with the true phase state and that with the false phase state based on the hypothesis test theory.

4AC.33

Superoxide Formation from Aqueous Reactions of Biogenic Secondary Organic Aerosols.

JINLAI WEI, Ting Fang, Cynthia Wong, Pascale Lakey, Sergey Nizkorodov, Manabu Shiraiwa, *University of California, Irvine*

Biogenic secondary organic aerosols (SOA) account for a substantial fraction of atmospheric particulate matter, posing significant impacts on air quality, climate and public health. Reactive oxygen species (ROS) including OH, superoxide, and H_2O_2 play a central role in aqueous-phase processing and health effects of SOA. Recent studies have revealed that biogenic SOA can release ROS in the aqueous phase, but kinetics and reaction mechanisms of superoxide formation is rarely quantified and hardly understood. Here we present simultaneous measurements of hydroxyl radical and superoxide from aqueous reactions of SOA generated by ozonolysis and OH oxidation of biogenic VOCs using electron paramagnetic resonance spectrometry. Kinetic modeling reproduced temporal evolution of OH and superoxide formation by considering decomposition of organic hydroperoxides, OH oxidation of alcohols, and unimolecular decomposition of α-hydroxyperoxyl radicals. SOA generated from ozonolysis tend to contain higher fractions of peroxides leading to a OH-dominated profile with molar yields of up to ~0.1%, while SOA generated from OH photooxidation mainly form with molar yield of 0.1-0.7% depending on precursors. These findings have significant implications on the atmospheric fate and particle-phase reactions of highly oxygenated molecules, affecting their role in particle formation and chemical transformation of organic aerosols. In addition, inhalation and deposition of SOA particles may lead to a substantial release of superoxide in lung lining fluid, which may contribute to oxidative stress in the human respiratory tract.

4AC.34

Nonrefractory Particulate Matter Detection Using the Dual-Vaporizer Configuration of the Soot Particle Aerosol Mass Spectrometer (SP-AMS). LEAH WILLIAMS, Anita Avery, Arthur J. Sedlacek, Timothy Onasch, *Aerodyne Research, Inc.*

The Soot Particle-Aerosol Mass Spectrometer (SP-AMS) can operate with one of two particle vaporizers: (1) the standard AMS resistively heated tungsten vaporizer for traditional detection of non-refractory particulate matter (NR-PM), and (2) an intracavity laser vaporizer for detection of absorbing, refractory materials, including black carbon (rBC) and metal nanoparticles, and associated NR-PM. The SP-AMS can also be operated with both vaporizers by sequentially turning the laser vaporizer on and off. The use of both vaporizers simultaneously is complicated by different collection efficiencies (CE) and different relative ionization efficiencies (RIE) of NR-PM species that can strongly affect the measured NR-PM signals from rBC-containing particles. This work describes a systematic investigation of mixed particles with varying ratios of ammonium nitrate, ammonium sulfate or levoglucosan to rBC. Particles were generated by atomizing aqueous solutions with specific mass ratios of NR-PM material to rBC and size-selecting with a differential mobility analyzer (DMA). The composition of the particles was confirmed with a Single Particle Soot Photometer (SP2) to be the expected mixture of NR-PM and rBC and to be an internal mixture. Particle bounce at the tungsten vaporizer was assessed with a quadrupole (Q-) AMS equipped with a light scattering module. NR-PM and rBC mass concentrations were measured with an SP-AMS in both laser on and laser off modes. This dataset shows that CE at the tungsten vaporizer varies strongly with composition due to increasing bounce for particles with a higher fraction of rBC for the particle sizes used here (300 to 400 nm). CE at the laser vaporizer also decreases with increasing rBC due to particle beam focusing, but not as strongly. The interplay of these two CEs, in addition to different RIEs, causes an apparent increase in NR-PM signal when the laser is on.

4AC.35

Direct Measurement of Ozone Sensitivity to Oxides of Nitrogen and Volatile Organic Compounds during COVID-19 Using a Mobile Smog Chamber System. SHENGLUN WU, Toshihiro Kuwayama, Michael Kleeman, *University of California, Davis*

Ozone (O3) is a secondary pollutant produced from a series of non-linear photochemical reactions. Nitrogen oxides (NOx) and volatile organic compounds (VOCs) are two main precursors affecting O3 formation, but the NOx to VOC ratio defines the chemical regime that determines ozone response to changing precursor emissions. Understanding the atmospheric chemical regime is a critical first step in the design of effective emissions control strategies for reducing O3 concentrations. Here we describe a field study that directly measures the sensitivity of O3 to NOx and VOC using a mobile trailer equipped with three identical Teflon smog chambers. Three parallel chambers (each 1 m3) were filled with ambient air at approximately 11am each day. One chamber was used as basecase measurement, one chamber had NOx added, and one chamber had a surrogate VOC added (ethylene, m-xylene, n-hexane). Chambers were irradiated with UV (50 W m-2) equivalent to midday summer conditions for three hours. O3, NOx, NOy, temperature, and relative humidity were measured in all three chambers each 10 min. Measurements at Sacramento from Apr - July 2020 find increased O3 formation in the VOC-perturbed chamber and lower O3 formation in the NOx-perturbed chamber on weekdays. This finding suggests that the VOC-limited ozone production dominates weekdays in Sacramento. Reduced NOx emissions associated with COVID-19 shelter-in-place orders did not significantly affect the atmospheric chemical regime. However, a significant change of O3 sensitivity from VOC-limited to NOx-limited was detected on the weekend, when NOx concentrations were reduced by a factor of approximately two. Measurements on days with different ambient temperature suggest that increasing temperatures reduce the NOx limitation and increase O3 production. The results from the current study demonstrate a system to aid in the design of emissions control programs for O3 reduction.

4AC.36

The Effect of Aerosol Acidity on the Volatility of Isoprene and Monoterpene-derived Secondary Organic Aerosol (SOA). ALLA ZELENYUK, David Bell, Matthieu Riva, Dan Imre, Marianne Glasius, ManishKumar Shrivastava, John Shilling, Jason Surratt, Joel A. Thornton, Emma D'Ambro, Rahul Zaveri, *Pacific Northwest National Laboratory*

Reactive uptake of isoprene and monoterpene-oxidation products by acidic sulfate particles has been identified as an important source of SOA that leads to the formation of low-volatility products, i.e. oligomers and organosulfates (OS).

We have previously investigated the reactive uptake of isomeric isoprene epoxydiols (IEPOX) by acidic ammonium bisulfate (ABS) and non-acidic deliquesced ammonium sulfate (AS) particles. Using single particle mass spectrometry, we demonstrated that IEPOX uptake by pure ABS and AS particles is a volume-controlled process, which results in particles with uniform composition across a wide range of sizes. In contrast, IEPOX uptake by ABS particles coated with α-pinene SOA is lower compared to that of pure ABS particles and is strongly dependent on particle size.

The measurements of room-temperature evaporation kinetics of size-selected particles indicate that nearly 90% of IEPOX-SOA formed on ABS seeds is non-volatile. IEPOX-SOA formed on ABS at low RH and evaporated at high RH exhibit slightly higher evaporative loses, retaining 75% of their volume after 24 hours of evaporation. In comparison, IEPOX-SOA particles formed on AS seeds retain only 50% of their volume after 24 hours, at which point the particles composition is dominated by OS. In all cases the volatility of IEPOX-SOA is ~3 orders of magnitude lower than that of SOA formed by gas-phase isoprene photooxidation.

To better understand the observed size-dependent IEPOX uptake by α-pinene SOA-coated ABS particles we examined the chemical interactions between ABS seeds and α-pinene oxidation products. We will present the results of experiments, in which we observed size-dependent reactive uptake of gas-phase monoterpene ozonolysis products, size-independent reactive uptake of α-pinene oxide, and quantified volatility of α-pinene SOA coatings as a function of coating thickness.

4AC.37

The Interconnection of Aerosol-Phase State and Chemical Composition Impact the Formation and Climate-Altering Properties of Isoprene-Derived Secondary Organic Aerosols. YUE ZHANG, Yuzhi Chen, Andrew Lambe, Nicole Olson, Ziying Lei, Zhenfa Zhang, Avram Gold, John Jayne, Douglas Worsnop, Timothy Onasch, Andrew Ault, Jason Surratt, *University of North Carolina at Chapel Hill*

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. Previous studies have systematically examined the reactive uptake probability of isoprene-derived epoxydiols (γ_{IEPOX}) onto acidic ammonium sulfate particles coated with α-pinene or surrogate SOA by coupling a flow tube reactor with an iodide-adduct high-resolution time-of-flight chemical ionization mass spectrometer (HR-ToF-CIMS). Given the complex chemical composition of atmospheric aerosols, a parameterized model is needed to address how chemical composition systematically impacts IEPOX-derived SOA.

A uniform layer of organics generated from selected atmospherically relevant SOA precursors was coated onto acidic sulfate particles in a potential aerosol mass (PAM) oxidation flow reactor, and confirmed by atomic force microscopy (AFM) and scanning electron microscopy (SEM). Measured γIEPOX was parameterized as a function of SOA coating type, coating thickness, oxidation state, and RH. Results show that certain pre-existing anthropogenic SOA coatings reduced γIEPOX to a higher extent than biogenic SOA coatings of the same thickness, in some cases by nearly an order of magnitude. A multivariate model combining the measured oxidation state and chemical composition of the aerosols was constructed to predict the viscosity of SOA as a function of chemical composition and aerosol water content. The multivariate model on viscosity was combined with a box model with ambient measurement input from the 2013 SOAS campaign to assess the effects of pre-existing organic coatings on IEPOX-derived SOA formation in the Southeast U.S. We show that the oxygen-to-carbon (O/C) and the hydrogen-to-carbon (H/C) ratios of organic shell impact both the phase state and the subsequent IEPOX-derived SOA formation in the presence of an existing SOA coating. 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.

4AC.38

Gas-phase Hydrogen Peroxide from Multiphase Ozonolysis of Unsaturated Lipids. ZILIN ZHOU, Jonathan Abbatt, *University of Toronto, Canada*

Gas-phase hydrogen peroxide (H_2O_2) is an oxidant in the atmosphere and an indoor air pollutant that is an irritant to the respiratory system at high concentrations. It is well known that the gas-phase ozone oxidation of gas-phase alkenes, such as limonene, leads to the formation H_2O_2 through the reaction between Criegee intermediates (CI) and water. However, the degree of H_2O_2 formation from multiphase ozonolysis on surfaces has not been reported. Here, we studied the heterogeneous ozonolysis reactions of multiple unsaturated lipids present in natural environments and on household surfaces. H_2O_2 formation and ozone consumption were simultaneously monitored online by a Picarro H_2O_2 analyzer and an ozone monitor during the reaction. Upon exposure to ozone, gas-phase H_2O_2 was only observed under high relative humidity, as a result of the decomposition of hydroxyhydroperoxides (α-HHP) that are generated through water reaction with CI. In addition, α-HHP can be stable over a few hours under dry conditions and their decomposition is facilitated by water vapor. The H_2O_2 yields vary, ranging from 7-35% for triolein, methyl oleate and squalene, with insignificant dependence on relative humidity between 50% and 80%. In contrast, the H_2O_2 yield in ozonolysis of oleic acid was negligible, presumably due to the rapid scavenging of CI by the acid head group of the fatty acid. The environmental implications of this chemistry will be discussed from the perspectives of the oxidizing ability in the atmosphere and indoor air quality.

4AC.39

Photochemical Uptake of Ozone by Organic-Coated TiO2 Particles: Influence of Atmospheric Transport on Mineral Dust Photochemistry. MAYA ABOU-GHANEM, Sarah Styler, *University of Alberta*

Mineral dust is one of the most abundant types of aerosols in our atmosphere, with an estimated 1600 Tg emitted annually. Since the atmospheric residence time of mineral dust ranges from days to weeks, it can travel thousands of kilometers before settling. During its transport, mineral dust provides a surface for reaction of gas-phase pollutant species, with many of these reactions promoted by light. These interactions can influence not only the chemical composition of the atmosphere but also that of mineral dust itself; for example, field observations have shown the presence of organic and inorganic coatings at the surface of mineral dust upon mixing with pollutant species. Organic coatings have been found to influence cloud condensation nuclei activity and optical properties of mineral dust; however, the implications of organic coatings for mineral dust photoreactivity are still poorly understood.

Here, we use a custom-built aerosol flow tube coupled to an ozone analyzer and a scanning mobility particle sizer to investigate the influence of organic coatings on the photochemical uptake of ozone by TiO_2, which we use as a simple photoactive model for mineral dust. In particular, we explore ozone photodecomposition at the surface of TiO_2 coated with a suite of anthropogenic alkanes of differing viscosities and find that the uptake of ozone is suppressed in comparison to uncoated TiO_2. This work provides new insights on the influence of organic coatings on mineral dust photochemistry, as well as the implications of these coatings on urban air quality.

4AC.40

A Two-city Study of Air Quality in Vietnam 2018-19: Source Apportionment Using PMF Applied to Offline AMS Data.

ZAINAB BIBI, James Allan, Thomas Bannan, Alex Baker, David Oram, Duong Huu Huy, To Thi Hien, Hugh Coe, Saleh Alzahrani, *University of Manchester, UK*

Hanoi and Ho Chi Minh City (HCMC) in Vietnam are very heavily polluted cities, with annual average PM2.5 concentrations of 50.5 and 42 µg m–3 respectively (Hein et al., 2019). As part of a collaborative project between the UK and Vietnam, “A Two City study of Air Quality in Vietnam”, PM2.5 was collected on glass fibre filters in 2018 and 2019 from different sites in Hanoi and HCMC. Filter extracts were then analysed using a High-Resolution Aerosol Mass Spectrometer (HR-AMS) to study organic and inorganic compounds. Positive Matrix Factorisation (Paatero and Tapper, 1994) was performed to discriminate between different sources of pollution, with the objective of informing policymaking decisions. The results of this study showed the highest concentrations of organics followed by nitrates, sulphates, ammonium and chloride while PMF analysis identified the data into four different sources in Hanoi and HCMC both. The first factor contains a marker associated with Mannitol, which can be associated with the ejection of the fungal spores. The second factor is highly oxidised organic fragments with the high peaks at m/z 28 and m/z 44 and representing the substantial fraction of organic matter from both sources i.e. natural biogenic emissions (Xu et al., 2015a; Chen et al., 2015) and anthropogenic sources mainly vehicle emissions (Presto et al., 2014). The third factor is semi-volatile oxygenated OA (SVOOA), which is a mixed factor mainly coming from the secondary sources. The fourth factor has peaks associated with levoglucosan which is a marker associated with biomass/wood burning. This study will provide an important additional information about sources of organic aerosols in both cities and will be helpful for policymaking in the future.

4AC.41

Deep Learning for Prediction of Multiphase Isoprene Oxidation Products.

MUNKHZAYA BOLDBAATAR, Mohamadamin Tavakoli, Dora Kadish, Karla Rojas Garcia, Pierre Baldi, David van Vranken, Sergey Nizkorodov, Annmarie Carlton, *University of California, Irvine*

Isoprene is the most abundantly emitted biogenic volatile organic compound in the atmosphere and its oxidation with atmospheric oxidants contributes substantially to the global secondary organic aerosol budget. Isoprene oxidation has been studied for many years, but despite the extensive studies, our mechanistic understanding is far from complete and the precise chemical identities of high molecular weight compounds of isoprene oxidation remain speculative. To understand the full extent of atmospheric reactions and the identity of isoprene oxidation products, we approach this problem from the nexus of computer science and chemistry by training and applying an intelligent system “Reaction Predictor.” Reaction Predictor, or shortly RP, is a machine learning-based system that utilizes a deep learning algorithm to predict the outcome of chemical reactions. Reactions are predicted at the level of elementary mechanistic steps that can be chained together to yield complex global reactions. RP is currently trained with 677 radical reactions (resonance, homolysis, abstraction, addition, recombination, hydride shift) and more than 12,000 polar reactions and reactions of atmospherically relevant gas-phase VOCs (α-pinene and isoprene). We apply RP to isoprene oxidation by a hydroxyl radical, OH. Here, we present our RP predictions with mass spectra from laboratory smog chamber experiments, with a focus on chemically identifying large molecular weight products.

4AC.42

Impact of Meteorological Models on Aerosol Liquid Water Predictions. ALYSSA BURNS, Virendra Ghate, Amy Christiansen, Annmarie Carlton, *University of California, Irvine*

Meteorological reanalysis datasets are critical to understanding the fate and transport of trace species in the atmosphere. For example, air quality models employ meteorological models nudged to reanalysis data to drive physical transport and some emissions. Relative humidity, temperature, and planetary boundary layer depth are routinely utilized in comparisons to remotely sensed aerosol optical depth (AOD) or paired with surface measurements of aerosol chemical composition to calculate aerosol liquid water content (ALW). A comprehensive investigation of reanalysis meteorological products in the context of particle chemical composition is necessary to ensure adequate predictive skill of air quality models. In this work, we investigate two reanalysis datasets, the North American Regional Reanalysis (NARR) and the European Centre for Medium-range Weather Forecasts (ECMWF) ERA5, and the resulting impacts on ALW predictions. We evaluate the NARR and ERA5 and subsequent estimates of ALW with measurements made during the Southern Oxidant and Aerosol Study (SOAS). Significant differences in ALW mass concentrations are observed when the different data products are used, and when RH is calculated using dew point versus specific humidity.

4AC.43

Aqueous Phase Reactions of Humic Like Substances (HULIS) Proxies with Photoproduced Reactive Oxygen Species (ROS). ANTHONY CARRASQUILLO, Wyndom Chase, David Noeckel, Amelia Schaeffer, Allison Wong, *Williams College*

Humic Like Substances (HULIS) have been identified as major light-absorbing components of aerosol formed from biomass burning events. This material is highly heterogenous, containing biopolymeric structures derived from the major components of cell walls (lignins, tannins, etc.). Aqueous phase reactions involving photolytically generated reactive oxygen species (ROS) within aerosol particles have the potential to degrade these structures, leading to the destruction of chromophores and in turn the alteration of their light-absorbing properties. While the major ROS previously identified in field studies include singlet oxygen ($^1O_2$), hydrogen peroxide (H_2O_2), superoxide (O_2^-), and organic radicals (RO), only the reaction of the hydroxyl radical (OH) with HULIS has received significant attention in the literature. Here we focus on the aqueous phase photochemical reactions of two HULIS proxies, gallic acid (GA) and egallic acid (EGA). Each proxy was irradiated with artificial sunlight in the presence of an ROS-specific photosensitizer to generate enhanced concentrations of each OH, $^1O_2$, H_2O_2, RO, and O_2^- in bulk solutions. A relative-rates method was used to measure the concentration of ROS generated in each experiment, and to determine the rate constant for reaction with each proxy as a function of pH. Finally, we will present preliminary assignments for major products determined using GC-MS along with potential reaction mechanisms to provide new insight into the role of ROS in the degradation of atmospheric HULIS.

4AC.44

Coupling Online Conductivity with Offline Ion Chromatography Measurements using the Particle-into-Liquid Sampler. EWAN CROSBIE, Michael Shook, Luke Ziemba, Taylor Shingler, Bruce Anderson, Claire Robinson, Edward Winstead, Armin Sorooshian, Connor Stahl, Alexander B. MacDonald, Rachel Braun, *SSAI*

A particle-into-liquid sampler has been combined with a flow through conductivity cell to provide a continuous, non-destructive, online measurement in support of offline ion chromatography analysis. The conductivity measurement provides a rapid assessment of the total ion concentration augmenting the slower batch data from the offline analysis and is developed primarily to assist airborne measurements, where fast time response is essential. A model of the conductivity was developed for measured ions and excellent closure is derived for laboratory-generated aerosols. The PILS-conductivity measurement was extensively tested during the NASA Cloud, Aerosol and Monsoon Processes: Philippines Experiment (CAMP2Ex) across nineteen research flights and the conductivity data was found to augment the temporal capability of the PILS instrument for assessing ionic species, allowing sub-minute variability to be resolved. Through the sampling of a diverse range of ambient aerosol, including biomass burning, fresh and aged urban pollution, the conductivity measurement offered additional useful information to untangle the composition of complex aerosol mixtures, specifically for assessing acidic aerosol conditions.

4AC.45

Comparison of Nitrate Radical Initiated Oxidation of Four Monoterpenes in a Laboratory Chamber Study to Gain Mechanistic Insight. MICHELIA DAM, Danielle C. Draper, Andrey Marsavin, Juliane L. Fry, James Smith, *University of California, Irvine*

A wide range of SOA and organic nitrate yields have been reported for different monoterpene systems, suggesting that the oxidation mechanisms depend the specific structures of the monoterpenes and illuminating a need to further investigate these mechanisms. To address this need and gain mechanistic insight by assessing yield and composition of oxidation products in both gas and particle phase, laboratory chamber studies were conducted of nitrate radical-initiated oxidation of four monoterpenes, delta-carene, beta-pinene, alpha-pinene and alpha-thujene. Time series of gas phase oxidation products were measured using an LTOF high resolution time of flight analyzer (Tofwerk, AG) and a home-built transverse chemical ionization inlet employing two different reagent ions sensitive to different stages of the oxidation mechanism. Nanoparticle composition was measured using a thermal desorption chemical ionization mass spectrometer (TDCIMS), and organic nitrates in gas and particle phases were measured using a thermal desorption cavity ring down spectrometer (TDCRDS). New particle formation was observed for all monoterpenes except alpha-pinene. Comparisons of organic nitrate yield in gas and particle phase were made between the four monoterpene systems. Relative abundance of highly oxidized gas phase compounds generally corresponded to observed particle mass, with delta-carene and beta-pinene producing many dimers and highly oxidized species and alpha-pinene producing no dimers and few detectable highly oxidized species. In contrast, alpha-thujene exhibited a high gas phase dimer yield but low particle yield. The number and ratios of C, H, N and O atoms were used to identify classes of possible reaction products and assess the dominance of specific mechanistic pathways. These ratios varied greatly between monoterpene systems, highlighting differences in competition between unimolecular and bimolecular radical propagation and termination reaction steps, some of which lead to the formation of low volatility reaction products and particle formation.

4AC.46

Simulations of Kinetically-Limited IEPOX-SOA Reactive Uptake with Glass Transition Temperatures Predicted by Volatility and Chemical Composition Implemented in CMAQv5.3.

SARA FARRELL, Quazi Rasool, Havala Pye, Yue Zhang, Ying Li, Yuzhi Chen, Chitsan Wang, Haofei Zhang, Ryan Schmedding, Manabu Shiraiwa, Jason Surratt, William Vizuete, *University of North Carolina at Chapel Hill*

A major assumption in air quality models is that organic and inorganic constituents found in fine aerosols are homogeneously mixed. In recent years studies have shown that these aerosols can in fact form organic coatings with an aqueous inorganic core. This core-shell morphology has implications for cloud condensation nuclei activation, human health, and secondary organic aerosol formation via reactive uptake. Schmedding and Rasool et al., 2020 used the Community Multi-Scale Air Quality Model (CMAQ), version 5.2, to implement a phase separation algorithm dependent on glass transition temperature (Tg) and the average oxygen to carbon ratios (O:C) of the whole aerosol. When conditions were favorable for phase separation, the Tg, calculated based off of Shiraiwa et al 2017, of the organic shell was used to predict the viscosity and thus diffusivity of the isoprene epoxydiol (IEPOX) into the particle. A key assumption in this study was that 10% of aerosol liquid water (ALW) would reside in the organic layer.
This current investigation aims to implement the aforementioned phase separation algorithm and Tg equation into the latest version of CMAQ, version 5.3 (CMAQv5.3), through which organic ALW is parameterized based on hygroscopicity parameters. Furthermore, this research also analyses various Tg equations in CMAQv5.3 from recently published studies that are based on O:C ratios, saturation vapor concentrations, and elemental composition. Taking advantage of these new equations, and new ALW estimates in CMAQv5.3, this study evaluates various Tg parameterization's effect on phase state and multi-phase chemistry reactions leading to IEPOX-derived SOA. Model output for each parameterization will be cross-compared and validated by observational data. The findings of this work support future model development of CMAQ and will inform future experimental work further investigating how oxygenated organic coatings can impact multiphase chemistry.

4AC.47

Photolysis of Aqueous Atmospheric Aerosol Mimics.

Jacqueline Sharp, Daisy Grace, Shiqing Ma, Joseph Woo, MELISSA GALLOWAY, *Lafayette College*

Aqueous reactions of small, water soluble aldehydes with amines or ammonium salts are important contributors to 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 supercritical fluid chromatography–tandem mass spectrometry. Photobleaching and photobrowning rates vary with wavelength and aldehyde identity, while mass spectrometry shows that the chemical composition changes significantly upon photolysis.

4AC.48

Ozonolysis of Unsaturated Products from Toluene Photo-oxidation Can Form Highly Oxygenated Organic Molecules (HOM). OLGA GARMASH, Matthieu Riva, Matti P. Rissanen, Pekka Rantala, Otso Peräkylä, Liine Heikkinen, Yanjun Zhang, Mikael Ehn, *University of Helsinki*

Recent studies have shown that highly oxygenated organic molecules (HOM) contribute to atmospheric particle formation and growth. HOM are formed in the gas phase through a chemical process called autoxidation and involve peroxy radicals generated from the oxidation of volatile organic compounds (VOCs). The highest HOM molar yields have been observed in the ozonolysis of monoterpenes that contain endocyclic double bond, such as α-pinene and limonene. In our initial study, we demonstrated that OH-initiated oxidation of aromatic VOCs yields HOM. More specifically, multiple OH oxidation steps of benzene were responsible for the significant increase in the observed HOM molar yields.

In this study, we explored the oxidation of toluene in presence of OH radicals and ozone (O_3) in a 2m^3 PTFE chamber for its potential to form HOM through “secondary” ozonolysis. We hypothesize that the initial OH attack forms non-aromatic, unsaturated ring products that can further react with O_3 and lead to larger HOM formation. While typically reaction with O_3 is orders of magnitude slower than with OH radicals, atmospheric concentration of O_3 is significantly larger. Using state-of-the art instrumentation, we observed an increase of HOM yield (in respect to consumed toluene by OH) when O_3 rised from 40 to 80ppb while OH radical concentration was maintained constant. Only C_7-monomer and C_{14}-dimeric-HOM were considered. Using simple calculations, we simulated the first and second generation of HOM produced in the chamber and we were able to reveal that observed HOM yield cannot be fully explained by typical first-generation oxidation products. In sum, our results contribute to understanding HOM and secondary organic aerosol formation from the oxidation of aromatic species. Finally, this study highlights the role of O_3 in the gas-phase oxidation of aromatics, which has been widely dismissed in the literature.

4AC.49

Impacts of Functional Group Identity on SOA Yields and Kinetics. ANDREW HALLWARD-DRIEMEIER, Jonathan Hall, Amelia Schaeffer, Spence Katie, LeClerc Paul, Nicholas Whitcomb, Petra Baldwin, Nandini Seetharaman, Chris Avila, Anthony Carrasquillo, *Williams College*

Much of the uncertainty in climate and air quality modeling derives from the challenges of modeling organic aerosol, particularly the Secondary Organic Aerosol (SOA) fraction which poses unique difficulties. SOA formation involves numerous possible oxidative pathways and multigenerational chemistry, further impeding modeling efforts. Initiation by the OH radical generally proceeds by H-abstraction, yielding an alkyl radical which couples with oxygen, generating an alkylperoxy radical, and finally reaction with NO to form an alkoxy radical. The alkoxy radical can then undergo a 1,5 H-abstraction and increase in oxidation state to form lower-volatility products that produce more SOA or fragment into smaller more volatile products that remain gaseous. Previous work has established that the structure of the alkoxy radical is key to determining branching ratios and therefore SOA yields and this work extends that analysis to the role of neighboring functional groups. Here, we take a structural approach to determine how varying the identity of a single functional group moiety influences the oxidative reaction pathways, especially with regards to the key fragmentation or abstraction step, and resulting properties of the products of different C-10 molecules: alkane, alkene, alkyne, alcohol, aldehyde, ketone, and halides. SOA was generated from each precursor VOC in a Teflon smog chamber via reaction with OH under low and high NOx conditions and the concentration of particles produced was measured. These results are discussed in the context of aerosol yields. Experimental data is supplemented with results of kinetics modeling of first-generation aerosol products and volatility measurements for each major product. By comparing the results from different precursor species we will provide new and valuable insight into the importance of functional group identity on SOA formation.

4AC.50

Growth of Fresh SOA Seed Particles by α-Pinene Ozonolysis. DEVON HAUGH, Michael S. Taylor, Michael J. Apsokardu, Murray Johnston, *University of Delaware*

Ambient nanoparticle formation and growth is an important source of cloud condensation nuclei. For this reason, understanding growth mechanisms is particularly important for predicting climate. For biogenic secondary organic aerosol (SOA), condensation of highly oxidized organic molecules (HOMs) contributes substantially to nanoparticle growth. However, particle phase reactions can also play a role. Recent work in our group has shown for SOA produced by a-pinene ozonolysis that size-selected aqueous droplets in the 40-100 nm size range grow about 20% faster than inert, solid particles. The work presented here extends these studies to the growth of size-selected seed particles consisting of fresh SOA. Depending on relative humidity, these particles can be glassy- or liquid-like, and in either case they are likely to be peroxide-rich, and therefore, highly reactive. The particle growth experiments to be presented use a dual flow tube reactor assembly, where the first flow tube generates fresh SOA seed particles from a-pinene ozonolysis that subsequently react in the second flow tube. Results from two types of particle growth experiments will be described: 1) growth proceeds by exposing seed particles to additional amounts of a-pinene and ozone, and 2) growth proceeds by exposing seed particles to vapors of specific compounds that are known to be produced by a-pinene ozonolysis. Growth mechanisms will be discussed in the context of measured diameter growth rates of the seed particles and chemical composition of the grown particles.

4AC.51

NH3 and PM2.5 Characteristics at an Agricultural Site. JOONWOO KIM, Haebum Lee, Taewoong Gong, Kihong Park, *Gwangju Institute of Science and Technology*

The majority of ammonia (NH_3) is emitted from agricultural sites by fertilizer application and livestock waste. NH_3 is one of the major precursors of particulate matter less than 2.5 μm ($PM_{2.5}$) since NH3 reacts with acidic compounds in the atmosphere, producing ammonium (NH_4^+) salts. While NH_3 affects the local environment with the lifetime of several hours, NH_4^+ have impacts on longer ranges with the lifetime of several days. NH_3 is oxidized to NO_x by soil bacteria activities in agricultural sites, which are important to O_3 and secondary aerosol formation. Field studies in agricultural sites were barely conducted but are necessary to understand the relationship between NH_3 and $PM_{2.5}$ considering that agricultural sites have the NH_3-rich atmosphere. In this study, the concentrations of NH_3, NO_2, and $PM_{2.5}$ were measured downwind of swine feedlots at an agricultural site in Korea in June and July, 2020. The monitoring site was 0.7 km east of the center of swine concentrated animal feeding operations (CAFOs) containing ~50,000 head. The concentrations of NH_3 and NO_2 were recorded by an open-path ultraviolet differential optical absorption spectroscopy (DOAS). The concentrations of $PM_{2.5}$ were measured using an optical particle counter. Wind speed, wind direction, temperature and relative humidity were also recorded using an automatic weather station (AWS). $PM_{2.5}$ concentrations from national air quality monitoring network stations operated by Korea Environment Corporation within ~20 km from the sampling site were collected to examine regional distributions. The results of the field measurements on NH_3, NO_2, and $PM_{2.5}$ concentrations will be displayed and the characteristics following meteorological conditions will be discussed. Further analysis on other measured parameters is ongoing and will be presented briefly.

4AC.52

Physicochemical Properties of Free Tropospheric Particles Collected at Pico Mountain Observatory and Their Role in Ice Cloud Formation. NURUN NAHAR LATA, Bo Zhang, Simeon Schum, Lynn Mazzoleni, Claudio Mazzoleni, Swarup China, *Pacific Northwest National Laboratory*

Free tropospheric particles after long range transport can contribute to ice nucleation affecting cloud properties and formation. Therefore, detailed physicochemical characterization of ice nucleating particles is fundamental to elucidate their effects on heterogeneous ice nucleation in clouds. In this study, we characterized free tropospheric particles collected from three different events in July, 2014 at the remote Pico Mountain Observatory. Pico Mountain Observatory is located at 2225 m above sea level in the summit caldera of Pico Volcano on Pico Island in the Azores archipelago in the North Atlantic. We performed FLEXPART retroplume modeling to investigate their transport pattern. Utilizing multimodal microscopy and spectroscopic techniques, we analyzed several physicochemical properties of the collected particle and investigate their ice nucleation propensity using a state of the art ice nucleation instrument coupled with an Environmental Scanning Electron Microscope operated at temperature and relative humidity values relevant to mixed phase and cirrus clouds. We conducted single particle as well as bulk analysis of the particles collected from three different sampling periods. The outcomes from both investigations indicates that the chemical compositions of the particles with different aging times are significantly different. Chemical imaging and microanalysis of individual particle using energy dispersive spectroscopy evidance the aging of the organic particles. The identified ice nucleating particles are comprised of mixtures of dust, organic and sulfate coating materials, and other carbonaceous particles. We observed an enhancement of ice nucleation activity for the sample dominated by mineral dust. Altogether, the results from this study provides a better understanding of the role of long range transported free tropospheric particles on ice cloud formation.

4AC.53

Effect of Particle Properties to the Atmospheric Visibility. WEN-BIN LEE, Yeou-Lih Yan, Hsin-Chih Lai, Shao-Hao Lu, Ming-Tung Chuang, Tang-Huang Lin, Chea-Yuan Yang, Ying-I Tsai, Chih-Chieh Chen, Wen-Yinn Lin, *National Taipei University of Technology*

Visibility degradation is a significant index impact of particle concentrations in atmospheric air. Scattering and absorption of visible light through suspended particles can be attributed to visibility degradation. However, different particle components may exhibit contrasting effect of extinction efficiency. This study aimed to determine the correlation between visibility and physical–chemical composition of particulate matter (PM)2.5. Four season samplings from November 2017 to July 2018 were obtained in Cianjin (urban) and Ciaotou (suburban) areas, Southern Taiwan. Aerosol optical properties were measured in terms of particle concentration, size distribution, and chemical compositions (e.g., NH4NO3, (NH4)2SO4, element carbon, and TOC) using an integrating nephelometer and an AE33 aethalometer. The variation in relative humidity may not directly influence the extinction coefficient of particles. Visibility reduction is mainly influenced by the increase in particle concentration. The particle extinction coefficient is correlated with the proportion of components. The concentration of particle compositions, such as (NH4)2SO4 and NH4NO3, in Cianjin is higher than that in Ciaotou. The size distribution in the visible region ranges from 0.4 µm to 0.7 µm. Therefore, the visibility in Cianjin is lower than that in Ciaotou. Visibility-related monitoring planning and strategy setting can be used to improve visual air quality by determining the correlation between PM2.5 properties and visibility.

4AC.54

Formation of Secondary Organic Aerosol from Nitrate Radical Oxidation of Phenolic Vocs: Implications for Nitration Mechanisms and Brown Carbon Formation.

RAPHAEL MAYORGA, Zixu Zhao, Haofei Zhang, *University of California, Riverside*

Volatile phenolic derivatives are substantially emitted from biomass burning and produced from photochemistry of atmospheric aromatic volatile organic compounds (VOCs). Oxidation of phenolic VOCs at night by nitrate radicals (NO_3) may represent a significant source of secondary organic aerosols (SOA) and brown carbon (BrC) formation in the atmosphere. In this study, NO_3 oxidation of five phenolic derivatives, including phenol, catechol, 3-methylcatechol, 4-methylcatechol and guaiacol are investigated in laboratory experiments. The SOA constituents from the NO_3 oxidation were analyzed using electrospray ionization ion mobility spectrometry time-of-flight mass spectrometry, which allows for characterization and identification of isomers in the oxidation products. Through these analyses, several classes of nitro-containing products in addition to the well-known nitrophenol compounds were observed, including: (1) the nitrophenol type of products with additional hydroxyl functional groups; (2) non-aromatic nitro-products with lower double bond equivalence; (3) phenol and catechol products from the C_7 phenolic VOCs with carbon-containing substitutions; and (4) nitrated diphenyl ether dimers. The present work indicates that new products from previously unrecognized pathways are formed during NO_3 oxidation of phenolic VOCs and may contribute an important portion of the SOA. Some of these products were also observed in ambient aerosols during biomass burning. We suggest that the ubiquity of the nitrophenol type of products in the SOA derived from phenolic VOC + NO_3 are responsible for the strong light absorption measured in this study. Therefore, elucidation of these pathways will be critical for understanding the nighttime oxidation and BrC formation mechanisms.

4AC.57

Nucleation and Growth of Particulate Matter from the Photooxidation of Aromatic Hydrocarbons.

ISSAK PROAñO LóPEZ, Murray Johnston, *University of Delaware*

The oxidation of volatile organic compounds (VOCs) in the atmosphere to produce low-volatility products that form secondary organic aerosol (SOA) through the nucleation and growth of nanoparticles is of great atmospheric importance. The majority of VOCs present in the atmosphere are of biogenic origin, however, in the industrial period the proportion of VOCs emitted from anthropogenic activities has increased, especially in areas where urbanization and industrialization are prevalent.

Anthropogenic VOCs that produce low-volatility products are typically from the aromatic hydrocarbon class, whose dominant oxidation mechanism in the atmosphere involves the hydroxyl radical (·OH). We are using multiple flow-through photooxidation chambers to generate ·OH for the study of particle nucleation and growth from anthropogenic VOCs. In initial work, the molecular composition of anthropogenic SOA is being characterized online by droplet-assisted ionization (DAI) interfaced with a Waters Synapt G2-S quadrupole ion mobility time-of-flight mass spectrometer and offline by particle collection and analysis by electrospray ionization (ESI) interfaced with an Orbitrap mass spectrometer. Particle-phase composition is reconciled with measurements of gas-phase oxidation products that have been previously reported using chemical ionization mass spectrometry. The results give insight into the mechanism of particle growth in an urbanized environment.

4AC.58

Sea Spray Aerosol Assessment of Atmospheric Corrosion in a Marine Environment. RAYMOND SANTUCCI, Christine Sanders, *US Naval Research Laboratory*

Marine atmospheric corrosion is facilitated by the deposition of salt-laden sea spray aerosols onto engineering materials. Aerosol deposition flux (mass / time-area) is clearly dependent upon atmospheric aerosol concentration (mass / volume) and deposition velocity (length / time), in accord with sample geometry and relevant fluid dynamics near the sample. A rigorous assessment of marine atmospheric corrosion at a controlled test site in Key West, Florida was conducted over the course of a year with the intent of elucidating the role of sea spray aerosols. Certain factors which have been previously implicated in the literature as controlling, or at least heavily influencing, the corrosion of engineering materials in atmospheric exposure were isolated and explored. In particular, the effect of sample geometry and orientation with respect to gravitational settling of sea spray aerosols, precipitation, and sea winds was explored. The effect of surface area on measured steel mass loss was explored to identify the veracity of the so-called “edge effect”. Efforts were made to correlate meteorological atmospheric conditions (Temperature, Relative Humidity, Wind Speed, Wind Direction, chloride deposition flux, etc.) to monthly assessments of corrosion damage. Interestingly, the summative, compounded monthly corrosion damage tends to significantly overshoot the observed cumulative corrosion damage for samples exposed over the same time period. The results of this study form the basis for new research regarding the role of sea spray aerosols in the marine atmospheric corrosion process. This “fresh look” into marine atmospheric corrosion and the way in which it is informed by the results of this research will be discussed. Future directions in the continued convergence between the fields of corrosion science and engineering and aerosol science and technology will be highlighted.

4AC.59

Multiphase Degradation of Levoglucosan Using 0-D Numerical Simulations: Degradation Time Scales and Effects on SOA and Other Gases. LOREDANA SUCIU, Robert Griffin, Caroline Masiello, *Rice University*

Biomass burning is an important source of gases and particles in the atmosphere that impact air quality and climate. Organic molecular tracers, such as levoglucosan (LEV) and its isomers are emitted as both gases and fresh particles. Their properties make them reactive and volatile, thus both chemistry and gas/particle (G/P) partitioning may simultaneously influence their gas-phase and aerosol-phase concentrations in the atmosphere, and implicitly, their atmospheric lifetimes which are still not fully understood. Using a zero-dimensional modeling framework, we developed multiphase chemistry and G/P partitioning mechanisms to study degradation time scales of LEV and the effects of its degradation on secondary organic aerosols (SOA) and other gases. We ran multiple chamber simulations initialized with conditions used in chamber experiments and varying the first-order heterogeneous reaction rate coefficient and the mass accommodation coefficient (α). We found that the model best predicted degradation of aerosol-phase LEV when the heterogeneous reaction rate was slowed down by 2-3 orders of magnitude, at a constant α value (0.001). For these conditions, the resulting degradation time scale varied by phase, respectively 1.5-3.5 days (gas-phase) and 8-21 hours (aerosol-phase). The resulting SOA yields ranged from 5-32%, implying that LEV chemistry can impact air quality. In addition, LEV chemistry influenced other gases such as increasing the mixing ratios of radicals and decreasing those of reactive nitrogen species. The enhanced decay of nitrogen oxides in the presence of multiphase LEV chemistry drove ozone to increase more rapidly compared to changes in volatile organic compounds. Varying the heterogeneous reaction rate suggests that longer degradation time scales of LEV are possible, but to evaluate this finding, more extensive data from chambers or fire plumes are needed in the future.

4AC.60

Chemical Characterization of Isoprene- and Monoterpene-Derived Secondary Organic Aerosol (SOA) Tracers in Marine Aerosols from the Galápagos Islands. TESSA SZALKOWSKI, Tianqu Cui, Karsten Baumann, Ryan Schmedding, Zhenfa Zhang, Jason Surratt, Jackson Seymore, William Vizuete, *University of North Carolina at Chapel Hill*

Atmospheric fine particulate matter ($PM_{2.5}$) plays a critical role in the global climate system, in which the oceans are an important primary and secondary source. The atmospheric processes that produce secondary remote marine $PM_{2.5}$, however, remain unclear. This is partly due to a lack of characterization of particulate organic constituents and understanding of their links with biogenic volatile organic compounds (BVOCs) produced by phytoplankton that participate in secondary organic aerosol (SOA) formation. An approach to access the marine contribution to $PM_{2.5}$ is to conduct concurrent atmospheric and marine measurements. The Galápagos Islands are an ideal location to make these measurements, as it is a pristine environment with few anthropogenic sources. Furthermore, the waters surrounding the islands harbor a diverse range of phytoplankton communities within small spatial scales.

This work presents the feasibility of using this site for real-time $PM_{2.5}$ mass and off-line $PM_{2.5}$ chemical characterization of marine aerosols. $PM_{2.5}$ samples were collected onto high-volume quartz filters and chemically characterized at the molecular level using a recently developed hydrophilic interaction liquid chromatography (HILIC) method interfaced to electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (ESI-HR-QTOFMS). $PM_{2.5}$ organic constituents showed a correlation with chloride, indicating some contribution from marine sources. Strong correlations with methanesulfonic acid and oxalic acid indicated that marine bioactivity, such as algal production, may have contributed to the observed $PM_{2.5}$ levels. We show, for the first time, evidence of isoprene-derived SOA contributing to $PM_{2.5}$ collected on the Galápagos Islands. Our findings also suggest the presence of other sources of organic aerosol, such as primary OA from bubble-bursting processes and oxidative aging (heterogeneous oxidation) products from particulate 2-methyltetrol sulfate diastereomers. The composition and correlations from our measurements can provide an estimation of marine sources and their contribution to $PM_{2.5}$, thus serving as model inputs for chemical and climate studies.

4AC.61

Modeling and Interpreting the Growth of Deliquesced Ammonium Sulfate Seed Particles by α-Pinene Ozonolysis. MICHAEL S. TAYLOR, Michael J. Apsokardu, Devon Haugh, Murray Johnston, *University of Delaware*

Particles in the Aitken mode size range (10-100 nm in diameter) often contribute the largest number fraction of particles to the air in ambient environments. Understanding the mechanisms responsible for the growth of these particles allows for cloud condensation nuclei (CCN) concentrations to be better predicted. Gas phase oxidation reactions of biogenic volatile organic compounds (BVOCs) such as α-pinene have been shown to produce low volatility organic compounds that contribute significantly to particle growth in this size range. By studying particle growth as a function of seed particle size and gas-phase mixing ratios for monoterpene ozonolysis reactions, a kinetic model can be used to explain the experimental growth. In recent work by our group, seed particle phase has been shown to affect the growth rate. For experiments performed at 60% RH, deliquesced ammonium sulfate seed particles grow about 20% faster than effloresced ammonium sulfate seed particles. For growth by α-pinene ozonolysis, the effloresced particles grow according to a condensational growth model with a highly oxidized molecule (HOM) yield of about 13% (Krasnomowitz et al., AS&T 2019). Deliquesced seed particle growth is modeled using a variety of particle phase processes that have been suggested in the literature. Our initial modeling has focused on the possibility of accretion reaction in the particle phase. By varying the volatilities and molar yields of the reactants, along with the reaction rate constant, we find that several permutations of these variables are able to explain the experimentally measured growth, but all rely on a very fast rate constant, even for highly reactive hydroperoxide functionalities. The insight gained from particle growth measurement and modeling be discussed.

4AC.62

Surfactant Effects on Hanging Droplet Aqueous-Phase Aerosol Mimic Direct Photochemistry. Thomas Beier, JOSEPH WOO, *Lafayette College*

Carbonyl-containing volatile organic compounds (CVOCs) have been demonstrated to exhibit a significant fraction of water-soluble organic carbon in aqueous aerosols and droplets, and are known to exhibit compositional changes under both dark and irradiated conditions. While condensed-phase photochemistry is often assumed to uniformly occur within a given phase, recent work has suggested that surfactant species in droplets may strongly react at the gas-liquid interface in hanging droplets. The prevailing bulk droplet chemistry may or may not be affected by the presence of a reactive surface. This study explores the direct photochemistry of aged glyoxal/ammonium-sulfate aerosol mimics, a non-surfactant CVOC aqueous reaction system, in the presence of additional non-reactive (sodium dodecyl sulfate) and reactive (nonanoic acid) surfactant compounds. UV/visible absorbance and dynamic surface tension measurements for small (10µL), RH-controlled mimic droplets are presented.

4AC.63

Atmospheric Nanoparticles: Optical Photothermal Infrared Spectroscopy of Determining Particle Sizes. Nicole Olson, YAO XIAO, Ziying Lei, Andrew Ault, *University of Michigan*

Atmospheric aerosol particles have a huge impact on climate by triggering multiple chemical reactions which are pH dependent, scattering solar radiation and nucleating clouds and ice crystals. Although the importance of aerosol particles has been addressed, determining particle sizes at the most abundant size level (<1µm) is still an analytical change due to their ultrafine size. Moreover, the traditionally used microspectroscopy techniques like scanning electron microscopy will perform under the vacuum which will distort the physicochemcial property of ambient samples. Therefore, in this study, we introduced the first application of Optical Photothermal Infrared Spectroscopy (O-PTIR) to determine properties of both lab-generated and ambient aerosol particles. A visible and a tunable IR lasers are aligned together to introduce the change of scatter Raman signal caused by the thermal expansion of the particles when the IR frequency matches the vibrational absorption of samples. Due to the change of signals, both Raman and IR spectra can be extracted from the samples under submicron resolution spontaneously. Microscopy substrates were tested and used to minimize the background interference and maximize the sample signals. Organic and inorganic functional groups were characterized for lab-generated and ambient aerosol particles. Mapping was also introduced to study the distribution of different groups in the multi-component particles. The results presented the strong capability of O-PTIR to study the atmospheric aerosols at submicron levels which is far beyond the traditional vibration spectroscopy like Fourier-transformed IR. Therefore, this study provides an important method to further understand the impact of aerosols on the climate and human health at a critical size range.

4AC.64

Composition of Isoprene and Nitrate Radical Reaction Products Using FIGAERO-CIMS. TIANCHANG XU, Masayuki Takeuchi, Yuchen Wang, Nga Lee Ng, *Georgia Institute of Technology*

Isoprene is one of the most abundant volatile organic compounds (VOC) in the atmosphere emitted from biogenic sources such as vegetations. Secondary organic aerosols (SOA) formed from isoprene reactions play essential roles in affecting global SOA production and budget. Among isoprene's possible reactions in the atmosphere, its reaction with nitrate radicals (NO3) is an important pathway owing to its high yields of SOA and contribution to gas and particulate organic nitrates. One useful tool to study oxidation product composition is Filter Inlet for Gases and AEROsols coupled to a High Resolution Time-of-Flight Iodide Chemical Ionization Mass Spectrometer (FIGAERO-CIMS) because FIGAERO-CIMS can offer us composition information in both gas and particle phases at the molecular level. In this work, we conduct laboratory chamber experiments with isoprene and NO3 radicals under dark condition. The gas-phase and particle-phase oxidation products are continuously measured by FIGAERO-CIMS over the course of the experiments. SOA yields and gas and particulate organic nitrates are examined and discussed.

4EJ.2

Advancing Air Quality Monitoring in Environmental Justice Communities of the South Coast Air Basin, CA: II. Design and Development of a Novel Multi-Metal Mobile Platform. MOHAMMAD SOWLAT, Sina Hasheminassab, Pami Mukherjee, Payam Pakbin, Steven Boddeker, Avi Lavi, Jamie Berg, Andrea Polidori, *South Coast Air Quality Management District, Diamond Bar, CA*

Ambient particulate metals are an important category of Hazardous Air Pollutants (HAPs) with known detrimental impacts on human health. Given the large spatio-temporal variability in ambient particulate metal concentrations, information from sparsely distributed fixed air monitoring networks may not adequately reflect their levels and trends, especially in disproportionately impacted (i.e., Environmental Justice (EJ)) communities. Mobile monitoring techniques are a potential solution, as they enable us to capture data in a short enough time period that can represent the spatial variations of the target pollutant. In this study, we developed a novel platform for mobile monitoring of multiple ambient particulate metals using an optimized X-Ray Fluorescence- (XRF) based instrument. The instrumentation aboard the platform also enables the measurement of aerosol characteristics, including particulate matter (PM) mass (PMx), particle number (PN), particle number size distribution, and black carbon (BC); trace gases, including NO_2 and CO_2; and meteorological parameters, including wind speed/direction; all in fine time resolutions (seconds to minutes). It is noteworthy that the mobile platform has been developed as a modular system able to switch and host other monitors as well. Since most pollutants of interest for this platform are in particulate phase, an inlet system was designed that is appropriate for both mobile and stationary measurements with minimum losses for relevant particle sizes (<10 µm). The efficiency of the designed inlet system was fully characterized using laboratory-generated polystyrene latex (PSL) particles. Here, we will provide an overview of the design criteria, features, and characterization of the platform, and discuss examples and challenges in the application of the platform for both mobile and stationary monitoring. In a companion presentation, we will present preliminary results of the full-blown application of the developed platform, and demonstrate a complex approach for concentration mapping, source identification, and source characterization.

4EJ.3

Composition and Source Characterization of Aerosols in an Environmental Justice (EJ) Community in California (Wilmington).

HOSSEIN PAZOOKI, Pami Mukherjee, Mohammad Sowlat, Payam Pakbin, Roya Bahreini, *University of California, Riverside*

Following the enactment of the Assembly Bill (AB) 617, California Air Resources Board (CARB) established the Community Air Protection Program (CAPP), aiming to reduce exposure in communities disproportionately impacted by air pollution. As parts of efforts to better characterize emission sources in Southern California Air Basin (SCAB), and through a collaborative study with the South Coast Air Quality Management District, a series of aerosol measurements were conducted in Wilmington, an EJ community in the SCAB selected under the AB 617 program, for three weeks during Fall 2019. The site was selected to examine the influence of nearby oil refineries, major highways, and the ports of Los Angeles and Long Beach on local air quality. Temporal concentration changes of various aerosol species were measured using a Compact Time-of-Flight Aerosol Mass Spectrometer (m-AMS, Aerodyne Research Inc.). The results showed that during the measurement period, the non-refractory composition of submicron aerosols was dominated by organics (average of 12.64 $\mu g/m^3$), followed by nitrate (5.16 $\mu g/m^3$) and sulfate (2.8 $\mu g/m^3$). Considering the ratios of m/z 43 and m/z 44 fragments to the total organics, the site was influenced predominantly by fresh hydrocarbon-like and slightly oxygenated organic species. Results from Positive Matrix Factorization (PMF) will be presented to further examine the composition of organics during different meteorological conditions and under the influence of different source regions. Specifically, organic and inorganic (e.g., sulfate) composition during times with a direct influence from the nearby oil refinery will be compared with those of other wind sectors to determine the direct influence of the refinery's emissions on local aerosols.

4SD.1

The Relationship between MAIAC Smoke Plume Heights and Surface Particulate Matter.

MICHAEL CHEESEMAN, Bonne Ford, John Volckens, Alexei Lyapustin, Jeffrey R. Pierce, *Colorado State University*

Biomass burning is a source of fine particulate matter ($PM_{2.5}$) air pollution, which adversely impacts human health. However, quantifying the health effects from biomass burning $PM_{2.5}$ is difficult. Monitoring networks generally lack the spatial density needed to capture the heterogeneity of smoke from biomass burning events. Satellite aerosol optical depth (AOD) can be used to fill the spatial gaps in monitoring networks; however, AOD is a column-integrated value that does not distinguish surface-level aerosols. Plume injection heights (PIH), however, may provide constraints on the vertical distribution of smoke. We hypothesized that the ratio of surface $PM_{2.5}$ and AOD would be correlated with the ratio of PIH and the planetary boundary layer height (PBLH), because when the smoke is aloft (i.e. PIH:PBLH >1) the surface may experience smaller $PM_{2.5}$ enhancements than if the smoke remained in the boundary layer (PIH:PBLH<1). We investigated the relationship between PIH, AOD, and surface $PM_{2.5}$, using PIH and AOD from the Multi-Angle Implementation of Atmospheric Correction (MAIAC) dataset and PBLH from the National Centers for Environmental Prediction (NCEP). We assessed regional characteristics of PIH and evaluated its correlation with co-located $PM_{2.5}$ and AOD measurements downstream of biomass burning events. PIH is generally highest over the western US. The ratio $PM_{2.5}$:AOD generally decreases with increasing PIH:PBLH, which indicates a lower surface $PM_{2.5}$ enhancement, on average, when plumes are injected into the free troposphere. Thus, we show that PIH has the potential to refine surface $PM_{2.5}$ estimates during smoke events; however, the relationship is only strong when averaging over large regions or longer time periods.

4SD.2

Infection vs Fatality of COVID-19 in New York State: Effects of Demographics and Poor Air Quality.

VIJAY KUMAR, Bridget Wangler, Chaya Chaipitakporn, Shantanu Sur, Supraja Gurajala, Suresh Dhaniyala, Sumona Mondal, *Clarkson University, Potsdam*

The coronavirus disease 2019 (COVID-19) caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has affected the world at an unprecedented scale, however, its impact on different countries and even on different regions within a country varies widely. A multitude of COVID-19 related risk factors have been identified including demographic factors and chronic exposure to air pollution but the specific contribution of these risk factors to infection and fatality is yet to be understood. In this work, we compared the incidence of COVID-19 in New York State (NYS) counties, and analyzed how various risk factor variables associate with the variation observed across different counties. Using publicly available data, we found that the rate of COVID-19 infection correlates well with the death rate, both being high in counties located near the New York City, the epicenter for the infection, and drops prominently in counties located farther away from the epicenter. However, in terms of death among the infected population, several other counties take up the topmost positions even having a low infection rate. To investigate this apparent discrepancy, we divided the counties into three clusters based on the infection rate, death rate, and death per infection, and compared the contribution of various potential risk factors such as ethnicity, age, population density, poverty, and air quality PM2.5 in each of these clusters. Furthermore, a regression model built on this data reveals ethnicity (African-American and Hispanic) and poverty are the major risk factors behind high infection rate, while disease fatality has a strong association with age and PM2.5. Our results show distinct contributions by various risk factors to the COVID-19 burden, and this information could be useful in designing control and mitigation strategies.

4VC.1

A New Framework for Modeling Emissions from Volatile Chemical Products.

KARL SELTZER, Elyse Pennington, Venkatesh Rao, Benjamin Murphy, Madeleine Strum, Kristin Isaacs, Havala Pye, *United States Environmental Protection Agency*

Volatile chemical products (VCPs) are an increasingly important source of anthropogenic organic emissions. Among these sources are everyday items, such as personal care products, household and institutional cleaners, architectural coatings, pesticides, adhesives, and fragrances. These emissions have long been accounted for in the US EPA's National Emission Inventory as the solvent sector, but new inventory methods suggest these estimates could be biased low by factors of 2-3. As the influence of VCPs on secondary air pollution grows in relevance, the need to resolve these differences becomes paramount. Here, we develop VCPy, a new framework to model emission factors from VCPs throughout the United States, with additional applications to spatially allocate these emissions to regional and local scales. In this framework, fate and transport assumptions are a function of the use timescale for assigned product categories and the evaporation timescales of individual compounds within these categories are a function of physiochemical properties. Since ingredients in these product categories are considered individually, determination of speciated emission profiles is explicit. This approach also enables quantification of emission volatility distributions and the abundance of different compound classes. We test the sensitivity of the magnitude of emissions to uncertain parameters, such as use and evaporation timescales, through Monte Carlo analysis, evaluate the inventory using ambient observations, and map emissions to common chemical mechanisms for ease of research use in the chemical transport modeling community.

4VC.2

Model Estimation of Indoor-to-Outdoor Migration of Volatile Chemical Products. AMIRASHKAN ASKARI, Arthur W. H. Chan, *University of Toronto*

Recent studies have revealed the importance of Volatile Chemical Products (VCPs) in determining air pollutant levels, specifically as precursors of secondary pollutants such as secondary organic aerosol or tropospheric ozone. However, since a considerable fraction of VCPs is consumed indoors, there is a knowledge gap regarding the effective fraction of indoor VCP emissions that, after possible attenuation through indoor reaction and partitioning phenomena, are transferred to outdoor air through building air exchange processes. In this work, we aim to parametrize the effective VCP emissions from different buildings and better estimate these emissions. Using a bottom-up approach, an estimation of the total weight of different classes of VCPs consumed annually in Canada is made. Subsequently, using the California Air Resources Board (CARB) emission inventories, the chemical profile of these emissions is investigated. Finally, by running a fugacity-based chemical fate model, an estimation of the effective steady-state VCP emissions in a typical year is presented. Lastly, the effects of building-specific parameters on the fraction of VCP migration to outdoor air are explored.

4VC.3

Characterization of Oxygenated Organic Compounds in SOA from the Photooxidation of n-Heptadecane in the Presence of NOx. MOHAMMED JAOUI, Michael Hays, Emily Li, Kenneth S. Docherty, Michael Lewandowski, Tadeusz Kleindienst, *U.S. Environmental Protection Agency*

While enhanced urban organic aerosol formation has been associated with alkane-rich conditions, the underlying chemistry and mechanisms remain poorly understood. Recent studies have reported that volatile chemical products (VCPs) are an important source of alkanes, in addition to traditional sources such as gasoline and diesel vehicles. This study focuses on the characterization at the molecular level of secondary organic aerosol (SOA) originated from n-heptadecane photooxidation in the presence of nitrogen oxide (NOx) and methyl nitrite (CH3ONO). The experiment was carried out in a 14.5 m3 smog chamber operated in flow mode. A Scanning Mobility Particle Sizer system (3936, TSI) and a Condensation Particle Counter (3025A, TSI) were used to study the SOA formation, and a filter/carbon strip denuder sampling system was used for collecting particle-phase products. The chemical characterization of the SOA was analyzed using (1) derivatized (BSTFA, BSTFA + PFBHA) and underivatized based methods followed by gas chromatography–mass spectrometry; (2) liquid chromatography-high resolution mass spectrometry; (3) Fourier-transform infrared spectroscopy; and (4) high resolution aerosol mass spectrometer. The analyses showed the occurrence of more than 100 oxygenated organic compounds in the particle phase tentatively identified. The SOA components belong to three major classes including: (1) cyclic hemiacetals/ethers and tetrahydrofuran/dihydrofurans; (2) hydroxyl/carboxyl/carbonyl compounds; and (3) organo-nitrates. While the focus of this study has been examination of the particle-phase, small carbonyls (aldehydes and ketones) in the gas-phase have also been examined as their 2,4-dinitrophenylhydrazones (DNPH) derivatives using a HPLC method. Detailed reaction schemes are presented to account for selected reaction products. The OM/OC ratio at an average aerosol load of 198.5 µg m–3 was 1.3.

4VC.4

Modification and Optimization on Environmental Chamber Experiments of Secondary Organic Aerosol Formation from LVP-VOCs and Volatile Consumer Products to Improve Model Prediction.

QI LI, Sophia Charan, Reina Buenconsejo, John Seinfeld, David R. Cocker III, *University of California, Riverside*

Recent studies show that non-vehicular sources such as volatile consumer products (VCPs) become to contribute a larger fraction of the total volatile organic compounds (VOCs) emissions in the urban areas than before. To better characterize the sources and evaluate their impacts on the ambient secondary organic aerosol (SOA) formation, in this study, a series of chamber experiments have been performed on a wide range of VCPs under urban relevant conditions. 12 VCPs-related VOCs (including some LVP-VOCs) are selected due to their high suspected potential on SOA formation and emission abundance. Experimental SOA formation data are presented from environmental experiments done under varying conditions of NOx, H_2O_2, and seed aerosol. Typical VCPs-related VOC benzyl alcohol shows a SOA yield of up to 60% at 291k, in the presence of H_2O_2, NOx, and ammonia sulfate seed (larger than previously reported 41% and 56% with surrogate). Well-controlled environmental chamber experiments are heavily relied for chemical mechanisms development. However, due to the features of the LVP-VOCs (low vapor pressure and high boiling point), environmental chamber studies with the LVP-VOCs can be hard. A detailed environmental chamber comparison between the UCR chamber and Caltech chamber has been performed to modify and optimize the experimental chamber experiments and refine the experimental protocol. The comparison and optimization have been done in various aspects including chamber construction features, instrument performance, experimental methods (including injection and sampling methods), and data analysis methods. Certain experiments performed under similar conditions in both chambers show a deduction of up to 60% in terms of the difference of the SOA yield before and after the optimization.

4VC.5

Temporal Evolution of Secondary Organic Aerosol Production from Volatile Chemical Products.

ALBERT PRESTO, Mackenzie Humes, Rebecca Tanzer Gruener, Rishabh Shah, Allen Robinson, Neil Donahue, *Carnegie Mellon University*

One of the key distinctions between volatile chemical products (VCPs) and traditional combustion sources is that the magnitude and composition of VCP emissions can evolve over time. Chemical transport models can reasonably assume that vehicles and power plants have consistent (or at least predictable) fuel-based emission factors (e.g., g-pollutant per kg-fuel). Activity based emission factors are less certain for evaporative emissions from VCPs such as paints, coatings, and sealants that are applied as a liquid and have solvent(s) that evaporate over time. In this study, we monitored the evolution of organic compound (I/S/VOC) emissions from paint samples and quantified secondary organic aerosol (SOA) formation and composition over time.

We painted a 1 square meter board with several paints (e.g., interior latex paint, spray paint) and characterized I/S/VOC emissions with a PTR-MS and sorbent tubes analyzed via GC-MS. We used an oxidation flow reactor to generate SOA from the paint emissions. In each experiment, the board was painted, and concentrations monitored until they returned to background levels. We hypothesized that the paint would act as a long-term source of IVOC and SVOC compounds, and that SOA formation would persist for days to weeks after painting. Instead, the results are consistent with the painting acting as a one-time emissions event followed by dilution of the emitted vapors. Both vapor concentrations and SOA formation in the OFR return to background levels within ~6-8 hours, consistent with the dilution rate in the room where experiments were conducted. The SOA formation experiments will be supplemented with emissions tests using a flux chamber to verify that the bulk of SOA-forming vapors are emitted quickly.

4VC.6

Connecting Composition to Reactivity for Fragrances and Their Emissions.

JAMES HURLEY, Gabriel Isaacman-VanWertz, *Virginia Tech*

Atmospheric oxidation of volatile consumer products (personal care products, cleaning agents air fresheners, etc.) has recently been shown to account for a substantial fraction of organic aerosol in urban environments. Many of these products include fragrances, which may contain reactive and/or volatile components, but their composition is often proprietary or unpublished. In this study, 11 commercially available fragrances were analyzed for their composition, and their evaporation and impacts on local chemistry were modeled. The components of the fragrance were identified by gas chromatography-mass spectrometry (GC-MS) and carefully quantified using a GC coupled to a flame ionization detection (FID). Each fragrance was found to be dominated by between 2 and 9 resolved and identified components, which on average accounted for approximately half of their mass (range: 25-93%). The evaporation of each fragrance was modeled to estimate the timescales and magnitudes of the evaporated mass, and the emission of hydroxyl and ozone reactivity. While only a small fraction of total fragrance mass was comprised of terpenes (primarily limonene), these components were found to dominate the emission of reactivity due to their high volatility and reactivity (with both hydroxyl radical and ozone). Given the dominance of terpenes, most reactivity is emitted in the first several hours, but lower levels reactivity may continue to be emitted for days from a fragrance. Due in large part to the varying presence of terpenes, the total amount of reactivity evaporated may differ by an order of magnitude between different fragrance formulations. Consequently, detailed composition analyses such as those presented here are critical for estimating the growing influence that consumer products exert on aerosol formation and air pollution in urban areas.

5AC.1

Acidity at the Nanoscale: pH Measurement of Individual Ultrafine Aerosol Particles. ZIYING LEI, Yao Xiao, Samuel Bliesner, Claire Mattson, Madeline Cooke, Nicole Olson, Julie Albert, Andrew Ault, *University of Michigan*

Aerosol acidity (pH) is a critical property that affects the composition of the atmosphere as many key multiphase chemical reactions are pH-dependent. Despite the importance of atmospheric aerosol has been addressed, determining aerosol pH remain a challenge especially for ultrafine particles that have great impact on climate and health. Additionally, due to differences in particle-to particle composition, further understanding of atmosphere aerosol acidity at a single particle level is needed.

This study developed novel pH measurement methods for individual ultrafine aerosol particles. The first method was explored using a pH-sensitive polymer, poly(ε-caprolactone), to determine the acidity of particles. Acidic particles with pH 0 were deposited on a polymer thin film (21-25 nm), and the degradation of the polymer was characterized by atomic force microscopy and Raman microspectroscopy. As particle size decreased, polymer degradation increased, indicating an increase in aerosol acidity at smaller particle diameters. This method presents the potential of studying submicron individual aerosol particles without constraints on complex chemical compositions and relative humidity. Another pH measurement method was developed to directly measure the pH of individual ultrafine particles down to 68 nm in diameter using an acid-conjugate base approach via atomic force microscopy with photothermal infrared spectroscopy. Heterogeneity in pH values was observed for particles generated from the same solution, particularly as a function of size. Both pH measurement methods will improve the fundamental understanding of individual ultrafine aerosol acidity and fill the current knowledge gap of characterizing atmospheric aerosol particles.

5AC.2

Tracking pH Changes in Real-time in Single Levitated Organic or Inorganic Acidic Droplets Undergoing Ammonia Uptake. HALLIE BOYER CHELMO, Walker Cage, Ryan Sullivan, *University of North Dakota*

Aerosol pH is one of the most consequential properties dictating the chemical processing atmospheric particles undergo, yet direct measurements of in situ aerosol droplet pH have remained an important challenge. pH can change considerably during atmospheric aging, requiring a real-time pH micro-probe to directly study this chemistry. We recently developed a novel method of pH measurement of levitated microdroplets using a custom-built aerosol optical tweezers (AOT) for a test system of partially dissociating bisulfate, achieving an accuracy of ±0.03 and a pH range of -0.36 to 0.76. Here, we apply the method to a new probe molecule, 3-methylglutaric acid, and monitor droplet growth and pH change by ammonia and water co-condensation. We demonstrate the new capacity to track droplet pH changes during exposure to ammonia by trapped organic and inorganic acidic droplets. Direct measurements of the rate (kinetics) and extent (thermodynamics) of ammonia uptake will be presented. The pH measurement method uses two independently measured quantities available in the AOT: spontaneous Raman spectra of the acid and base modes and the stimulated Whispering Gallery Modes. Together, these quantities enable measurements of the acid/base concentration ratio and the refractive index, where refractive index is used to determine total anion concentration. The ammonia vapor induces a change of up to 1 measurable pH unit in a bisulfate droplet, a large increase relative to the ~0.1 pH unit change due to changes in relative humidity alone. This work advances our ability to assess aerosol buffering capacity by closely tracking pH in aerosol droplets, such as during important atmospherically relevant processes of gas-particle partitioning, liquid–liquid phase separation, and multiphase chemical reactions.

5AC.3

Models Underestimate the Increase of Acidity with Remoteness Biasing Radiative Impact Calculations.

BENJAMIN A. NAULT, Pedro Campuzano-Jost, Douglas Day, Duseong Jo, Roya Bahreini, Huisheng Bian, Simon Clegg, Jack Dibb, Alma Hodzic, Alma Hodzic, Joseph Katich, Agnieszka Kupc, Eloise Marais, J. Andrew Neuman, John Nowak, Brett Palm, Fabien Paulot, Jeffrey R. Pierce, Gregory Schill, Joel A. Thornton, Kostas Tsigaridis, Paul Wennberg, Christina Williamson, Jose-Luis Jimenez, et al., *CIRES, University of Colorado, Boulder*

The inorganic fraction of fine atmospheric aerosol affects numerous physical and chemical processes. However, due to limited global measurements, there is large uncertainty in its burden, composition, and lifetime. Here, extensive airborne observations are used to investigate how two measures of aerosol acidity, the fraction of anions neutralized by ammonium (ammonium balance), and aerosol pH, change from polluted to remote regions. Both parameters strongly decrease with remoteness (distance from source) at all altitudes. Chemical transport models tend to show more neutralized aerosols and higher pH than observed. We show that part of the discrepancy is due to a frequent high bias in ammonia emissions or lifetime, and/or the incorrect assumption of internally mixed sea-salt. The observations suggest very different aerosol properties and impacts, including higher water content and a smaller direct radiative effect. These results indicate the need for better constraints on the emissions and lifetime of inorganic aerosol precursors, especially ammonia.

5AP.1

Homogeneous Nucleation of Carbon Dioxide from 30-90 K: The Transition from Barrier-Controlled to Barrierless Nucleation.

KAYANE DINGILIAN, Martina Lippe, Ruth Signorell, Barbara Wyslouzil, *The Ohio State University*

Characterizing the nucleation of carbon dioxide (CO_2) from the gas phase is crucial to understanding processes as diverse as carbon capture, refrigeration cycles, and cloud formation on Mars. Here, we explore the homogeneous phase transition of CO_2 for temperatures ranging from ~30 to ~90 K and pressures spanning about four orders of magnitude. The broad range of conditions is achieved by combining results from experimental setups at OSU and ETH, where both experiments rely on a supersonic expansion to rapidly cool selected gas mixtures. In the OSU experiments, nucleation occurs within the diverging portion of the nozzle, and particle formation rates are based on the results of pressure trace measurements and small angle X-ray scattering experiments. In the ETH experiments, nucleation occurs in a uniform post nozzle flow and nucleation is characterized using single-photon ultraviolet ionization coupled with mass spectrometry. Despite the differences in experimental setups and gas compositions, there is excellent agreement between the onset data in the region of overlap. Experimental nucleation rates measured in the OSU setup are, however, two to three orders of magnitude higher than those determined in the ETH apparatus. This difference is consistent with the degree to which non-isothermal nucleation effects play a role. In particular, if the measured rates are scaled by non-isothermal correction factors to determine the intrinsic nucleation rates, remarkable consistency is achieved between the data sets. Furthermore, the combined data suggests that, in this measurement range, the nucleation process changes from one in which particle formation is controlled by a barrier to one in which the barrier vanishes and the kinetics of dimer formation controls the phase transition rate.

5AP.2

Freezing of Aqueous-Alcohol Nanodroplets. TONG SUN, Barbara Wyslouzil, *The Ohio State University*

The freezing of ice in supercooled aqueous droplets is a phenomenon frequently encountered in nature and industry. Since water is not necessarily pure, understanding the role of other species in enhancing or suppressing ice nucleation is important. Amphiphilic alcohols are particularly interesting due to their increasing prevalence in the atmosphere, and their propensity to be highly enriched at the surface. Thus, the temperature at which aqueous-alcohol nanodroplet freeze will be influenced both by the presence of the alcohol and its distribution throughout the droplet.

In the current study, we generate aqueous-alcohol aerosols in a supersonic nozzle with overall mole fractions of the short-chain alcohols n-propanol and n-pentanol up to 0.08, and examine how the freezing process changes relative to that of pure water. Condensation and freezing are characterized by two complementary techniques, pressure trace measurements and Fourier transform infrared spectroscopy. When an alcohol is present condensation occurs earlier in the expansion, largely due to the decrease in interfacial free energy of the binary critical clusters relative to the pure water critical clusters. FTIR results suggest that when 12 nm particles freeze, the tetrahedral structure of the ice core is well preserved for overall alcohol mole fractions up to 0.031 for n-propanol and 0.043 for n-pentanol. For n-propanol, ice nucleation is systematically delayed and the rate is gradually reduced as the alcohol mol fraction increases. In contrast, the freezing kinetics are not altered for n-pentanol until mole fractions reach ~0.03. For each alcohol we estimated the partitioning of alcohol between the surface and the interior or bulk as a function of overall composition. For nanodroplets with comparable bulk concentrations, n-pentanol perturbs the ice freezing process more than n-propanol, consistent with the longer alkyl chain length of the C5 alcohol.

5AP.3

Concentration Depth Profile (CDP)-Based Multi-Sorption Layer Surface Tension Model. SHIHAO LIU, Cari Dutcher, *University of Minnesota*

Surface tension plays a significant role in atmospheric aerosols, including aerosol nucleation, phase transitions, activation into cloud condensation nuclei. Recent predictive surface tension models using a mono-sorption layer framework is available for both organic and inorganic solutions (1). The model, however, considers the partitioning of solute and water molecules only between one surface layer and the bulk region, overlooking the continuous distribution of surface molecules at the surface. Here we discuss a binary-solution model that further divides the surface region into several layers to capture the continuity of molecule spatial distribution near the surface. Partition functions are established for both water molecules and solute molecules based on the molecule displacement. Treating the average number of displaced surface water molecules, the energy of bulk solute molecules, as well as energy difference of bulk and surface solute molecules as model parameters gives accurate prediction of surface tension of aqueous solutions. Published experimental and simulated results of concentration depth profile and number density of molecules/ions near the surface are used to obtain the parameters relevant to the number of solute molecules at each surface layer. Furthermore, the complexity of chemical compound of atmospheric aerosols motivates us to extend the model to predict surface tension of mixture solutions without additional parameter fitting. Coupled nonlinear equations are solved using neural network to predict surface tension with calculated number of molecules at the surface or in the bulk. Both binary and mixture models can predict surface tension over a wide range of concentrations, which can benefit the understanding of aerosol processes in the atmosphere.

[1] Boyer, H. C.; Dutcher, C. S. Atmospheric Aqueous Aerosol Surface Tensions: Isotherm-Based Modeling and Biphasic Microfluidic Measurements. J. Phys. Chem. A 2017, 121 (25), 4733–4742. https://doi.org/10.1021/acs.jpca.7b03189.

5CO.1

A Molecular Dynamics Study of Inception and Growth of Soot during Combustion. Akaash Sharmaa, Khaled Mosharraf Mukut, Eirini Goudeli, SOMESH ROY, *Marquette University*

Accurate prediction of soot formation and growth in combustion systems is very important for reasons ranging from reduced combustion efficiency to the global climatic forcing of soot. Unfortunately, the fundamental physico-chemical processes behind the formation of soot are still not completely understood. In this study, a detailed and systematic investigation of inception and growth of soot is conducted by full-atom reactive molecular dynamics (rMD) simulations using reactive force-field (reaxFF) interatomic potentials for bond breakage and new bond formation upon collisions. The simulations show the formation and evolution of several precursors and incipient soot clusters with time starting with acetylene at different temperatures. The number of 5-, 6-, and 7-membered aromatic rings increase with time as the size of the incipient soot clusters grows. The majority of the aromatic rings are found at the core of the clusters, while the aliphatic branches are found mostly on the surface. The gyration diameter, Sauter-mean diameter, and the fraction of the aromatic rings within the incipient cluster increase substantially with time, while the C/H ratio remains approximately constant at about 2.5, consistent with the literature. The incipient clusters also show a decrease in the relative shape anisotropy with time leading to a more spherical shape as the aliphatic branches on the particle surface become shorter. Additionally instances of sintering were observed specifically for certain ranges of temperature and incipient cluster sizes.

5CO.2

Impact of Dilution Temperature on Size-Resolved Aerosol Emissions from Lignocellulosic Biomass. LUKE MCLAUGHLIN, Erica Belmont, *University of Wyoming*

Biomass burning events, such as wildland fires and prescribed burns, are complex combustion phenomena consisting of four main stages: pyrolysis, flaming combustion, primary char oxidation, and smoldering. These fire events produce significant amounts of particulate matter which influence global radiative forcing, decrease air quality and visibility, and have negative health impacts. Biomass burning aerosol emissions consist predominantly of elemental carbon and organic carbon, the quantity, size distribution, and volatility of which are influenced by the combustion mode and ensuing dilution process of the emissions mixing into ambient air. As the number and size of wildland fires increase each year, and as prescribed burning is used as a forest fire management technique across the United States, there is an increased need to characterize the quantity, size, and volatility of the emissions from burning lignocellulosic biomass to better understand environmental and health effects. This work examined the emissions from lignocellulosic biomass and its major constituents under laboratory pyrolysis conditions to understand biomass composition and dilution temperature influences on aerosol formation. The major constituents of lignocellulosic biomass were pyrolyzed and the resultant aerosol emissions were characterized in terms of particle size, quantity, and volatility under variable dilution temperatures and at a fixed dilution ratio and rate. The aerosol emissions formed from the biomass constituents were then compared to those of wood and grass biomasses, and an additive model for predicting characteristics of biomass burning emissions from the behavior of individual constituents was assessed. Results showed a significant influence of dilution temperature on particle size, number, and distribution, with the nucleation mode of particle formation dominating at low dilution temperatures. The additive model performed well in predicting the trends and magnitude of aerosol emissions from native biomass samples with variable lignocellulosic constituent distributions.

5CO.3

The Effects on Emissions of Modified Operation of Pellet-Fed Gasifier Stoves. STEPHANIE PARSONS, Ky Tanner, Andrew Grieshop, *North Carolina State University*

Field tests of biomass pellet-fed stoves in Rwanda found lower emissions compared to other biomass stoves, in many cases approaching that of current “gold standard” technologies such as liquefied petroleum gas. However, emission factors (EFs) of particulate matter ($PM_{2.5}$) and carbon monoxide (CO) during high emitting pellet tests were as high as those during low emitting wood and charcoal tests, emitting the most $PM_{2.5}$ and black carbon (BC) at the startup and the end of cooking (i.e. the burnout phase). We conducted two sets of laboratory tests, based on the Water Boiling Test and the International Organization for Standardization Laboratory Sequence, to observe how varying stove operation affects emissions of $PM_{2.5}$, CO, organic and elemental carbon (OC, EC), BC, and particle number. Three different variations were examined: startup operation, shut down operation, and refueling. Using kindling to ignite the stove produced almost three times higher CO and $PM_{2.5}$ emissions compared to using kerosene. Low, medium, and high fan speeds during the burnout phase resulted in CO EFs 71%, 92%, and 118% higher than with the fan off, respectively. Likewise, a slight increasing trend in $PM_{2.5}$ EFs was observed between the fan off and low speed compared to the medium and high speeds. Refueling with hot pellet embers blocking the gasifier holes (highest refuel height) resulted in 300% (50%) higher CO ($PM_{2.5}$) EFs than the lowest refuel height. Particle number emissions increased with increasing fan speed during burnout, with the high speed emitting five times more particles than the fan off, and with increasing height of hot embers used for refueling, with the highest refuel height emitting 50% more particles than the lowest. We will communicate results to the stove manufacturer to possibly influence the stove design and operation specifications to decrease improper use.

5EJ.1

Advancing Air Quality Monitoring in Environmental Justice Communities of the South Coast Air Basin, Ca: III. Community-Scale Monitoring of Particulate Metals and Other Air Pollutants Using a Recently Developed Mobile Platform. SINA HASHEMINASSAB, Mohammad Sowlat, Payam Pakbin, Steven Boddeker, Avi Lavi, Faraz Ahangar, Christopher Lim, Julia Montoya-Aguilera, Andrea Polidori, *South Coast Air Quality Management District*

In this study, a recently developed mobile platform was deployed for near-source and community-scale monitoring of ambient particulate metals and other air pollutants (i.e., particle number and mass, black carbon (BC), CO2, and NO2) in two Environmental Justice (EJ) communities within the South Coast Air Basin (SCAB). The monitoring scheme consisted of sequential steps, including area-wide mobile monitoring to broadly identify the local hotspots; investigative mobile monitoring for identification of potential sources; and subsequent stationary monitoring downwind of the identified sources to characterize their emissions. As these measurements were typically conducted during the day and on weekdays, they lacked information on concentrations outside of these hours. They were also, by design, not collected at one location, complicating direct comparison between measurements while accounting for variations due to changes in emissions and meteorological conditions. Therefore, fixed sites were established for continuous monitoring of particulate metals and other air pollutants to account for those variations. In addition, to ensure data representativeness, sample size (i.e., number of data points in each location for stationary monitoring and number of passes for mobile monitoring) calculations were done using statistical techniques, taking into account the desired confidence limits, confidence intervals, and the standard deviations of air pollutant concentrations. In this presentation, we report the hyper-local, spatio-temporal variations of ambient particulate metals in the EJ communities of the SCAB and demonstrate how this approach has enhanced our capabilities to identify and characterize potential emission sources in the study area. Results from this study will be used for future community-scale source apportionment and source-specific exposure/risk assessment studies. Our findings can also be used to support development of strategies and policies to reduce the exposure to air pollutants in EJ communities.

5EJ.2

Pandemic-Induced Changes in Traffic Patterns and Localized Air Quality in Inland Southern California.

ARASH KASHFI YEGANEH, Shams Tanvir, Kanok Boriboonsomsin, Khanh Do, Matthew Barth, Cesunica E. Ivey, *University of California, Riverside*

Due to high population density, various sources of emissions, unique topography, and atmospheric conditions in the South Coast Air Basin (California), this region historically experiences the worst air quality in the United States. Poor air quality of the region combined with minorities and underserved communities being disproportionally exposed to pollutants makes health conditions much worse for this susceptible part of society. While governmental agencies are doing extensive research to find out the most effective scenario to improve human exposure to pollutants, lockdowns due to COVID-19 presented an opportunity to investigate the relationship between air quality, meteorology, and emissions to design regulatory plans. Lockdown orders to prevent the spread of COVID-19 led to traffic volume reduction of more than 50% on some California highways. In this work, we quantify the changes in traffic due to COVID-19 lockdowns to estimate traffic-related emissions (CO, NO_2, $PM_{2.5}$) precisely at the corridor level in the cities of Riverside and San Bernardino, CA. By aggregating traffic-related emissions at the census tract level, we relate localized air quality to localized transportation emissions and disproportionate impacts on environmental justice communities using GIS spatial clustering and joins. Results are provided for the 2020 pre-COVID-19 period and phases 1-3 of government reopenings.

5EJ.3

Comparing Local and Regional-Scale Particle and Gas-Phase Pollutant Exposure Disparity in a Long-Term Mobile Monitoring Campaign.

SARAH CHAMBLISS, Carlos Pinon, Kyle Messier, Shahzad Gani, Brian LaFranchi, Melissa M. Lunden, Julian Marshall, Ramon Alvarez, Joshua Apte, *University of Texas at Austin*

We utilize mobile monitoring of ultrafine particles (UFP), black carbon (BC), NO, and NO_2 in eighteen neighborhoods within the San Francisco Bay Area to characterize both highly localized and broader urban scale variation in outdoor air pollution. Mobile laboratories were deployed on weekdays throughout a 32-month campaign, recording over 3,100 hours of data. We derive long-term spatial patterns using a temporal aggregation algorithm that calculates the median of individual drive passes within 10 m of each census block. We calculate the distribution of concentrations among the entire population of each neighborhood and among five census-based racial-ethnic groups: Hispanic/Latino, and non-Hispanic Asian, Black, White, and Other groups.

We find high within-neighborhood heterogeneity in census block-based exposure concentrations relative to between-neighborhood differences. Even with a 10-fold difference in median NO between "background" and high-emission neighborhoods, the interquartile range of NO in highly polluted neighborhoods is comparable to the absolute difference between neighborhoods. BC shows a similar trend. For UFP there are several distinctly high and distinctly low neighborhoods and a high degree of exposure overlap among intermediate-concentration areas. Concentrations of NO_2 show the least overlap among neighborhoods but still exhibit substantial within-neighborhood heterogeneity.

Considering racial-ethnic exposure disparity, we find that the White non-Hispanic group experiences lower average concentrations for all pollutants, especially in comparison with Black and Hispanic/Latino populations. Population-weighted average concentrations for those groups are 10% higher for BC, over 25% higher for UFP and NO2, and over 50% higher for NO. Majority non-White neighborhoods tend to be ranked highest in median concentrations, and within some high-concentration neighborhoods the White population constitutes a disproportionate share of the lowest exposure categories. This work illustrates the complementary interaction between spatially dense measurements and coverage of a large, diverse set of neighborhoods to better understand population exposure and identify issues of environmental justice.

5ID.1

Quantifying the Relative Risk of Aerosol Generating Procedures in Clinical Settings. FLORENCE GREGSON, Jules Brown, Bryan R. Bzdek, Andrew Shrimpton, Tony Pickering, Jonathan P. Reid, *University of Bristol*

The risk of SARS-CoV-2 transmission to and by healthcare workers in clinical settings is a pressing issue. Many activities are classified as Aerosol Generating Procedures (AGPs), including (in the UK) intubation, extubation, and manual ventilation. These procedures are thought to produce aerosols and droplets that may spread disease. Consequently, such procedures require enhanced personal protective equipment (PPE, including facemask respirators, fluid resistant gowns, and face shields) and strategies to minimise exposure of other staff have been implemented (e.g. minimal staff present during AGPs; delays after each AGP to allow air changes). These enhanced safety precautions increase cost, decrease throughput, and inhibit communication among clinicians. However, the actual exposure (and risk of disease transmission) during many AGPs is unknown because the evidence base is lacking. For instance, the concentration and size distribution of aerosol produced during AGPs is poorly known.

In this study, a Condensational Particle Counter (CPC, < 1 µm particles) and Optical Particle Sizer (OPS, 300 nm – 10 µm) were deployed to quantify the number concentration (CPC, OPS) and size distribution (OPS) of aerosol produced during AGPs in a laminar flow operating theatre over a period of several weeks. The near-zero particle background in the operating theatre allowed sensitive measurements of aerosol production from individual coughs (showing a characteristic particle size distribution) and concentration. Aerosol production during intubation and extubation were compared to aerosol production from voluntary coughs. We will present our data quantitating the relative risk of aerosol production associated with AGPs which should prompt a re-evaluation of current practice.

5ID.2

Evaluating the Presence of Airborne Virus in Common Upper Airway Surgical Procedures. TOFIGH SAYAHI, Chris Neilson, Yuan Yu, Kayden Neurberger, Michael Seipp, Matt Firpo, Albert Park, Kerry Kelly, *University of Utah*

The risk of COVID-19 transmission through aerosols generated during upper airway (UA) surgical procedures is a great concern to healthcare workers due to high viral loads in oral and nasal secretions of the infected patients. This study uses a murine cytomegalovirus (mCMV) model for infection to: 1) investigate whether common UA surgeries can generate aerosolized virus and whether the virus is viable, and 2) quantify aerosol generation. We inoculated BALB/c mice with saline (3 mice) or mCMV (14 mice), and after 5 days we performed the following four procedures on each mouse: drilling, microdebrider, coblation, and electrocautery. We used an Aerosol Device Biospot sampler to collect aerosol samples for virus detection using viral culture (viable) and for viral titer using polymerase chain reaction (PCR). We also evaluated the particle size distribution (using SMPS/APS and GRIMM) and PM2.5 concentration (using DustTrak II and GRIMM). The results showed coblation and electrocautery generated the highest aerosol concentrations, with over 100,000- or 35,000-fold increases in PM2.5 concentration compared to background levels, and over 350- or 1200-fold increases in the total particle counts compared to background levels, respectively. We identified viral DNA in samples from coblation and drilling procedure, however, the preliminary tests did not identify viable viruses in samples from any of the procedures.

5IM.1

Measuring Humidification Effects on Ammonium Sulfate – Nigrosin Mixtures with a Novel Humidity Controlled Albedometer. TYLER CAPEK, Christian Carrico, Kyle Gorkowski, Jared Lam, James D. Lee, Allison Aiken, Timothy Onasch, Andrew Freedman, Claudio Mazzoleni, Manvendra Dubey, *Michigan Technological University*

Water can have a significant influence on the optical properties of atmospheric particles by altering their ability to scatter and absorb sunlight. Water can condense on these particles, increasing their size and altering their overall morphology. Some absorbing particles can be hydrophobic; however, hydrophilic coatings on these particles can lead to water uptake and enhancements in both absorption and scattering. Accurate assessment of these enhancements is key for determining the particles' impact on the climate. We have developed a cavity attenuated phase-shift albedometer (RH-CAPS-SSA), operating at 450 nm, integrated with a humidifier to study humidification effects on the optical properties of atmospheric particles. We have characterized the optical properties and hygroscopicity of two benchmark aerosol, ammonium sulfate, and nigrosin. Ammonium sulfate (AS) is a hygroscopic aerosol that scatters strongly in the visible spectrum. Nigrosin ink is used as a proxy for strongly absorbing and weakly hygroscopic atmospheric particles, providing a reproducible model particle to study and better understand the fundamental behaviors of more complex absorbing atmospheric particles such as black and brown carbon. Mixtures of nigrosin and AS can lead to a particle that is more hygroscopic than pure nigrosin and more absorbing than pure AS. We compare the measured enhancements of pure aerosol and mixtures to models incorporating Mie theory and κ-Köhler theory with an eye on characterizing the performance of the RH-CAPS-SSA and developing a model for characterizing humidified atmospheric aerosol mixtures. Enhancements in absorption were observed for each sample containing nigrosin when relative humidity was increased. For example, absorption enhancement as high as 1.12±0.02 in pure nigrosin, which compared favorably to the Mie estimate of 1.15±0.08. As relative humidity increased, we also observed increasing single scattering albedo (SSA) in each of the samples containing nigrosin.

5IM.2

Scattered Light Truncation Issues in the CAPS PM Single Scattering Albedo (CAPS PMssa) Monitor: Effects of Particle Size Distribution and Fefractive Index. FENGSHAN LIU, Joel Corbin, Prem Lobo, Gregory Smallwood, *National Research Council Canada*

The cavity attenuated phase shift particulate matter single scattering albedo (CAPS PMssa) monitor has been increasingly used to measure aerosol absorption and single scattering albedo (SSA) based on the extinction-minus-scattering (EMS) principle for different applications. As with other nephelometers, CAPS PMssa also suffers from truncation issues in its scattering channel: part of the scattered light in the forward and backward directions cannot be detected. To achieve accurate measurements of both aerosol absorption and SSA, it is important to develop accurate truncation correction models to correct the measured aerosol scattering, especially for aerosols with a high SSA.

To date, limited numerical and experimental studies have been conducted to investigate the truncation issue of CAPS PMssa. To gain a more comprehensive and quantitative understanding of CAPS PMssa truncation, a numerical study was carried out to investigate the effects of aerosol particle size distribution and refractive index using our previously developed truncation model based on the radiative transfer equation (RTE). The aerosol particles considered in this study include both polydisperse non-absorbing and absorbing spherical polystyrene latex (PSL) particles and polydisperse absorbing fractal soot aggregates.

For aerosol measurements using CAPS PMssa, it is challenging to perform truncation correction to the measured scattering coefficient since the morphology, refractive index, or even the composition of aerosol particles are often unavailable. In most cases, only SSA and particle mobility or aerodynamic size distribution data are available. Our previous study showed that the truncation of CAPS PMssa correlates well with the asymmetry factor of the aerosol particle scattering phase function. To develop a practically usable truncation correction model, an attempt was made to estimate the range of asymmetry factor of aerosol particle scattering phase function based on SSA and particle mobility size distribution assuming PSL and soot particles represent two extreme types of aerosol particles in terms of morphology and refractive index.

5IM.3

Dual Cavity Spectrometer for Monitoring Broadband Light Extinction by Atmospheric Aerosols. AISWARYA SASEENDRAN, Susan Mathai, Shreya Joshi, Anoop Pakkattil, Tyler Capek, Gregory Kinney, Claudio Mazzoleni, Ravi Varma, *Michigan Technological University*

Atmospheric aerosols directly influence Earth’s climate by scattering and absorbing solar radiation. To study the broadband optical properties of aerosols, we developed a dual cavity enhanced extinction spectrometer that uses a supercontinuum laser source and a compact spectrometer. The spectrometer measures the extinction coefficient over a broad wavelength region from 420 to 540 nm simultaneously. A dual cavity approach is employed to account for changes in background signal and for spectral and intensity fluctuations of the laser. Polystyrene latex spheres and aerosolized salt particles were used to test the system, and the measured extinction showed good agreement with Mie calculations. Furthermore, we favorably compared the scattering coefficient of non-absorbing aerosols measured using a nephelometer with the extinction coefficient measured using the dual cavity system. The spectrometer was also used to measure the extinction Ångström exponent of laboratory generated soot particles that was found to be equal to ~1.6, comparable to values previously reported in the literature. The broadband dual-cavity extinction spectrometer is simple and robust and should be particularly useful for laboratory measurements of the extinction coefficient of brown carbon aerosol. In the future, the instrument could be deployed in the field to study the optical properties of brown carbon such as smoke particles emitted from biomass burning.

6AC.1

The Surface Tension of Surfactant-Containing, Finite Volume Droplets.

BRYAN R. BZDEK, Jonathan P. Reid, Jussi Malila, Nonne Prisle, *University of Bristol*

Surface tension influences the fraction of atmospheric particles that become cloud droplets. Although surfactants are an important component of aerosol mass, the surface tension of activating aerosol particles is still unresolved, with most climate models assuming activating particles have a surface tension equal to that of water. By studying picoliter droplet coalescence, we demonstrate that surfactants can significantly reduce the surface tension of finite-sized droplets below the value for water, consistent with recent field measurements. Significantly, this surface tension reduction is droplet size-dependent and does not correspond exactly to the macroscopic solution value. A fully independent monolayer partitioning model confirms the observed finite-size-dependent surface tension arises from the high surface-to-volume ratio in finite-sized droplets and enables predictions of aerosol hygroscopic growth. This model, constrained by the laboratory measurements, is consistent with a reduction in critical supersaturation for activation, potentially substantially increasing cloud droplet number concentration and modifying radiative cooling relative to current estimates assuming a water surface tension. The results highlight the need for improved constraints on the identities, properties, and concentrations of atmospheric aerosol surfactants in multiple environments and are broadly applicable to any discipline where finite volume effects are operative, such as studies of the competition between reaction rates within the bulk and at the surface of confined volumes and explorations of the influence of surfactants on dried particle morphology from spray driers.

6AC.2

Enhanced Reactivity in Droplets Relative to Bulk Solution Studied by Droplet Assisted Ionization Mass Spectrometry.

YAO ZHANG, Murray Johnston, *University of Delaware*

Droplet Assisted Ionization (DAI) is a relatively new method for online analysis of aerosol droplets that enables measurement of the rate of an aerosol reaction. It is an inlet ionization method, where ions are formed when droplets pass through a temperature-controlled capillary inlet to a mass spectrometer. Here, we used DAI to study the reaction of carbonyl functionalities in secondary organic aerosol (SOA) with Girard’s T (GT) reagent. Varying the droplet transit time between the atomizer and mass spectrometer allowed the reaction rate constant to be determined, which was found to be 4 orders of magnitude faster than what would be expected from bulk solution kinetics. Mechanisms of reaction acceleration on the droplet were investigated by varying DAI conditions including: i) increasing temperature applied on the capillary inlet, ii) decreasing the relative humidity of the air surrounding the droplets in between the atomizer and the mass spectrometer, and iii) varying the size of the droplets. It was found that the product formation was enhanced by heating the capillary inlet and decreasing the relative humidity of the air, suggesting that removing water from the droplets increased the reaction rate. Decreasing the droplet diameter increases the surface to volume ratio and can distinguish reaction on the particle surface from that in the bulk volume. The results suggest that reaction on the droplet surface plays an important role to increase the reaction rate in droplets relative to bulk solution.

6AC.3

Direct Quantification of the Effect of Ammonium on Aerosol Droplet pH. QISHEN HUANG, Haoran Wei, Linsey Marr, Peter Vikesland, *Virginia Tech*

Aerosols and droplets with high water content are important systems that dictate many atmospheric processes. pH is arguably a key controlling parameter as its effect on aerosol physicochemical properties (e.g., size, surface tension, and mixing state) ultimately impact climate, human health, and aerosol reactivity. pH has been reported to correlate with many atmospheric processes such as secondary aerosol formation, cloud condensation nuclei activity, and liquid-liquid phase separation. Ammonium sulfate (AS) is a major component of atmospheric secondary aerosols. As such, sulfuric acid plays an important role in the formation of new atmospheric particles, and ammonia is significant in the heterogeneous neutralization of acidic aerosols.

Aerosol pH is frequently evaluated via analysis of field-collected aerosol composition or is indirectly predicted by proxy methods such as thermodynamic models. In this study, the impact of ammonium ion on aerosol droplet pH was directly quantified using pH nanoprobes and surface enhanced Raman spectroscopy (SERS). Sample solutions were prepared by mixing 1 M ammonium sulfate (AS), ammonium nitrate (AN), sodium sulfate (SS), or sodium nitrate (SN) solutions with 1 M phosphate buffer (PB) at different volume ratios. The pH of the 10 – 50 µm aerosol droplets generated from these solutions was measured to determine how ionic composition affects droplet pH. When the ammonium concentration (AS or AN) was increased, the centroid pH within the droplets decreased from ≈11 to 5.5. Such a decrease was not observed in sodium (SS or SN) systems and no pH differences were observed between sulfate and nitrate. Formation of ammonia and its partitioning to the gas phase in ammonium containing droplets appeared to be negligible. The pH difference between ammonium-containing droplets and ammonium-free droplets suggests that the presence of ammonium alters the system ion distribution. The role of the air-water interface and the interfacial preference of different cations and anions in ion distribution were investigated and discussed using surface tension measurements and 2D Raman spectra.

6AP.1

Light Backscattering from Post-flame, Cooled Soot Particles. PRAKASH GAUTAM, Justin Maughan, Christopher Sorensen, *Kansas State University*

We studied light scattering due to soot particles generated by ethylene, propane and oxygen combustion via a pre-mixed burner. The measurements were made at a wavelength of 532 nm with vertically polarized incident light in the scattering angle range from 0.32° to 157°. The scattering volume was in a post-flame region where the soot was nearly at room temperature. The results showed a fractal dimension of -2.00 ± 0.15 with an enhancement in the backscattering, a result not observed theoretically. For analysis, soot particles were collected from the scattering volume region using a thermophoretic sampling devices. The size distribution shown by transmission electron micrographs (TEM) was in good agreement with the size distribution given by an aerodynamic particle sizer (APS 3321) and consistent with Guinier analysis of the scattering. Further, the micrographs indicated that some soot particles were dense aggregates while others were ramified fractal aggregates. We propose that these represent water coated and dry aggregates, respectively. Based on our TEMs, we further propose that our experimentally observed backscattering is due to the dense aggregates which results from the presence of water in the soot aerosol.

6AP.2

Phase Shift Parameter Controls Light Absorption Enhancement for Coated Fractal Aggregates. PAYTON BEELER, William Heinson, Rajan K. Chakrabarty, *Washington University in St. Louis*

The mass absorption cross-section (MAC) of black carbon (BC) aggregates is an important parameter in many climate models. Failure to account for the complex morphology and mixing state of BC aggregates will result in significant underestimation of their MAC, and ultimately errors in global radiative forcing calculations. Consensus holds that organic compounds can coat the surface of BC aggregates and alter their morphology towards an increase in phase shift parameter. However, the detailed evolution pathway of MAC during the coating-induced BC restructuring remains understudied till date. Here, we perform computer simulation to comprehensively probe the MAC enhancement factor ($E_{MAC,BC}$) for coated BC aggregates with changing phase shift parameter and amount of coating. Three aggregation models: diffusion-limited cluster-cluster aggregation, percolation, and simple cubic lattice stacking, were adopted to generate aggregates mimicking real-world BC in the freshly-emitted, partially-collapsed, and fully-collapsed states, respectively. The simulated aggregates were subsequently coated with non-refractory organics, and their optical properties were calculated with the Amsterdam discrete dipole approximation. Our results show that the amount of coating determines the magnitude of $E_{MAC, BC}$ per a universal scaling relationship. Finally, we find that the phase shift parameter determines whether $E_{MAC, BC}$ is positive or negative (i.e. increased or decreased absorption) over the atmospheric lifetime of BC aggregates, and determines whether core-shell model overestimates or underestimates light absorption by coated BC aggregates.

6AP.3

Quantifying Brown Carbon Measured in Real-world Biofuel Combustion Emissions. MOHAMMAD MAKSIMUL ISLAM, Alyssa Sanderson, Andrew Whitesell, Ashley Bittner, Rawad Saleh, Andrew Grieshop, *North Carolina State University*

Biomass burning is considered an important source of light-absorbing organic carbon (OC), also known as brown carbon (BrC). Although BrC affects earth’s radiative balance, its absorption properties remain uncertain for many sources. In this work, we used methanol (ME) to extract organic carbon from ~60 filters collected during ‘real-world’ biofuel combustion in India and Malawi from emissions tests of various wood stoves (traditional, rocket, gasifiers and chimney) and artisanal charcoal kilns. We then used a spectrophotometer to collect the absorption spectra (239 to 800 nm wavelengths) to characterize BrC absorption.

Mass absorption coefficients ($MAC_{\lambda\text{-}ME}$) of extracted OC from chimney stoves and charcoal kilns are significantly lower than those of traditional and improved non-chimney stoves at near-ultraviolet to blue wavelengths. Traditional and chimney stove emissions have the lowest and highest absorption angstrom exponent (AAE_{ME}), respectively. $MAC_{\lambda\text{-}ME}$ in the UV wavelengths shows positive correlation with elemental-to-organic carbon ratio (EC/OC), although weaker than that observed in lab cookstove studies. Unlike EC/OC, modified combustion efficiency (MCE) exhibits weak positive correlation with $MAC_{\lambda\text{-}ME}$, showing that EC/OC is a better indicator of combustion conditions associated with brown carbon production. At near-ultraviolet to blue wavelengths, imaginary refractive indices of BrC ($K_{BrC\text{-}ME}$) are anti-correlated with wavelength dependence, w (≈AAE-1), suggesting that less wavelength-dependent BrC has higher light absorptivity. $MAC_{\lambda\text{-}ME}$ correlated with the fraction of OC evolving at 615°C (OC3/OC; r = 0.54 at 500 nm) and anti-correlated with OC evolving at 310°C (OC1/OC; r = 0.49 at 500 nm). This association is consistent with a link between absorptivity of brown carbon and OC volatility, and hence, suggests that BrC absorption may be parameterized by using existing OC data. We apply a simple radiative forcing model to provide an estimate of BrC’s climate impacts relative to co-emitted black carbon.

6CO.1

Investigating the Formation of Primary and Secondary Aerosols from Heavy Duty Vehicles (HDVs) Using Smog Chamber.

SAHAR GHADIMI, Hanwei Zhu, David R. Cocker III, Thomas D. Durbin, Georgios Karavalakis, *University of California, Riverside*

Heavy duty vehicles (HDVs) are major contributors to urban air pollution. Fuel types and driving conditions—Urban Dynamometer Driving Schedule (UDDS) cycle, refuse cycle and Cruise cycle— are known to impact vehicle emissions, while their influence need further investigation particularly on secondary organic aerosol (SOA) formation. In this study, the secondary and primary aerosol formations from different fuel types including Liquefied Petroleum Gas (LPG), Compressed Natural Gas (CNG), Renewable Diesel (RD), and Ultra-low Sulfur Diesel (ULSD) and different aftertreatments such as Three-Way Catalyst (TWC), Diesel Particulate Filter (DPF) and Selective Catalytic Reduction (SCR), were investigated using the 30 m^3 Mobile Atmospheric Chamber (MACh) at UC Riverside. The physiochemical properties of the emissions and aerosols were evaluated using variety of particle and gas phase instrumentations such as Scanning Mobility Particle Sizer (SMPS), Kanomax Aerosol Mass (APM) analyzer, High-Resolution Time-of-Fight Aerosol Mass Spectrometer (HR-ToF-AMS), and LI-840A CO_2/H_2O gas phase analyzer. All of the experiments were performed under cold start conditions.

For all the fuel types, cruise mode produced lower primary and secondary emissions comparing to the UDDS and refuse driving cycle. Higher secondary organic mass observed in ULSD vehicles bearing DPF aftertreatment compered to RD vehicles with the same after treatment. Inorganic ammonium nitrate (NH_4NO_3) aerosols were extremely low (or negligible in some cases) in primary emissions and MACh-mediated photo-oxidation of diesel (RD and ULSD) exhaust. On the other hand, LPG and CNG vehicles were equipped with TWC aftertreatment produced higher ammonia (NH_3) which further generated secondary ammonium nitrate particles (NH_4NO_3) upon reacting with HNO_3. The combined impact of fuel type, aftertreatment strategies, and driving mode on primary and secondary emissions will be evaluated and discussed in detail.

6CO.2

Effects of Blended Fuel on Diesel Engine Exhaust Particles: From Bulk to Single Particle Compositions.

LAURA-HELENA RIVELLINI, Mutian Ma, Nethmi Kasthuriarachchi, Wenbin Yu, Yichen Zong, Wenming Yang, Markus Kraft, Alex Lee, *National University of Singapore*

Diesel engine emissions are important sources of fine particulate pollutant, causing negative impacts on climate and human health. Recent studies have shown reduction in emissions of black carbon (BC) and organic aerosol (OA) when blended fuels were used. This work investigates the effects of polyoxymethylene dimethyl ethers (PODE) blended fuels (0%, 10%, 20% and 30% by volume) on the emission characteristics of diesel engine exhausts under various engine loadings using a soot-particle aerosol mass spectrometer (SP-AMS). In addition to the ensemble measurements, a novel single-particle mode of SP-AMS was used to determine the chemical compositions of individual particle, and thus the particle mixing state. This work identified three particle types in the emissions based on a single-particle clustering analysis. While one particle type presented higher BC content (>50 wt% of BC), the rest were dominated by OA that can be further classified by their molecular weight. The distributions of these particle types varied with both engine loadings and fuel compositions. In particular, a global increase of rBC-containing particle mass fractions with engine loadings, except for the blended fuel with 30% PODE whose BC-rich particle fractions remained <10% for all tested conditions. Although increasing the blended volume of PODE to 20% or higher could reduce the BC-rich particle fractions, the blended fuel with 10% PODE enhanced the BC-rich particle fractions compared to that from diesel. Furthermore, increasing the blended volume resulted in decreasing of particle size of each particle type. The chemical characteristics of traffic-related particle observed in urban environment matched well with the particles types identified here, especially for those containing > 50 wt% of BC, hydrocarbon-like OA, and high molecular weight OA. Our observations provide insight into the changes in emission characteristics and environmental implications of diesel engine particles caused by the application of blended fuel.

6CO.3

Determining Fleet-based Vehicle Emission Factors Using Low-cost Sensor Packages: A Case Study across Three Parking Garages. Bingqi Liu, 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, NO_2, CO_2, O_3 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 CO_2 signals were converted to fuel-based emission factors for the five pollutants measured by the RAMP monitors and to measure the relative impact of cold-start. We report $PM_{2.5}$, CO, and NO_x emission factors in-line with previously calculated emission factors using regulatory grade instruments. We also found that emission factors from vehicles leaving the garages in the evening (simulated cold start) were up to 50% higher than emission factors from vehicles entering the garages in the morning.

6EJ.1

Advancing Air Quality Monitoring in Environmental Justice Communities of the South Coast Air Basin, Ca: I. Overview of Approaches, Technologies, and Community Engagement. Sina Hasheminassab, PAYAM PAKBIN, Faraz Ahangar, Mohammad Sowlat, Steven Boddeker, Julia Montoya-Aguilera, Avi Lavi, Christopher Lim, Andrea Polidori, Jason Low, *South Coast Air Quality Management District*

The regional air quality improvement in the South Coast Air Basin (SCAB) is well documented. However, disproportionate exposure to elevated levels of air pollution in Environmental Justice (EJ) communities of the SCAB continues to have serious public health consequences. In 1997, the South Coast Air Quality Management District (South Coast AQMD) began its EJ initiatives to conduct enhanced air monitoring and to take a more systematic approach to reduce the disproportionate impact of air pollution in disadvantaged communities. Since then, South Coast AQMD has developed strong relationships with EJ communities to learn about their local air quality concerns and develop solutions jointly with community members. More recently, in 2017, the enactment of Assembly Bill (AB) 617 provided additional opportunities and resources to accelerate the efforts to address air pollution issues in EJ communities throughout the state of California.

Thus far, five EJ communities have been selected in the SCAB under the AB 617 program. Depending on the specific needs of each community, South Coast AQMD develops a tailored Community Air Monitoring Plan (CAMP) to identify and implement the most appropriate air monitoring strategies to support actions for emissions and exposure reduction. As part of these efforts, the South Coast AQMD has been developing and evaluating some of the most advanced air monitoring technologies to enhance its capability to measure community-scale criteria and toxic air pollutants. Considering that most of the EJ communities in the SCAB cover a vast geographical area and encompass a wide range of air pollution sources, an approach that integrates multiple air monitoring strategies and technologies seems appropriate. In this presentation, we will provide an overview of the AB 617 air monitoring program in the SCAB and discuss the monitoring approaches, technologies, and the community engagement process. In two companion presentations, we will also present the preliminary results of the community-scale air monitoring projects that have been conducted so far as part of this new program.

6EJ.2

Framework for Selecting Data Analytic and Modeling Methods for Environmental Justice Analysis.

RIVKAH GARDNER-FROLICK, Amanda Giang, *University of British Columbia*

Environmental justice (EJ) and health analyses present a unique set of requirements for using data analytic and modeling approaches beyond selecting methods that are suitable for the available data and pollutant of interest. Techniques that may be appropriate for other applications might not be useful for the EJ questions being considered by researchers, communities, and other stakeholders, or worse, they could result in misrecognition of EJ communities. As a result, EJ communities may not receive the aid they need to improve their environmental conditions. Additionally, improper techniques could falsely label a place as harmful or degraded, or unfairly blame community residents for environmental hazards. With this in mind, we perform a scoping review of available literature to create a framework for selecting between common and emerging data analytic and modeling methods for use in EJ analysis, given the purpose of analysis, users, and resources available.

Upon critically synthesizing the literature, we identify three main dimensions on which to evaluate a data analytic or modeling technique when considering its use in EJ analyses. The key components that form the basis of this framework are the accuracy and interpretability of the results, the spatiotemporal features of the method, and the usability of the method. Techniques should be evaluated on accuracy and interpretability by their ability to describe real life concentrations, how reliably they identify EJ communities, and the ease of determining which factors are affecting concentrations and identification of communities. Spatiotemporal features demand appraisal of the available spatiotemporal resolution and domain of a method. Finally, the usability of a method is assessed through an examination of the accessibility, computational efficiency, and cost. We illustrate the framework with case studies from the literature. By locating different methods along these dimensions, we provide a framework for matching methods to analytical needs, resources, and users.

6EJ.3

Future Air Pollution and Environmental Justice in California: Achieving Equity for all Socio-economic Classes.

YITING LI, Anikender Kumar, Yin Li, Michael Kleeman, *University of California, Davis*

California has committed to an 80% reduction in GHG emissions by the year 2050. This massive reduction will require a transformation in the energy system that will also impact air quality. The optimal future energy portfolio will not only reduce climate change and improve air quality at minimum economic cost, but it should also seek to provide equal benefits for all socio-economic classes by achieving environmental justice (EJ) principles.

Predicting how different energy scenarios affect air quality for each socio-economic class requires analysis at neighborhoods scales, which poses a major computational challenge for the chemical transport models CTMs) used in such studies. We start our analysis by using the source-oriented WRF/Chem (SOWC) model at 250m, 1km, 4km, and 12km spatial resolution to analyze air quality and EJ in California during the year 2016. Exposure to PM0.1 and PM2.5 concentrations is estimated for different socio-economic classes based on income and race-ethnicity. The model spatial resolution needed to bring EJ issues into focus at the smallest computational cost is identified. The modeling system is then used to study EJ in the year 2050 under two different energy scenarios to achieve GHG reductions: (i) a Business as Usual (BAU) scenario and (ii) a low-carbon GHG-Step scenario. Future year 2050 air quality simulations were carried out for 32 randomly-selected weeks between 2046-2055 (to account for effects of medium-term meteorological cycles such as ENSO). Population exposure to PM2.5, PM0.1 total mass, primary PM was then estimated for different socio-economic classes under the BAU and GHG-Step scenarios. The results from this study identify the optimal spatial resolution needed for EJ analysis in California, and compare the benefits of future BAU and GHG-Step energy scenarios across socio-economic classes.

6ID.1

Fluid Mechanics and Droplet Transport from the Production of Unvoiced Fricatives. TANVIR AHMED, Andrea Ferro, Amir A. Mofakham, Brian T. Helenbrook, Goodarz Ahmadi, Deborah M. Brown, Byron D. Erath, *Clarkson University*

The COVID-19 pandemic has highlighted the importance of airborne droplet transport as an efficient vector for virus transmission. Recent work has identified how human speech produces droplet size distributions that are remarkably similar to coughing, and which are capable of staying suspended in aerosol form for long periods of time, thereby increasing infection risk. Missing, however, is a description of how these droplets are transported from the mouth exit, into the ambient environment. Although the time-averaged velocity at the exit of the mouth has been quantified for various English phrases, this prior work does not provide the temporal resolution that is needed to fully elucidate the highly transitory, unsteady fluid mechanics that are produced during human speech. This work identifies how specific utterances of speech (e.g., phones) are capable of producing unique fluid mechanics that are effective at transporting expirated droplets over distances that are longer than previous time-averaged measures have identified. Emphasis is placed on investigating the phones [*f*] and [ϑ], which are produced by the consonant production at the end of words such as “huff”, and “with”, respectively. These unvoiced fricatives are shown to produce a transient, high velocity jet of air at the mouth exit, due to the narrow constriction that is formed at the mouth during their pronunciation. The quantity and size distribution of human droplet production for these consonants are quantified and reported based on measurements using an aerodynamic particle sizer. Particle image velocimetry (PIV) of the velocity field at the exit of the mouth is also acquired from human intonations, as well as in physical models, to quantify the resultant jet momentum, elucidating how these transient speech behaviors entrain and advect droplets into the surroundings. These results are necessary for predicting infection risk from airborne viruses as a function of speaker distance.

6ID.2

Making Music: Aerosols, Droplets and the Risks of SARS-CoV-2 Transmission. JONATHAN P. REID, Florence Gregson, Bryan R. Bzdek, Declan Costello, Natalie Watson, Christopher Orton, Pallav Shah, James Calder, *University of Bristol*

Abruptly in late March 2020, live musical performances and rehearsals were suspended in the UK after the emergence of the COVID-19 pandemic, threatening the livelihoods of many musicians and the viability of established institutions. During the easing of restrictions imposed during lockdown, the implications of relaxing the restrictions on rehearsals and live musical performances involving singing, and brass and woodwind instruments were widely debated. These concerns focused on the potential of spreading the SARS-CoV-2 virus through droplet and aerosol transmission, with numerous cases of transmission widely reported in choirs. Despite these concerns, very little information was available about the aerosol and droplet concentrations generated by singing and musical instruments. The correlation between the loudness of speech and the number of generated respirable particles and droplets, spanning a continuum in size from 100s nanometres to 100s of micrometres, had been reported previously. However, expiratory events such as speaking, coughing and sneezing, generate very small number of aerosol particles and droplets, so few that they are normally unmeasurable against a much larger background concentration. Benefiting from access to the extremely clean environment of an orthopaedic operating theatre in a hospital, with a background particle concentration of 0 cm^{-3} for particles larger than 300 nm in size, we will report measurements of aerosol particle and droplet concentrations generated by singers, and woodwind and brass instrument musicians. Measurements were undertaken with over forty professional performers from the Royal Opera House and the BBC Chorus. Uniquely, we will report measurements of the size distributions and distance dependencies from singing and instruments, measured synchronously by up to three aerodynamic particle sizers and two optical particle sizers, probing the dispersion of the aerosol jet. We will reflect the policy implications of this work for the reopening of the performing arts.

6ID.3

Aerosol Generation and Transmission from Performing Singing and Wind Instruments. JUN WANG, Tiina Reponen, Sergey A. Grinshpun, John Singletary, Michael Yermakov, *University of Cincinnati*

During the COVID-19 pandemic, concerns were raised with potential airborne virus transmission during musical performances, particularly during singing and playing wind instruments. Past studies suggest aerosol emissions from singing with magnitudes varying by person and vocal pitches. Aerosol emissions from wind instruments remain unclear. The objective of this study is to examine the spatial and temporal changes of aerosol concentration in a musical performing environment when singing and wind instruments are involved. College-Conservatory of Music (CCM) at University of Cincinnati hosts various music education programs, where the lecturer and students have to be face-to-face in a teaching room. Four condensation particle counters were strategically placed throughout the teaching room. Besides singing, six instruments (trumpet, trombone, horn, clarinet, saxophone, and flute) were performed by professionals at CCM. Two types of tests were conducted for each instrument: 10 minutes of playing; 10 minutes of combined playing and talking to mimic the teaching session. The results showed singing elevated aerosol concentration as high as 3.9×10^{3} cm^{-3} at the performing point, more than three times of the background (1.2×10^{3} cm^{-3}). Most instruments acted as an interceptor of aerosols, with aerosols presumably impacted in the complex airway inside the instrument. Some instruments, such as flute, which leaks air by design, contributed to aerosol emission, but not as much as singing and talking. Particle concentrations away from the performing point stayed relatively the same during the test, while aerosol concentration at performing point reduced quickly after the test with adequate ventilation (around 12 air changes per hour). Future studies include measuring aerosol emissions in a controlled low-background chamber so instrument differences will be easier to detect, as well investigations a larger setting such as an orchestra hall. The results will be used to devise corresponding administrative strategies and control techniques at performance sites.

6IM.1

Operation of a Condensation Particle Counter under the Low-pressure Condition. FAN MEI, Maynard Havlicek, Mikhail Pekour, Andrea Tiwari, Jason Tomlinson, Beat Schmid, Oliver F. Bischof, Patrick Roth, *Pacific Northwest National Laboratory*

Given that the aerosol population is heterogeneous in the vertical and horizontal dimension, detailed time and space-resolved measurements are needed to characterize aerosol properties adequately. Traditionally, condensation particle counters (CPC) have been used to measure the aerosol particle number concentration. In this study, the counting efficiency of a TSI 3789 CPC operated with water as working fluid was assessed in the pressure range of 100-1000 hPa. This study will also explore the counting efficiency dependence on the aerosol composition. Additionally, the counting efficiency under different operating temperatures will also be investigated. The main goal of our study is to determine the operational envelope of the CPC for in-situ airborne measurements.

6IM.2

Modification of a Water-based Condensation Particle Counter to Rapidly Measure Sub 3 Nanometer Atmospheric Clusters through Pulse Height Analysis: Laboratory and Field Measurements. CHONGAI KUANG, Darielle Dexheimer, *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 using new working fluids and modified 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 and properties. To address this measurement need, a light-weight, compact, and battery-operated commercial water-based CPC 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. Vertically-resolved nanoparticle measurements obtained from deploying the modified water CPC on a tethered balloon system will be also be presented.

6IM.3

A Mobility Particle Size Spectrometer to Access the 1nm Particle Size Range: The PSMPS. GERHARD STEINER, Joonas Vanhanen, Joonas Enroth, Lothar Keck, Minna Väkevä, *Grimm Aerosol Technik Ainring*

Here, we present the final, commercially available, version of a mobility particle size spectrometer that is able to access the 1 nm particle size range for ambient atmospheric measurements. The instrument originates from a collaboration of Grimm Aerosol Technik, Germany and Airmodus Ltd, Finland, combining a Grimm SMPS+C system with the Airmodus Particle Size Magnifier (PSM). Accordingly, it is named: PSMPS. The main system components are: a modified version of the short Grimm Differential Mobility Analyzer (Grimm S-DMA), the diethylene glycol-based PSM (Airmodus A10) and the new butanol-based CPC (Grimm 5417). The modified S-DMA is specially optimized for the transmission of small ions. Typically, it is 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 1.1-55.7 nm. The PSM is used to lower the detection efficiency of the Grimm CPC below 2 nm in electrical mobility equivalent diameter. The new Grimm 5417 CPC is an upgraded version of the well-known 5416 CPC, that features two switchable aerosol sample flow rates of 0.3 and 0.6 L/min and also supplies the S-DMA with sheath airflow rates of either 3.0 or 10.0 L/min. The overall system performance was tested in a multitude of laboratory experiments, determining various size dependent parameters like: DMA’s transfer function, DMA penetration efficiency, PSM and CPC counting efficiency. With the knowledge of these parameters, we are able to define a well-known overall system performance. In this presentation, we will introduce the features and performance of the PSMPS system and will highlight some laboratory and ambient aerosol number size distribution measurements.

7AC.1

The Role of Hydrates, Competing Chemical Constituents, and Surface Composition on ClNO2 Formation. HALEY ROYER, Dhruv Mitroo, Sarah Hayes, Savannah Haas, Kerri Pratt, Patricia Blackwelder, Thomas Gill, Cassandra Gaston, *University of Miami*

Atomic chlorine (Cl*) is a potent oxidizer that can affect air quality. A common source of Cl* is nitryl chloride ($ClNO_2$) that forms when chloride-containing aerosol reacts with dinitrogen pentoxide (N_2O_5). The formation of $ClNO_2$ presumably occurs only in urban coastal regions where both chloride (Cl^-) from sea spray aerosol and N_2O_5 from anthropogenic activity are abundant. However, recent research has shown that $ClNO_2$ formation also occurs inland, for example when N_2O_5 reacts with Cl^- in saline lakebed (playa) dust. Recent research also has shown that current parameterizations poorly predict $ClNO_2$ formation based on Cl^- content from playa dust. To understand this phenomenon, we utilized Scanning Electron Microscopy with Energy Dispersive X-Ray Spectroscopy (SEM/EDS), X-Ray Diffraction (XRD), and Single Particle Aerosol Mass Spectrometry (SPAMS) to determine the chemical composition and mineralogy of playa dust from the southwest United States. SEM and SPAMS both revealed the presence of highly hygroscopic Cl-containing minerals (e.g. carnallite) which can deliquesce at low relative humidity (RH), thereby facilitating $ClNO_2$ formation at low RH. XRD revealed the presence of 10Å clay minerals (a mineral category including illite, muscovite, and bioite) in samples with high N_2O_5 uptakes but low $ClNO_2$ production, suggesting for the first time that clay minerals can outcompete Cl^- for N_2O_5. SPAMS analysis detected high levels of soil organic matter (SOM) in samples with high Cl^- content and low N_2O_5 uptake, suggesting that SOM inhibits N_2O_5 uptake . Finally, comparisons of $ClNO_2$ yields and Cl^- content from bulk and surface analytical techniques indicate that surface analytical techniques predict $ClNO_2$ formation better than bulk analytical techniques, implying that $ClNO_2$ formation occurs on the surface rather than in the bulk aerosol. Our results suggest that current parameterizations for $ClNO_2$ formation must be updated with the additional controlling factors found in this study.

7AC.2

Characterization of Particle Charge from Aerosol Generation Process: Investigations of Material Reactivity. ERIN M. DURKE, Monica McEntee, Meilu He, Suresh Dhaniyala, *US Army CCDC CBC*

Aerosols are one of the most important and significant surfaces in the atmosphere. They can influence weather, absorption and reflection of light, and reactivity of atmospheric constituents. A notable feature of aerosol particles is the presence of surface charge, a characteristic imparted via the aerosolization process. The existence of charge can complicate the interrogation of aerosol particles, therefore many researchers remove or neutralize aerosol particles before characterization. However, the charge is present in real world samples, and likely has an effect on the physical and chemical properties of an aerosolized material. In our studies, we aerosolized different materials in an attempt to characterize the charge imparted via the aerosolization process and determine what impact it has on the aerosolized materials' properties.

The metal oxides, TiO_2 and SiO_2, were aerosolized expulsively and then characterized, using several different techniques. Particle charge distribution measurements were conducted via the employment of a custom scanning mobility particle sizer. Determination of the degree of surface charging led to the use of non-traditional techniques to explore the impact of additional surface charge on the overall reactivity of the metal oxides, specifically TiO_2.

TiO_2 was aerosolized, again expulsively, onto a gold-coated tungsten mesh, which was then evaluated with transmission infrared spectroscopy in an ultra-high vacuum environment. The TiO_2 aerosols were exposed to O_2, H_2 and CO, respectively. Exposure to O_2 resulted in a decrease in the overall baseline of the aerosol spectrum, suggesting O_2 removed some of the surface charge imparted during aerosolization. Upon exposure to H_2, there was no observable rise in the baseline of the IR spectrum, as is typically seen for TiO_2, due to the population of electrons into the shallow trapped states and subsequent promotion of the electrons into the conduction band. This result suggests that the additional charge imparted via aerosolization fills the trapped states, therefore no rise is seen upon exposure to H_2. Dosing the TiO_2 aerosols with CO showed no adsorption of CO on the surface, even at lower temperatures (~100 K), indicating the additional charge on the aerosol surface prevents the CO molecules from adsorbing to the TiO_2 surface.

The TiO_2 was also exposed to methanol vapor. The reaction was performed on both aerosolized TiO_2 and unmodified TiO_2 powder. The results for the reaction with the aerosolized sample differ drastically from those recorded for the methanol exposed powder. The results observed for the exposure of aerosolized TiO_2 suggest that the additional charge imparted via aerosolization impacts the reaction with methanol, causing a divergence from the known, well-documented pathway.

Finally, a high-flow dual-channel Differential Mobility Analyzer (HDDMA) was employed to determine the particle charge distribution for the polydisperse TiO_2 samples. The HDDMA data indicates as many as 230 charges per particle for a 700 nm particle of TiO_2. Also of note is the polarity of the aerosol particles. The concentration of positively charged particles versus negatively charged particles appears to be dependent upon the material being aerosolized, as opposed to the generation process simply resulting in an even bipolar distribution.

7AC.3

Chemical and Microphysical Properties of Windblown Dust near an Actively Retreating Glacier in Yukon, Canada. PATRICK HAYES, James King, Colm Wickham, Marie-Pierre Bastien-Thibault, Malo Bernhard, Jill Bachelder, Kevin Wilkinson, Madjid Hadioui, *Universite de Montreal*

Airborne mineral dust 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 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 are performing a series of studies on the physico-chemical properties and emissions of mineral dust from a sub-Arctic proglacial dust source. Soil and aerosol samples (PM10, PM2.5, TSP and deposited mineral dust) were collected in May 2018 and May 2019 near the A'Ay Chu (Slims River), a site exhibiting 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 measured at more well-characterized, low-latitude dust sources. In addition, mineralogy and elemental composition of ambient PM10 were characterized; PM10 elemental composition was enriched in trace elements as compared to dust deposition, bulk soil samples, and the fine soil fractions (d<53 µm). This enrichment is even more pronounced in PM2.5 samples. Finally, through a comparison of the elemental composition of PM10, dust deposition, and both fine and bulk soil fractions, as well as of meteorological factors measured during our campaign, we propose that the primary mechanisms for dust emissions from the A'ay Chu Valley are the rupture of clay coatings on particles or the release of resident fine particulate matter. This field study highlights the need to include high-latitude mineral dust sources in climate and chemical transport models in order to correctly predict future climate feedbacks, for example, increases in atmospheric ice nuclei concentrations or the deposition of light absorbing mineral dust on snow and ice.

7CA.1

Efficient Nighttime SOA Formation from Mixed Biogenic and Anthropogenic Emissions. RAHUL ZAVERI, John Shilling, Jerome Fast, Stephen Springston, *Pacific Northwest National Laboratory*

Organic nitrates formed from nighttime reaction between anthropogenic nitrate radicals (NO3) and biogenic volatile organic compounds (BVOCs) are an important but highly uncertain source of secondary organic aerosol (SOA). Here we report on the enhanced nighttime biogenic SOA formation observed in a polluted residual layer over Sacramento, California, the morning of 15 June 2010 during the Carbonaceous Aerosols and Radiative Effects Study (CARES). Trajectory analysis showed that the residual layer air, containing trace amounts of isoprene and monoterpenes left over after nighttime oxidation, was influenced by the San Francisco Bay Area emissions the previous evening. The residual layer aerosol was also enriched in nitrate, with about 64% of it estimated to be in the form of organic nitrates. The nitrate:organic mass ratio of the SOA was about 0.47±0.044, which corresponds to the range typically found in isoprene mononitrates. Assuming the SOA was composed of organic mononitrates, its nominal molecular weight was estimated at 186±11 g mol^{-1}, consistent with the highly functionalized isoprene hydroxynitrates that have been observed in the particle phase in the southeast United States. Overall, our findings show that the efficiency of nighttime biogenic SOA formation, expressed as the change in organic aerosol mass relative to carbon monoxide (ΔOA/ΔCO), equals ~100 µg m^{-3} $ppmv^{-1}$ and is comparable to the range previously estimated for enhanced daytime SOA formation from mixed anthropogenic and biogenic emissions during CARES. Assuming the SOA was formed from isoprene oxidation by NO3, we estimated mass yields of up to 0.55, consistent with previous field estimates.

7CA.2

High Time-Resolution Measurement of Carbonaceous Aerosol in Central Los Angeles With New TC-BC Method. MARTIN RIGLER, Matic Ivančič, Gašper Lavrič, Sina Hasheminassab, Payam Pakbin, Tony Hansen, *Aerosol d.o.o.*

Measurements of carbonaceous aerosols are of vital importance for local, regional, and global air quality monitoring. Because of their diverse physical and chemical properties, they directly impact air quality, visibility, cloud nucleation and cloud optical properties, the planetary radiation balance, and public health. The amount of carbon found in carbonaceous aerosols is called total carbon (TC), which is commonly categorized into fractions of organic carbon (OC) and elemental carbon (EC). Particulate OC can be directly emitted to the atmosphere (i.e., primary OC) or can be formed in the atmosphere from gas-to-particle conversion of (semi)volatile organic compounds after oxidation and condensation/nucleation (i.e., secondary OC). The chemical and physical processes associated with secondary organic aerosols (SOA) formation are complex and, therefore, represents a major research challenge in atmospheric science. Highly time-resolved SOA measurement techniques are required to evaluate its impact on atmospheric processes, climate and human health (Hallquist et al., 2009).

Newly developed online TC-BC method (Rigler et al., 2019), which combines an optical method for measuring mass equivalent black carbon (eBC) by the AE33 Aethalometer (Drinovec et al., 2015; Hansen et al., 1984), and a thermal method for total carbon (TC) determination by the Total Carbon Analyzer TCA08 was used for this study. The TC-BC method determines equivalent organic carbon (eOC) fraction of carbonaceous aerosols defined as eOC = TC – eEC, where eEC = b·eBC is equivalent to elemental carbon and the determined proportionality parameter b is a slope of regression analysis between EC and eBC.

In collaboration with the South Coast Air Quality Management District, an air monitoring campaign was conducted at an air monitoring station in central Los Angeles from March 2018 to December 2019. In this study, TCA08 and AE33 were used on 1h time resolution. eOC and eEC results were compared to 24h filter-based carbon measurements (sampled every third day) and other PM and meteorological parameters. In this study the diurnal patterns for eEC and eOC concentrations are compared for different seasons. Both eEC and eOC exhibit considerable daily, monthly and seasonal variations. The effect of morning rush hour peak in eEC is particularly pronounced in colder months, when higher traffic density is coupled with shallower mixing height. During warmer months eOC concentrations exhibit mid-day peak, which is associated with generation of secondary OC through photochemical processes in the atmosphere. Less pronounced peak of eEC in the evening is mostly caused by evening rush hour and a lower mixing height.

7CA.3

Exploring the Regional-scale Atmospheric Fate and Transport of Per- and Polyfluoroalkyl Substances (PFAS).

EMMA D'AMBRO, Havala Pye, Chris Allen, Kevin Talgo, Lara Reynolds, Kathy Brehme, Robert Gilliam, Jesse Bash, Benjamin Murphy, *Environmental Protection Agency*

Per- and polyfluoroalkyl substances (PFAS) are a class of man-made compounds whose emissions to air may contribute, via transport and deposition, to concentrations in surface water, ground water, and private well water in the vicinity of large point sources. Air quality modeling techniques can be used to quantify air concentrations and deposition fluxes to help parse the role of exposure pathways such as direct inhalation and ingestion via contaminated water. We apply the Community Multiscale Air Quality model (CMAQ) version 5.3.1 to a case study in Eastern North Carolina to model the PFAS emissions and transport at fine scale (1 km) from the Chemours Inc. Fayetteville-Works. The 23 PFAS with the largest emissions by mass are identified and added explicitly to CMAQ, along with an aggregate “other PFAS” species to represent the balance of the emissions. An updated deposition parameterization (Surface Tiled Aerosol and Gaseous Exchange, STAGE) is utilized along with estimated chemical properties for each species to simulate the deposition flux to specific, sub-grid land surface types. Thus, the updated model (CMAQ-PFAS) captures the dynamic transformations and removal processes that affect the extent of atmospheric transport of PFAS. We evaluate model performance against deposition sampling and quantify the model uncertainty with these measurements. Different emissions scenarios and species lumping configurations are explored to bound the model behavior and determine the level of detail required to accurately model emissions from other facilities. Our results are an important step in understanding the behavior of significant PFAS emissions from a point source, and can be used to inform studies quantifying exposure and biological effects.

Disclaimer: The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA.

7CO.1

Size Dependence of Mass Absorption Cross-Section (MAC) in Aviation-Turbine-Engine Soot.

JOEL CORBIN, Gregory Smallwood, Mark Johnson, Fengshan Liu, Prem Lobo, *National Research Council Canada*

The mass absorption cross-section (MAC) is a key intensive property of soot or black carbon (BC). Most commonly, the MAC is used to transform light absorption measurements to equivalent black carbon mass (eBC) concentrations by assuming a reference MAC from literature. The reference MAC is defined implicitly when instruments are calibrated against a reference sample, as they are in the aviation community. If the MAC of a given sample is lower than the reference MAC, such instruments will report eBC concentrations that are biased low relative to other measurement techniques.

Although many combustion sources produce soot with an average MAC of 8.0 ± 0.7 m^2g^{-1}, previous laboratory work has reported that the MAC of mass-classified soot increased with single-particle mass. Here, we use a similar technique to show that MAC also varies with size for an aviation-turbine engine and for an Argonaut miniature inverted soot generator (MISG), but appears to reach a plateau for larger particles. The MAC values observed for the smallest particles (~0.5 fg or 40 nm) were 40% lower (MISG) and 20% lower (aviation turbine engine) than those of the largest particles (~1 fg or 100 nm). This range is similar to the 30% enhancement in MAC predicted for soot aggregates versus isolated spheres. Therefore, we propose that the observed size-dependence of MAC is related to the number of primary particles in the soot aggregates, in addition to other potential factors. These results imply that (i) regulation-compliant measurement systems may report 20% lower eBC mass for engines producing smaller particles and that (ii) laboratory inverted burners may continue to be a useful proxy for producing aircraft-turbine-like soot.

7CO.2

Examining Chemical Composition of Gas Turbine-Emitted Organic Aerosol using Positive Matrix Factorization (PMF).

LIAM SMITH, James Allan, Hugh Coe, Ernesto Reyes-Villegas, Mark Johnson, Andrew Crayford, Eliot Durand, Paul Williams, *University of Manchester*

The organic matrix of volatile particulate matter (vPM) emissions from gas turbine engines is poorly characterized, except for lubrication oil. In this presentation, the characteristics of non-refractory aerosol emitted from two relevant aeronautical sources are reported; a turboshaft helicopter engine and a developmental combustor rig. Positive Matrix Factorisation (PMF) analysis was applied on Aerosol Mass Spectrometer (AMS) Unit Mass Resolution (UMR) organic aerosol (OA) data to identify three chemical factors; one unburnt fuel factor (AlkOA; Alkane Organic Aerosol) and two factors formed through oxidative processes; Semi Volatile Oxygenated Organic Aerosol (SV-OOA) and Low Volatility Oxygenated Organic Aerosol (LV-OOA). The AlkOA factor correlated with incomplete combustion tracers (i.e Elemental Carbon (EC)). The SV-OOA factor correlated with AMS-detected sulphate and Sunset OCEC Analyser-detected total Organic Carbon (OC) and coincided with higher OC converted to CO_2 at lower temperatures in the OCEC Analyser. Conversely, the LV-OOA factor mass corresponded with higher percentages of OC converted to CO_2 at the highest temperature during the OCEC analysis protocol. Factors were found to be a strong function of operating condition. In addition, a variety of techniques were used toward isolation the presence of the presence lubrication oil from other OA factors present during the engine testing. Lubrication oil was concluded to be negligible or non-derivable in the sampled exhaust with four potential hypotheses will be presented.

7CO.3

An Overview of Smoke Detection and Spacecraft Fire Safety in Low Gravity. CLAIRE FORTENBERRY, Marit Meyer, David Urban, Daniel Dietrich, Gary Ruff, *Universities Space Research Association*

Spacecraft fires pose a major risk to human activity in space. Flames behave differently under low gravity conditions; for example, materials classified as non-flammable on Earth may exhibit different flammability limits in low gravity. Additionally, the lack of gravity in space challenges spacecraft smoke detection. In an indoor fire under normal gravity, buoyant smoke particles rise to form a layer at the ceiling, where commercial smoke detectors are typically placed. In low gravity, however, this stratification does not occur, and longer timescales are needed for smoke particles to reach sufficiently high concentrations to induce detector responses. Furthermore, suspended dust in low gravity can trigger false alarms because of long particle settling timescales, confounding detector placement within the spacecraft.

The next lunar landing is targeted for 2024 as the primary goal of NASA's Artemis program. Plans for a future long-term human presence on the moon motivate the need for improved smoke detection technology in low and partial gravity. In this presentation, we provide an overview of spacecraft fire safety and smoke detection studies to date, and we review current efforts to improve our understanding of smoke particle detection under low gravity conditions. Finally, we discuss anticipated challenges for ensuring fire safety in a future lunar habitat.

7DP.1

Thermodynamic Equations of State for the Dust Grain Using Langevin Dynamics Simulations. VIKRAM SURESH, Zhibo Liu, Ranganathan Gopalakrishnan, *The University of Memphis*

The complex plasma is modeled as an isotropic system of N charged grains (radius a_p and charge Z_p) interacting with each other through a screened Coulomb potential with a fixed Debye length λ_D in an isotropic periodic domain, without including a confining potential and the systematic drift of charged species. The equilibrium thermodynamic state is investigated using Langevin Dynamics simulations to capture the effect of grain-neutral gas interactions (parameterized by the grain Knudsen number $Kn \equiv \lambda_g/a_p$) across the various $\Gamma \equiv (Z_p^2 e^2/(4\pi\varepsilon_o n_p^{-1/3} k_b T_d))$, $\kappa = n_p^{-1/3}/\lambda_D$ -based electrostatic coupling regimes, where n_p is number concentration and T_d is the kinetic temperature of the grains. The Langevin-computed internal energy u_d, pressure p_d and $k_b T_d$ of the grain phase are parameterized as equations of state $\boldsymbol{f(u_d, p_d, k_b T_d)}$ and compared with experimental reports of dust kinetic temperature to refine the modeling assumptions. The non-trivial influence of grain-neutral gas interactions is discussed by calculating the pair correlation functions in the gas, liquid, and solid-like regimes of grain correlated behavior. A unified thermodynamic model will further the understanding of phase transitions and the transport properties of the dust phase across the entire **Γ, κ, Kn** regimes.

We thank The University of Memphis High Performance Computing Cluster for providing computational resources to carry out this research. Funding for this work was provided by DOE Office of Fusion Energy Sciences Award DE-SC0021146

7DP.2

The Addition of a Downstream DC Bias to an Atmospheric-pressure, Flow-through RF Plasma for Enhanced Charging of Aerosol Nanoparticles.

SUKRANT DHAWAN, Abhay Vidwans, Girish Sharma, Nabiel Abuyazid, R. Mohan Sankaran, Pratim Biswas, *Washington University in St Louis*

Electrostatic precipitators (ESPs) are widely employed in industry and indoor environments for the removal of aerosol particles. ESPs typically use a corona discharge to charge the particles and allow them to be removed by a DC electric field. However, corona discharges are weakly ionized plasmas with plasma densities of the order of 10^{14}-10^{16} #/m^3. In comparison, other types of atmospheric-pressure plasmas including radio frequency (RF) microplasmas are characterized by orders of magnitude higher plasma densities ~10^{20} #/m3. We have recently shown that high charging efficiencies (>90%) can be achieved by these plasmas for particles larger than 100 nm, while the charging efficiency of particles smaller than 100 nm was low. A two-stage charging mechanism based on a characteristic time scale analysis suggested that while particles were predominantly charged negatively in the plasma volume, the relatively faster rate of loss of the electrons in the spatial afterglow resulted in neutralization by positive ions.

Here, we present a new design concept for aerosol particle charging in atmospheric-pressure plasmas: a DC field downstream of the plasma volume in the spatial afterglow to potentially remove the positive ions and prevent neutralization of the particles. The overall charge fraction and polarity were measured as a function of particle diameter at different downstream DC voltages of a flow-through, RF atmospheric-pressure plasma. We find that when the magnitude of the applied DC voltage was higher than a critical value, the charge fraction of particles increased, and the charge polarity shifted from bipolar to unipolarly negative. The results were supported by analyzing the characteristic timescales for neutralization by and loss to the walls of positive ions in the spatial afterglow at different downstream DC voltages.

Reference:
[1] Sharma, G. et al (2020). J Phys D. 53(24), 245204.

7DP.3

Understanding the Depletion of Electron Density in Dusty Plasmas at Atmospheric Pressure.

NABIEL H ABUYAZID, Xiaoshuang Chen, Davide Mariotti, Paul D Maguire, Christopher J. Hogan, R Mohan Sankaran, *University of Illinois*

Dust formation in plasmas, once an undesired phenomenon, is now relatively well-established for the gas-phase synthesis of stabilizer-free, high-melting point nanoparticle materials including carbon and silicon.[1] These complex multiphase systems are characterized by two-way interactions between plasma species and the precursor vapor and nucleated particles. For example, it has been shown that nanoparticles preferentially obtain a negative charge because of the higher mobility of electrons as compared to ions, which leads to a decrease in the electron density and other effects on the plasma.[2] However, many of these studies have focused on low-pressure plasmas where the concentrations of nanoparticles and plasmas species as well as the nature of plasma-particle interactions may be very different from those at atmospheric pressure.

Here, we present a combined experimental and modeling study of nanoparticle-containing plasmas at atmospheric pressure. A tandem plasma system was set up consisting of a RF-powered plasma to nucleate and grow carbon nanoparticles from hexane vapor, and a second, identical plasma where the particles were introduced. On-line, non-contact diagnostics were applied to both plasmas including ion mobility spectrometry to measure particle size distributions, electrical conductivity to obtain electron density, and optical emission spectroscopy to obtain gas temperature, electron density, and electron temperature. A constant number Monte Carlo (CNMC) simulation was developed to predict nucleation and growth in the first plasma and particle charging in the second plasma. Nanoparticle formation was confirmed both experimentally by IMS measurements and by CNMC simulations in the first plasma. Electrical conductivity and spectroscopic measurements show that there is an observable electron depletion in the second plasma when the particle-laden flow from the first plasma is introduced. However, control experiments supported by simulations reveal that the main contribution to electron depletion is a molecular vapor species that is either unreacted precursor or a reaction byproduct. Based on these results, we present a unifying picture for particle charging in a plasma at different pressures that shows that at atmospheric pressure, in contrast to low pressure, the electron density in the plasma is too high relative to the particle concentration for the particles to have a significant impact.

[1] Kortshagen, Sankaran, Pereira et al., Chem. Rev. 2016
[2] Woodard, Shojaei, Berrospe-Rodriguez et al., J. Vac. Sci. Technol. A 2020

7ID.1

Multiscale Models for Aerosol Transmission of Highly Infectious SARS-CoV-2 Novel Coronavirus.

SUKRANT DHAWAN, Huang Zhang, Renhui Ruan, Pratim Biswas, *Washington University in St Louis*

The highly infectious SARS-CoV-2 novel coronavirus has resulted in a global pandemic. More than ten million people are already impacted, with infected numbers expected to go up. There is a lot of discussion underway with conflicting opinions examining the airborne nature of the SARS-CoV2 virus. Coughing, sneezing and even breathing emit respiratory droplets which can carry infectious particles. It is important to understand how exhaled particles move through air to susceptible person to get answers regarding airborne transmission of SARS-CoV-2. Surprisingly, important phenomena prevalent with respect to aerosols (suspended droplets) have not been considered in recent SARS-CoV-2 studies. There are many studies conducted on the airborne spread of viruses causing diseases such as SARS and measles, however there are very limited studies that couple the transport characteristics with the aerosol dynamics of the droplet.

In this study, a comprehensive model for simultaneous droplet evaporation and transport, due to diffusion, gravitational settling, and ambient air flow, is developed. The considerations for viral load in droplets and virus decay are accounted for in the model to determine the spatial and temporal concentration of viable virus exhaled by the infected individual. The exposure to viable virus and risk of infection is determined using respiratory deposition curves. The effect of the different parameters such as ambient air velocity, relative humidity, viral load is determined on the risk of exposure as the function of separation distance from the infected person.

The model is further evolved to study the risk of virus exposure in a ventilated classroom. The droplet dispersion in a ventilated classroom is simulated by CFD with a validated Eulerian-Eulerian method. The effect of humidity, room temperature, droplet size, separation, and layout of ventilation system on the droplet transportation and subsequent risk of exposure is studied.

7ID.2

SARS-CoV-2 Aerosol Transmission and Infection Risk Estimation of In-Person Lectures in a University Classroom. BO YANG, Khaled Hashad, K. Max Zhang, *Cornell University*

Many schools were closed due to the worldwide COVID-19 pandemic, which caused by the Coronavirus, SARS-Cov-2. Recent but limited studies showed that the virus can be transmitted by aerosol particles generated from human breath. A lot of interventions, such as social distancing, facial masks, and handwashing have been measured to slow down the transmissions. However, there is no direct measure to prevent aerosol transmission. The situation might become worse given many universities announced the in-person lectures will be resumed in the 2020 fall semester. Students, faculty, and staff are becoming vulnerable and the medical system is facing huge potential pressure. The goal of this study is to simulate the SARS-Cov-2 aerosol transmission in a typical university classroom, estimate the infection risk and propose potential interventions. Airflow pattern in a university classroom was analyzed using computational fluid dynamics (CFD) coupled with the aerosol dynamics. Aerosol particles generated from sneezing, coughing, talking, and breathing will be simulated with considering parameters including classroom occupancy, ventilation rate, temperature, humidity, with or without wearing masks, and infectious person number. The CFD and aerosol dynamics simulation results will be compared with the Fate and Transport of Indoor Microbiological Aerosols (FaTIMA) tool developed by the National Institute of Standards and Technology (NIST). The minimum ventilation rate and the maximum occupancy rate will be provided to keep students and faculty safe in the classroom.

7ID.3

Accurate Representations of the Microphysical Processes of Aerosols and Droplets from Exhalation Events and the Impact on the Sedimentation Distance. JIM WALKER, Justice Archer, Florence Gregson, Bryan R. Bzdek, Jonathan P. Reid, *University of Bristol*

The role of droplets and aerosols in the spread of respiratory viruses such as SARS-CoV-2 is well established, contaminating surfaces and sometimes leading even to an opportunistic airborne mode of transmission. Large droplets and small respiable aerosol particles span a continuum in size from 100s nanometres to 100s of micrometres, and are generated from coughs, sneezes, speaking and even breathing. On expiration, a competition between evaporation, sedimentation and forward momentum, governs the sedimentation of large droplets, while small aerosol particles remain airborne for many hours. We will report measurements of the hygroscopic response of surrogate respiratory fluids, including an examination of kinetically impaired moisture loss, crystallization, and the temperature dependence of evaporation rates. With these improved models of the aerosol microphysics, we then examine the impact on sedimentation distances using a model that captures the transport of the aerosol and droplets, including air buoyancy, and evaporative mass and heat transfer. We will report on the differences observed when accurately representing the kinetics of moisture content of the aerosols and droplets composed of respiratory fluids rather than their often used treatment as aqueous sodium chloride or water droplets. The impact of phase behaviour on drying kinetics will be reviewed along with the dramatic sensitivities to environmental relative humidity and temperature. Consequences for physical distancing guidelines will be considered.

7IM.1

Yearlong Performance of Six PM Air Sensor Models across Seven U.S. Sites. KAROLINE BARKJOHN, Cortina Johnson, Samuel Frederick, Robert Yaga, Brittany Thomas, William Schoppman, Andrea Clements, *ORISE fellow, U.S. EPA Office of Research and Development*

Particulate air sensor performance is often evaluated at a single site or in a single region over a time period from weeks to a few months. However, sensor performance is typically dependent on environmental conditions, pollutant concentrations, and particle properties. In addition, performance may change due to seasonal variations in particle properties, environmental conditions, and degradation of the sensor. To study these impacts on air sensor performance, five models of gas and particulate sensors, were set up in August 2019 for a yearlong study. An additional sensor type was deployed March 2020. Sensors were collocated alongside a Federal Equivalent Method Monitor for $PM_{2.5}$ at seven air monitoring stations throughout the United States and across climate regions. The sensor models were the Maxima from Applied Particle Technology, Clarity Node from Clarity Movement, PA-II-SD from PurpleAir, the AQY1 from Aeroqual, and the RAMP from SENSIT, with QuantAQ's ARISense sensor deployed at the later date. $PM_{2.5}$ sensors were evaluated for accuracy, precision, and the influences of environmental conditions, including temperature and relative humidity. Prior to deployment, sensors were evaluated and normalized based on a collocation period in Durham, North Carolina so that performance could be compared across sites independent of differences among sensors of the same type. Accuracy was evaluated monthly at each site so that comparisons could be made over time. Initial results suggest significant seasonal changes in performance, low precision between sensors of the same type for some sensor models, and large differences in sensor performance across sensor types. This work provides insights to improve sensor accuracy across optical PM sensors across the United States.

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.

7IM.2

Evaluation Methods for Low-Cost Particulate Matter Sensors in Rural Oklahoma. JEFF BEAN, *Phillips 66*

Understanding and improving the quality of low-cost sensor data is a crucial step before low-cost sensors can be used to fill gaps for air quality management. This study focused on methods for understanding and improving data quality for low-cost particulate matter sensors using the results of 10 months of side-by-side measurements between reference instruments and low-cost sensors in Bartlesville, Oklahoma. At this site in rural Oklahoma the instruments typically encountered only low (under 20 $\mu g/m^3$) concentrations of particulate matter, however higher concentrations (50-400 $\mu g/m^3$) were observed on three different days during what were likely agricultural burning events. The data offered insights on how averaging time, choice of reference instrument, and the observation of higher pollutant concentrations can impact performance indicators (R^2 and root mean square error) for a sensor evaluation. The influence of these factors on performance metrics should be considered when comparing one sensor to another or when determining whether a sensor can produce data that fits a specific need. Though R^2 and root mean square error remain the dominant metrics in sensor evaluations, an alternative approach using a prediction interval may offer more consistency between evaluations and a more direct interpretation of sensor data following an evaluation. Ongoing quality assurance for sensor data is needed to ensure data continues to meet expectations. Observations of trends in linear regression parameters and sensor bias were used to analyze calibration and other quality assurance techniques.

7IM.3

Identification of High-emitting Heavy-duty Diesel Trucks with Low-cost Sensors and the Plume Capture Method.

REBECCA SUGRUE, Chelsea V. Preble, Thomas W. Kirchstetter, *University of California, Berkeley*

The exhaust plume capture method used to characterize pollutant emissions from in-use heavy-duty diesel trucks can serve as a surveillance tool to remotely identify high emitting trucks that may warrant inspection and maintenance. Lower cost sensors offer an opportunity for wider deployment of this approach, but have not been well evaluated in this application. This study compares black carbon (BC) emission factors measured with multiple BC and carbon dioxide (CO_2) analyzers for thousands of trucks at the Port of Oakland. Though the distributions of emission factors were similar across different pairs of BC/CO_2 analyzers, the identification of high-emitting trucks varied and depended more on the BC than CO_2 analyzer performance. For example, 90% of the high emitters classified by the Magee Scientific AE33 and LI-COR LI-7000 were also identified by the AE33 and the lower cost PP Systems SBA-5. In contrast, the lower cost BC analyzers misclassified more than half of their high emitters compared to the AE33.

The plume capture method measures only a snapshot of a passing truck's emissions, which are transient in nature and depend on the prevailing driving conditions. An analysis of emission rates from trucks that were sampled more than once shows that a single low-emission instance does not guarantee that a truck is not occasionally high-emitting; conversely, a high-emitting truck may not always be highly polluting. Consequently, this method is unlikely to identify all high-emitting trucks with a single measurement, yet is unlikely to falsely identify a clean truck as a high emitter.

8AE.3

Correcting Biases in Speciated PM2.5 Simulations Using a Geographically Weighted Regression. CARLOS HERNANDEZ, Ksakousti Skyllakou, Pablo Garcia, Brian Dinkelacker, Spyros Pandis, Allen Robinson, Peter Adams, *Carnegie Mellon University*

The ability to provide speciated and source-resolved $PM_{2.5}$ estimates make chemical transport models an alluring alternative, or complement, to empirical models for exposure assessments. Correcting characteristic biases in simulated $PM_{2.5}$ could encourage the adoption of chemical transport models in this area. We use geographically weighted regression, similar to van Donkelaar et al. [Environ. Sci. Technol., 2015, 49, 17, 10482-10491], to predict the bias between speciated $PM_{2.5}$ simulations and observations in the continental U.S. The regression model is trained by comparing simulated annual averages of NH_4, NO_3, SO_4, EC and OA in 2010 and 2001 to corresponding observations from the CSN and IMPROVE networks. Biases for speciated $PM_{2.5}$ simulations are predicted at U.S. census tract geographies. Corrected simulations are then aggregated to population-weighted averages for metropolitan statistical areas (MSAs). Correlations between MSA-level simulated total $PM_{2.5}$ and empirical estimates [Kim et al. PLOS ONE. 2020, 15, 2, e0228535] improve from 0.70 to 0.89 in 2010, and from 0.62 to 0.90 in 2001. On average, errors in fractional composition between speciated monitors and simulations were reduced by 40% in 2010, and 50% in 2001. A leave-one-out cross-validation shows a reduction of biases across all simulated components at speciated monitors. For OA and NO_3, normalized mean biases ranged from -20% to -35% before correction, and 0% to 3% after correction. For EC, normalized mean biases ranged from -10% to 25% before correction, and 2% to 5% after correction. For SO_4 and NH_4, normalized mean biases ranged from 3% to 10% before correction, and -2% to 1% after correction. Results from a ten-fold cross-validation are consistent with those from the leave-one-out cross-validation.

8AE.4

Exposure to Marijuana and e-Cigarette Aerosol in a Home. LANCE WALLACE, *US EPA (retired)*

Vaping, either marijuana or e-cigarettes, is rapidly growing in popularity worldwide. Secondhand exposure to the aerosols from vaping was studied for more than a year in an experimental room within a home. Research-grade monitors such as the SidePak (TSI Inc) and the Piezobalance (Kanomax) were employed together with a low-cost monitor (PurpleAir) to estimate the emission rates and decay rates of the aerosol.

Seven e-cigarette fluids ranging from 0-100% "VG" (vegetable glycerin) and "PG" (propylene glycol) were heated using a vaping pen and exhaled by a human vaper. Peak PM2.5 concentrations were high (1 mg/m3), but decay rates were extremely high and increased with time. About 88% of the exhaled aerosol was volatile and evaporated over a short time, so secondhand exposure was negligible. The Piezobalance recorded both the high initial concentration and over the next few hours also recorded the loss of particles from the crystal’s surface, a unique capability of this instrument.

Marijuana fluids ranging from 2:1 to 8:1 CBD/THC were heated in an electronic vaping pen either for 6 or 15 seconds producing PM2.5 emission rates of about 2.5 and 6.5 mg/puff, respectively. Peak concentrations were again high, volatility was low, and secondhand exposures were thus extensive. The decays were relatively slower compared to e-cigarettes.

The low-cost PurpleAir monitor performed well in relation to the research-grade monitors. An alternative method of calculating PM2.5 from the PurpleAir raw data performed better (higher precision, lower limit of detection) than the PM2.5 estimates provided by PurpleAir.

8AE.5

Optical Trapping-Raman Spectroscopy for Detection of Chemical and Biological Agents in Air. CHUJI WANG, Yukai Ai, Haifa Alali, Gorden Videen, Yong-Le Pan, *Mississippi State University*

Chemical and biological agents (CBAs) and other aerosolized infectious disease are a significant threat to humans, animals, and the environment. Detection, characterization, and identification of aerosolized CBAs in air in low density is a persistent challenge. For a given dangerous and or highly infectious CBA or disease such as the COVID-19 virus, the detection methods which typically depend on hands-on sampling are impractical in reality; thus highly sensitive, chemically selective, and hands-free sampling and detection techniques are needed. We report on an exploratory study on characterization and identification of aerosolized CBA simulants based on the newly developed optical trapping - Raman spectroscopy (OT-RS) technique. OT enables the capture of single aerosolized CBA or simulant particles in air for several minutes or longer, and RS detects and identifies chemical compositions based on molecular fingerprints. The OT-RS also minimizes potential interference from the background. Simultaneously, an integrated imaging system can monitor the single trapped CBA particle in real-time. Results from four surrogates: Bacillus globigii (BG), Yersinia rhodei, MS 2, and Bacillus subtilis (BS), are presented. We show that the four CBA surrogates can be well - classified by using the principle component analysis (PCA) method. The results demonstrate that the OT-RS system can be used for potential detection of aerosolized CBAs in air.

8AE.6

Statistical Analysis and Geospatial Exposure Model of Air Pollution Derived from Brake and Tire Wear. JONATHAN LIU, Irish Del Rosario, Michael Jerrett, Jonah Lipsitt, Farzan Oroumiyeh, Suzanne E. Paulson, Beate Ritz, Yifang Zhu, *University of California, Los Angeles*

In the realm of air pollution, due to regulations and technological advancements reducing tailpipe emissions, there is an increased focus on non-exhaust automobile emissions, consisting of particulate matter which contain heavy metals capable of oxidative stress. The following reports statistical and geospatial analyses on a dataset generated from two sampling campaigns across 51 different sites in southern California.

Data analyzed include particulate matter and speciated metals data from gravimetric samplers, time-series data from low-cost Purple Air sensors, and filter-based passive NO2 samplers from OGAWA USA. Through a review of prior literature, we identified a priori 31 primary and secondary tracers of brake wear, tire wear, tailpipe emissions, and dust and soil particulates.

Primary statistical analysis reveals a high level of correlation between tracers of automobile activity (Pearson R2 ranging from 0.71 to 0.95 in the fine fraction, 0.70 to 0.96 in the coarse fraction) not found between automobile activity and tracers of dust and soil particulates in both fine and coarse fractions. Similarly, dust and soil tracers are extremely positively correlated with one another (Pearson R2 > 0.8). We also found that levels of correlation between NO2, a gas phase pollutant typically used as a marker for vehicle activity, and tracers of brake wear, tire wear, and tailpipe emissions exceeded that between NO2 and dust and soil particulates.

Incorporating data on intersection density, car traffic intensity, truck traffic intensity, slope semivariance, we have generated an exposure surface of brake and tire wear generated co-kriging within a Bayesian hierarchical framework. Moving forward, our exposure surface will be used within existing epidemiological cohort data and government birth records to better understand the relationship between heavy metals in air pollution and negative health outcomes.

8AE.7

Assessing the Impact of Urban Transformations on Exposure to Air Pollutants in the City of Bogotá: Cable Car implementation and Renewal of the BRT System Fleet. DANIELA MENDEZ, Ricardo Morales Betancourt, Olga Lucia Sarmiento, Juan Manuel Rincón, Boris Galvis, *Universidad de los Andes*

Assessing personal exposure to air pollutants in large cities is particularly relevant as commuters are often exposed to higher aerosol particle concentrations than those reported by central monitoring sites. In this work, we analyzed the potential impacts on personal exposure of two urban transformations that took place in Bogota, Colombia, between 2018-2019. A cable car system was built to connect peripheral neighborhoods to the bus rapid transport-system (BRT). Simultaneously, a new bus fleet replaced almost 1400 18-year-old diesel buses with a mix of CNG and DPF equipped EURO-V diesel buses. For this, 136 personal exposure measurements spanning 408 hours were carried out. The measurements were performed before and after the intervention for both, the cable car system, and the completion of the BRT renewal process. A 50% decrease in the concentration of $PM_{2.5}$, eBC and CO was observed after the fleet renewal process, each species decreasing from 176 to 92 $\mu g/m^3$, from 90 to 45 $\mu g/m^3$ and from 4.8 to 3.3 ppm, respectively. Commuters in the BRT system were exposed to much higher concentrations when riding vehicles with more than 682 thousand vehicle kilometers traveled. In the cable car implementation, significant differences (p-value <0.05) among concentration in the different transport modes analyzed were observed, with those of the cable cabins being the lowest. When carrying out a classification analysis through binary trees, it was observed that BC exposure for commuter that were walking or inside the cable car cabins were exposed to the lowest concentrations (11.1 $\mu g/m^3$). On the other hand, commuters in another motorized transport mode were exposed to higher concentrations (30.9 $\mu g/m^3$). This work demonstrated the substantial reductions achieved when implementing urban interventions that involve cleaner transportation modes, can be used as input for decision-makers.

8AE.8

Cooking Fuel Transitions in Rwanda and Impacts on Exposure to Particulate Matter (PM2.5). CHERYL WEYANT, Joseph Pedit, Ashley Bittner, Leena Nylander-French, Sudhanshu Handa, Karin Yeatts, Zoe Frolking, Pamela Jagger, *University of North Carolina*

Exposure to pollutants from household cooking with solid fuels is a major cause of illness and mortality in the Global South. At the same time, many households are transitioning away from these fuels and adopting clean fuels, such and LPG, electricity, or pellets. However, these transitions are rarely closely observed outside of a trial or intervention. Here, a four-panel study, where households were surveyed over five years, was designed to study adoption of pellet stoves, but also captured unexpected observations of a rapid uptake of clean fuels, mostly LPG. In 2015, the first year of the panel, 8% of households used clean fuels (as primary, secondary, or tertiary fuels), and by 2019 41% were using a clean fuel. These households represent early stage adopters and measurements of their 24-hr exposure to $PM_{2.5}$ (N = 658) and CO (N = 2,777) capture an important aspect of this transition and may help predict the impacts of ongoing fuel transitions, globally. We observe significant differences in exposure to $PM_{2.5}$ and CO, depending on the primary fuel used for cooking, and also find an exposure trend that matches the “energy ladder” when accounting for multiple fuels. For example, households that used both LPG and charcoal were exposed to $50 \mu g m^{-3}$ less $PM_{2.5}$ per day compared to pure charcoal users (p = 0.008) and exposure by pure LPG users was even lower by $15 \mu g m^{-3}$. We also observed that the adoption trends are dynamic; some households adopted a clean fuel for a short time, then switched back to solid fuels as their primary stove. However, most kept their clean fuel stove in the household and would use it as a secondary or occasional stove. This has exposure and health implications that may not be apparent when only considering primary fuel.

8AE.9

Characterization of Airborne Nanoparticulate Matter in Semiconductor Manufacturing Environments. ZHAOBO ZHANG, Pierre Herckes, Paul Westerhoff, *Arizona State University*

Occupational exposure to airborne nanoparticles in semiconductor fabrication facilities is of emerging concern and has only recently been addressed in a few studies. To date, there is limited information on the airborne concentrations, the source or the physical and chemical properties of nanoparticles in these environments and potential worker exposure.

We will present initial findings from observations in a research and a pilot plant manufacturing facility. Filter samples were collected for offline analysis using Transmission Electron Microscopy and Inductively Coupled Plasma Mass Spectrometry, to determine the size, shape, and elemental concentration of collected nanoparticles. A Scanning Mobility Particle Sizer was used to monitor size resolved airborne nanoparticle concentrations during routine tool operations and maintenance activities. The results show low but measurable concentrations of nanosized particles in the clean rooms investigated during normal operations. Select maintenance operations, particularly on plasma-enhanced chemical vapor deposition tools, let to substantial particle concentrations (1000s /cc), most in the sub 20nm range. The particles appear to mainly be silicate although nanoparticulate metallic particles were also observed during the studies. A complete discussion of these results will be provided.

8BA.3

Taxonomic Characterization and Quantification of Personal Bioaerosol Exposures using Five Different Personal Samplers. NIRMALA THOMAS MYERS, Taewon Han, Hyeon-Ju Oh, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

A study comparing a newly-developed Personal Electrostatic Bioaerosol Sampler (PEBS; developed at Rutgers University) and four existing personal aerosol and bioaerosol samplers - CIP 10-M sampler, Ultrasonic Personal Aerosol Sampler, NIOSH Personal Bioaerosol Cyclone Sampler 251, and Button Aerosol Sampler - was conducted to estimate personal bioaerosol exposures at three different sites for long-term sampling (up to 4 hours): a horse barn, outdoors, and a greenhouse on Rutgers campus. These locations had different wind speeds, temperature, relative humidity, and local microenvironments. Two sets of these five samplers were placed on chests of two mannequins to represent sampling in an individual’s breathing zone, and a total of 96 samples were collected. Samples were then forwarded to an external laboratory for extraction of genomic DNA, sequencing of the rRNA genes for bacteria (16s) and fungi (ITS), and quantitative polymerase chain reaction (qPCR) analysis. Total DNA concentration estimate by qPCR analysis was performed using the SYBR Green ROX Mix (ThermoScientific) in a StepOnePlus Real-Time PCR System (Applied Biosystems Inc.).

The five samplers measured total DNA concentrations ranging from 10^2 to 10^5 copies/m^3. Linear regression models of total DNA concentrations stratified by locations indicated that the five samplers measured similar concentrations of bacteria ($p = 0.782$) and fungi ($p = 0.648$). The bacterial and fungal diversity differed by location and personal sampler ($p<0.05$). A total of 428 bacterial genera were identified by 16s sequencing, including *Pseudomonas*, *Acinetobacter*, and *Bacillus*. ITS sequencing detected 43 fungal genera with higher frequencies of *Epicoccum*, *Cladosporium*, and *Aspergillus*. In conclusion, we found that bioaerosol exposures in terms of microorganism taxonomy and quantification differed by choice of a personal bioaerosol sampler and sampled microenvironments. These findings would be very useful when choosing tools for personal bioaerosol exposure assessments in various occupational environments.

8BA.4

Investigating Seasonal Effects on the Spread of Antibiotic Resistant Bacteria in Dairy Farms using Computational Fluid Dynamics.

HYOUNGMOOK PAK, Maria King, *Texas A&M University*

Dairy farms are well known to harbor various bacteria species that could be pathogenic or resistant to antibiotics. Especially in a free stall dairy farm, these bacteria can disseminate into the open environment, causing nearby animals and people to be exposed to severe health risks. This study aimed to investigate the effects of seasonal factors on the development and spread of antibiotic resistant bacteria (ARB) in a dairy farm. Computational fluid dynamics (CFD) was utilized to assemble an airflow model and experimental air velocity measurements were taken and used for validation.

Two sampling campaigns at different seasons were taken to a dairy farm, which had about 400 cows and 36 axial fans, to measure air velocities and collect aerosolized bacteria at various locations. ANSYS was used to model the turbulent airflow patterns and experimental air velocity measurements were used to validate the CFD model. The airflow models at different seasons closely resembled their respective experimental results. Kirby-Bauer test revealed that bacteria on the southern side of the farm were most resistant to antibiotics, such as ampicillin, cephalothin, and tetracycline. Microbiome analysis was performed on the extracted bacterial DNA to determine which bacteria genus and species were present and carried antibiotic resistant genes. Seasonal factors, such as temperature and relative humidity, were observed to be triggering antibiotic resistant in aerosolized bacteria. On days of sampling, a southerly wind and wind generated by fans were shown to reintroduce certain ARB species back into the dairy farm. Principal coordinate analysis revealed that each seasonal factor had a significant and distinct effect on how ARB were being developed and disseminated in the dairy farm.

8BA.5

Design of an Electrical Gelation Chamber to Synthesize Alginate Microparticles for Inhalational Delivery of Anti-tubercular Drug.

CHETHANI ATHUKORALA, Hema Ravindran, Shantanu Sur, Suresh Dhaniyala, *Clarkson University*

Inhalational delivery of antitubercular drugs using polymeric carrier particles is emerging as an attractive therapeutic option for pulmonary tuberculosis (TB). For such approach to be successful, the size of the particles needs to be optimized for their delivery to the lung alveoli and enhanced uptake by macrophages, where TB bacteria reside. Previous reports suggest nebulized particles in the size range of 500-700 nm are most effective in reaching the alveolar region. The objective of the present work is to synthesize alginate microspheres within a narrow size range and relevant for pulmonary drug delivery application using a custom-designed electrical gelation chamber. Aerosols of alginate were first generated by atomization, which were collected in a chamber under electrostatic precipitation, and cross-linked to gel by exposure to $CaCl_2$ solution. The chamber was designed to collect alginate aerosols of <1 µm in size under an electric field of 5 kV/cm. Flow behavior and collection of alginate aerosols in the chamber was estimated by CFD simulations and its design was optimized for improved collection efficiency. The collection efficiency of the gelation chamber was examined as a function of the electric field and ionization of alginate aerosols. We achieved a collection efficiency of >90 % for aerosol of size <1 µm as estimated by APS measurements. Collected particles were further characterized by microscopy and dynamic light scattering experiments. We will present the design and performance details of the gelation chamber from our ongoing work.

8BA.6

Microorganism in Atmospheric Water and How They Drive Formaldehyde Transformation.

THUONG CAO, Pierre Herckes, Ferran Garcia-Pichel, *Arizona State University*

Research on the microorganism-mediated conversion of organic compounds in atmospheric water (clouds and fogs) has recently emerged in the bioaerosol community. Most existing work focused on observations in pristine environments (mainly Puy de Dôme, France) and few observations exist on microorganisms and bacterial biotransformation in more polluted environments such as urban fogs. In this study, bacterial strains isolated from samples collected in Bakersfield (California, USA) were used to investigate the biodegradation rate of formaldehyde. The initial results showed that the biodegradation of formaldehyde occurred at both 4 °C and 17 °C and ranges from 10^{-21} to 10^{-19} mol $cell^{-1}$ s^{-1}. These observations are consistent with the rate reported in Puy de Dôme clouds, implying that the redox reaction rate of formaldehyde promoted by microorganisms in atmospheric water does not depend strongly on sample locations. Moreover, the bacterial community composition was identified by 16S rRNA sequencing, and Proteobacteria (Alpha-, Beta- and Gamma-), Firmicutes, and Actinobacteria largely dominated in our samples. Although there are differences in the population, the presence of microorganisms in both Bakersfield (US) and Puy de Dôme (France) suggests the global occurrence of these species.

8BA.7

Compressible Flow-based Virtual Impactor towards Bioaerosol Sampling.

MYEONG-WOO KIM, Jaesung Jang, *Ulsan National Institute of Science and Technology, Korea*

Airborne viruses and bacteria cause allergies and infectious diseases, and their sampling with high concentration and safe capture is an important issue for their rapid measurements. One way to concentrate airborne biological particles coming into the sampler is to pass them through a virtual impactor. Although it is a well-known device, most studies have been focused on one with micrometre-sized cut-off diameter. Only few studies have dealt with virtual impactors with submicron cut-off diameters (Sioutas et al, 1994; Lee et al, 2002).

In this study, we present a virtual impactor with 0.45 µm cut-off diameters for 12 litres per minutes (LPM) using computer (FLUENT 18.2) simulation and experiments. The nozzle diameter (D_n) of the virtual impactor was computed using the Stokes number at the minor to total flow rate ratio of 0.1 and the Stokes number of ~0.4 (Marple and Chien, 1980). Another important parameters are the collection probe diameter (D_c), the distance from the collection probe to the nozzle (S), and collection probe angle (Θ_c). Computer simulation was performed at the following conditions: $D_C = 1.0\text{-}1.8{*}D_n$, $S= 1.2\text{-}2.0{*}D_n$, and Θ_c= 5-30°. We observed from the simulation and experiments that the cut-off diameter was around 0.4-0.55 µm, and the separation efficiency reached more than 98% at the particle size larger than 1 µm. The separation efficiency depended on the ratio of D_c/D_n, and its slope decreased with increasing ratio of D_c/D_n. The virtual impactor showed the highest collection efficiency at $D_c/D_n = 1.4$, and the collection efficiency depended on the collection probe angle. The experimental results for the virtual impactor showed similar value with simulation results. The optimized collection efficiency showed more than 78.4% at particle size larger than 1µm. This will be used for bioaerosol samplers with high collection efficiency and high concentration for high throughput.

This work was supported by the National Research Foundation of Korea(NRF) grant (2020R1A2C1011583), by the ITRC(Information Technology Research Center) support program (IITP-2020-2017-0-01635) supervised by the IITP (Institute for Information & communications Technology Promotion), by Basic Science Research Program through the NRF funded by the Ministry of Education(2020R1A6A1A03040570), and the Institute of Civil Military Technology Cooperation funded by Defence Acquisition Program Administration and Ministry of Trade Industry and Energy of Korean government (UM19402RD4).

8BA.8

Environmental Effects Triggering Antibiotic Resistance in Bacteria. BROOKE SMITH, Maria King, *Texas A&M University*

The world is currently in an antibiotic crisis due to the development of antibiotic resistance in bacteria. Antibiotic resistance poses a threat in many institutions such as hospitals, meat processing units and other agricultural and occupational entities. This study focuses on the environmental factors that may cause Escherichia coli (E. coli) MG 1655 to express antibiotic resistance genes (ARGs). These conditions include temperature, relative humidity, the absence or presence of light, airflow and duration of aerosolization. The fresh mid-log phase bacterial suspensions were aerosolized by the 6-jet Collison atomizer for 5, 10, 15, 30 and 45 minute periods into a 27 L sterile box at constant airflow of 80 L/min and collected using the 100 L/min wetted wall cyclone bioaerosol collector that maintains the culturability of the bacteria. Each sample was analyzed and compared based its response to each environmental factor by susceptibility testing and polymerase chain reaction using specific primers to target different ARGs (marR, rfaC, katE). The goal of this research is to uncover how bacteria react to certain environmental conditions, and delineate the factors that may trigger resistance. The Kirby Bauer susceptibility test results indicated the strongest resistant response to ampicillin, cephalothin, and gentamicin, which are cell wall or protein synthesis inhibitors. More resistance was detected in E. coli aerosolized for 5 minutes versus 45 minutes, but a similar number of resistant E. coli was found in the 15 minute and 30 minute aerosolizations indicating that after 30 min period the bacterium didn’t respond further to the increased amount of aerosolization stress. However, high susceptibility was maintained to imipenem and cefoperazone, both cell wall synthesis inhibitors, in all nebulization durations. This information will help mitigating antibiotic resistance in bacteria by optimizing environmental conditions to prevent the development of ARGs.

8BA.9

Study of Airborne Microbes in University Environment Using a Portable Electrostatic Bioaerosol Collection Device. KAVINDRA KUMARAGAMA, Hema Ravindran, Nueraili Kuerbanjiang, Shane Rogers, Shantanu Sur, Suresh Dhaniyala, *Clarkson University Potsdam, NY, USA*

We have developed a portable, low-power, and low-cost device for environmental bioaerosol monitoring. Our device called Trace Real-time Aerosol Concentration sensor and Biological sampler (TRAC- B), is capable of real-time air quality monitoring and capturing airborne particles for offline analysis. TRAC-B uses a low-cost sensor for real-time aerosol measurements and an electrostatic precipitator for the collection of bioaerosol for offline analysis. We have performed detailed characterization of the electrostatic precipitator-based bio-sampler section of the device, such as the impact of an ionizer on collection efficiency, effect of precipitation voltage on viability, and dependency of particle capture and recovery on the collection substrate used. We have deployed multiple TRAC-B units for a year-long study in various indoor and outdoor locations on Clarkson University campus. A culture and sequencing-based analysis of the collected samples was conducted to determine the diversity, abundance, and seasonal variation of the airborne microbial population in various indoor and outdoor environments. Our preliminary results (Sanger sequencing) show that bacterial species belonging to the genus *Bacillus* are the most abundant cultivable bacteria in the collected samples. Furthermore, our data suggests the highest microbial abundance in the spring and the summer seasons for both indoor and outdoor sampling locations.

Keywords: Bioaerosol, low-cost sensor, electrostatic precipitator

8BA.10

Fabrication of Silver Nanowire Coated Fibrous Air Filter Medium via a Two-Step Process of Electrospinning and Electrospray for Anti-Bioaerosol Treatment.

KYUHYUN PARK, Jungho Hwang, *Yonsei University, Republic of Korea*

Airborne microorganisms have been lots of interesting issues in any environment than 20 years ago. Also, particle filtration field has been growing up together as airborne microorganism occurs problem as SARS or MERS. Therefore, various filters have been developed and invented for figuring out problems of airborne microorganism.

Electrospinning and electrospraying method are used for fabricating and coating the web. Electrospinning and electrospraying process stand to reason for making and coating the filter because two processes can be used by only replacing the solution in the syringe.

Silver nanowire coated nanofiber web's filtration efficiency and pressure drop were measured to evaluate performance test. Aerosolizing prepared bacteria which were bacillus cereus, staphylococcus aureus, and micrococcus luteus and virus which was MS2 bacteriophage carried out for performance test of silver nanowire coated nanofiber web. Filtration efficiency of prepared nanofiber webs was measured upstream and downstream of the particle concentrations by aerosolizing prepared bacteria and virus. The concentration of bacteria and virus was measured by using an aerodynamic particle sizer (APS) and a scanning mobility particle sizer (SMPS). By using a differential pressure gauge, the pressure drop was measured between upstream and downstream.

For anti-microorganism test, pristine nanofiber filter and silver nanowire coated filter were used for comparison. Colony counting method and plaque counting method were used to get anti-bacterial efficiency and anti-viral efficiency. These efficiencies show a similar tendency which anti-microorganism was increased with increase of silver nanowire's coating time.

Filtration test of silver nanowire coated electrospun nanofiber web is evaluated by using APS and SMPS. Anti-bacterial and anti-viral ability of the web are also evaluated by using CFU and PFU assay. The silver nanowire coated electrospun nanofiber web is evaluated to prove increase of the filtration efficiency and antimicrobial ability with increase of coating areal density of silver nanowire and slightly increase of pressure drop.

8BA.11

Exposure to Bacterial Aerosols with Antimicrobial Resistance at Septic Systems.

GABRIELA RAMOS, Maria King, *Texas A&M University*

The aim of this study is to understand the role of aerosolization on the potential spread of antimicrobial-resistant bacteria and genes (ARB/ARGs) from wastewater effluents. During the spraying process aerosolized ARB/ARGs can spread far from septic tank systems into houses, degrading indoor air quality and posing risks to residents. Bioaerosols from common wastewater treatment plants can be found 10 km downwind of the plant boundaries. However, a septic tank system is required to be only 5 ft away from the house. It is critical to evaluate the aerosolization of ARB/ARGs from septic tank effluents to evaluate their potential contamination of the indoor air quality in nearby residences. The system in this study consists of four tanks connected by a filtration system. Aerosol samples at each tank were collected in the winter and summer with open and closed lids to observe the effect they may have on the emission of bioaerosols. The water inside each septic tank was also sampled to compare the bacteria concentration to the bioaerosol samples. The results of culturing, Kirby-Bauer antimicrobial testing, quantitative real-time polymerase chain reaction, and microbiome analysis showed lower concentrations of bacteria in the aerosols compared to the water samples. Aerosolized bacteria showed resistance to less than 50% of the antibiotics tested, lower in comparison to the 87.5% resistance in the water samples. Seasonality has also affected the antimicrobial resistance of the aerosolized bacteria. In the winter season, higher levels of resistance were detected mostly against beta-lactam antibiotics, while the summer season displayed lower levels of resistance. Operational conditions, discharge methods, humidity, temperature, airflow, and quorum sensing may all have an effect on the composition of the microbiome. After further analysis of septic tank effluents to surrounding outdoor and indoor air, mitigation methods of ARB/ARGs exposure will be applied and tested.

8BA.12

Assessment of a Bioaerosol Test Platform for the Evaluation of Biothreat Sensor Performance in Identifying Live BSL-3 Threat Agents.

LEAH CAROL, Benjamin Alvarez, Felix Sage, Thomas Pilholski, Elizabeth Corson, Brian Damit, *Johns Hopkins University Applied Physics Laboratory*

Robust evaluation of infectious bioaerosol sensors requires homogenous flow velocities and aerosol concentrations at sensor sampling locations. To support such testing, the Johns Hopkins Applied Physics Laboratory (JHU/APL) is currently designing and constructing a new Biological Safety Level (BSL-3) test platform for closed-circuit wind-tunnel exposures via inlet immersion of multiple instruments in series. A scaled-down prototype was described previously. The prototype includes 3D-printed honeycombs for flow straightening with minimal aerosol losses and a static mixer to promote aerosol mixing/uniformity. Results from the evaluation of the prototype system are reported here.

To evaluate velocity profiles and aerosol concentration uniformity, measurements were taken in a grid pattern at several points laterally along the flow path both upstream and downstream of the honeycombs. Coefficient of variation (COV) was calculated from these measurements and compared to industry standards provided by the Environmental Protection Agency (EPA) and American National Standards Institute (ANSI). For both velocity and aerosol concentration, EPA dictates COV no greater than 10% while ANSI allows COV up to 20%. Wind tunnel velocities of 1.5 m/s and 4 m/s were used to assess a typical condition and an extreme condition, respectively. Unobstructed flow as well as flow around a bluff body comprising 15% of the cross-sectional area were also examined. Use of the bluff body represented a worst-case scenario for perturbations.

Velocity COV met ANSI standards at all locations except the cross-section immediately following the bluff body (COV ~30%). Velocity COV also met EPA standards at most locations under unobstructed flow conditions. Meanwhile, aerosol COV met ANSI standards for all tested conditions and locations. When only the centermost grid points were examined, aerosol COV also met EPA standards. These results indicate the use of honeycombs and a static mixer can ensure homogenous flow velocities and aerosol concentrations at all sampling locations.

8HA.1

Fate of Inhaled Biological-agent Containing Aerosol Droplets in the Human Respiratory Tract.

BAHMAN ASGHARIAN, Owen Price, Jennifer Chesnutt, Gene McClellan, Jason Rodriguez, *Applied Research Associates, Inc.*

Aerosolized biological agents originating in a liquid suspension potentially have hygroscopic properties. These hygroscopic aerosols undergo phase change during which the size (and mass) of an aerosol changes depending on the relative humidity of the environment in which the aerosols are suspended. When the size of an aerosol changes, so do its deposition characteristics in the respiratory tract. To assess the fate of inhaled biological agents in the respiratory tract, size change during transport and deposition in the entire respiratory tract were modeled during inhalation, pause, and exhalation. Existing models for insoluble, non-hygroscopic aerosols were modified and extended to account for the influence of size change on deposition in lung airways. The behavior of agent containing droplets depended additionally on the temperatures of the droplet and air as well as the relative humidity of the air in the entire respiratory tract. Thus, a comprehensive model for aerosol size change and deposition was developed to predict aerosol deposition for agent exposure health risk. Major mechanisms of deposition were inertial impaction, Brownian diffusion, and gravitational settling. Droplets continued to grow in the respiratory tract. As a result, deposition characteristics of hygroscopic droplets were different from those of insoluble particles. When compared to insoluble particles, deposition fractions of hygroscopic droplets in the respiratory tract were found to decrease for initial sub-micrometer aerosols and increase for fine and coarse droplets. This study aids in developing an exposure-dose-response model for inhaled biological agents. This study was funded by Defense Threat Reduction Agency, contract HDTRA1119C0022.

8HA.2

Characterization of Water-Insoluble Oxidative Potential of PM2.5 Using the Dithiothreitol Assay.

DONG GAO, James Mulholland, Armistead G. Russell, Rodney J. Weber, *Georgia Institute of Technology*

Both water-soluble and insoluble components of ambient particulate matter (PM) have been shown to contribute to the oxidative potential (OP) of PM. In this study, we used the dithiothreitol (DTT) assay to assess the water-soluble (OP^{WS-DTT}) and total OP ($OP^{total-DTT}$) of ambient fine particles ($PM_{2.5}$), with water-insoluble OP (OP^{WI-DTT}) determined by difference. Ambient $PM_{2.5}$ filter samples were collected daily during 2017 in urban Atlanta and were analyzed for OP and major PM components. Results from measurements suggested a measurable contribution of water-insoluble components to OP^{DTT}, which comprised on average 20% of total PM OP. Strong seasonal trends were observed in both volume- and mass-normalized $OP^{total-DTT}$ and OP^{WI-DTT}, with higher values in the winter than in the summer, possibly driven by biomass burning emission seasonality. Correlation analysis indicated that all forms of OP^{DTT} measurements were related to organic species and metals. $OP^{total-DTT}$ and OP^{WI-DTT} were correlated with brown carbon (BrC) and total metals, especially total crustal elements. A multivariate regression model was developed for $OP^{total-DTT}$ based on particle composition data. The model suggested that the variability of $OP^{total-DTT}$ was primarily affected by BrC, followed by EC, total Cu and an antagonistic interaction between BrC and total Cu.

8HA.3

Development a New Health Metric for Ambient Fine Particles Based on Differential Toxicities among Different Sources.

MINHAN PARK, Kihong Park, *Gwangju Insitute of Science and Technology*

Fine particulate matters less than 2.5 µm ($PM_{2.5}$) in the ambient atmosphere are related with adverse health effects such as mortality and cardiovascular, respiratory, and allergic disease. A number of studies reported that the toxicity of fine particles differs depending on their sources due to different sizes and chemical components, suggesting that $PM_{2.5}$ mass concentration ($\mu g/m^3$) which is a current regulation standard should not be sufficient for monitoring health effects of $PM_{2.5}$. A new health metric was derived here based on the differential toxicities among different sources of fine particles including exposure levels of $PM_{2.5}$. The differential toxicity scores for fine particles from various sources (diesel and gasoline engines, biomass burning, coal burning, road dust, secondary organic aerosols, ammonium sulfate, and ammonium nitrate) were determined by using results obtained from in-vitro toxicity data (oxidative potential, cell viability, mutagenicity, DNA damage, oxidative stress, and inflammation) (Park et al., 2018). The new metric (risk score) was applied to local and regional mortality data (all-cause, COPD, lung cancer, asthma, and respiratory disease) for estimating association between new metric and health. The association was also compared with an association between ambient $PM_{2.5}$ mass concentration levels and health. The new health metric can be potentially served as a useful indicator to estimate the adverse health effects caused by different fine particle types although it should be continuously improved, and provide practical management of $PM_{2.5}$ beyond what can be achieved using $PM_{2.5}$ mass only. More results will be discussed in this presentation.

8HA.4

Reactive Oxygen Species in Fresh and Aged Biomass Burning Organic Aerosol. Shunyao Wang, Carolyn Liu-Kang, Jonathan Abbatt, Peter Gallimore, ARTHUR W. H. CHAN, *University of Toronto*

Biomass burning is an emerging issue all over the world in recent decades, threatening global climate and human health. The dynamic toxicity of biomass burning organic aerosol (BBOA) upon atmospheric processing remains poorly understood. For the first time, oxidative potential (OP) of primary and aged organic aerosol (by heterogenous OH oxidation) from wood burning were investigated by the dithiothreitol assay (DTT). In parallel, electron paramagnetic resonance (EPR) was applied to the direct measurement of reactive oxygen species (ROS) in primary and aged biomass burning aerosol. Results showed that the OP of organic aerosol from biomass burning is significantly enhanced upon aging equivalent to less than one day of oxidant exposure. Consistent with acellular OP measured by DTT, EPR ROS quantification using different spin trap techniques also showed a higher abundance of ROS in aged BBOA. After applying radical speciation and spin fitting, carbon centered radicals were found to be the most abundant radical species in primary organic aerosol from biomass burning while oxygen-centered radicals were found to be the dominant ROS in BBOA during atmospheric aging. Detailed chemical characterization performed by the high-performance liquid chromatography-high resolution mass spectrometer (HPLC-HRMS) illustrated that primary BBOA is predominantly consisted of less oxygenated multi-ring aromatic compounds while aged BBOA presents significantly higher abundance of oxygenated aromatic compounds with an elevated oxygen to carbon ratio, which contributes to an enhanced level of particle-bound ROS.

8HA.5

The Effect of Dust Storm Particles on Human Lung Epithelial Cells. KARIN ARDON-DRYER, Ayomide Tairu, Zyanya Ramirez-Diaz, Xueting Xia, Xueting Zhang, *Texas Tech University*

Dust is one of the most common natural atmospheric aerosol particles. During dust storm events there is an increase in particle concentration, many are breathable and can penetrate deep into our lungs. Once in the lung, it can cause our lung cells to overstress and die, which can manifest in inflammation. Therefore, exposure to dust particles can lead to respiratory complications, particularly for people with asthma. In this project, we are investigating the impacts that dust storm particles from different sources and concentrations (doses) have on human lung cells under different exposure times. These findings will help us to better understand the health-related consequences of exposure to dust storm events and will help us to set new regulations in areas with dust storms. We hope to better understand the implications of dust particles in different geographical locations around the globe.

8HA.6

Mutagenicity- and Pollutant-Emission Factors of Pellet-Fueled Gasifier Cookstoves: Comparison with Other Combustion Sources.

WYATT CHAMPION, Sarah Warren, Ingeborg Kooter, William Preston, Todd Krantz, David DeMarini, James Jetter, *ORISE, U.S. EPA*

Emissions from solid-fuel burning cookstoves are associated with premature mortality and climate effects. Pellet-fueled gasifier stoves have emission factors (EFs) approaching those of gas-fueled (liquid petroleum gas) stoves. However, their emissions have not been evaluated for biological effects. Here we use a new International Organization for Standardization (ISO) testing protocol to determine pollutant- and mutagenicity-EFs for a stove designed for pellet fuel—the Mimi Moto—and for two forced-draft stoves, Xunda and Philips HD4012, burning pellets of hardwood or peanut hulls. The Salmonella assay-based mutagenicity-EFs (revertants/megajoule$_{\text{delivered}}$) spans three orders of magnitude and correlates positively (r=0.99; n=5) to the sum of thirty-two polycyclic aromatic hydrocarbons (PAHs) EFs. Compared with data published previously for the Philips stove burning hardwood, the Mimi Moto/hardwood pellet combination shows total-PAH- and mutagenicity-EFs that are 99.2 and 96.6% lower, respectively and 100 and 99.8% lower, respectively, compared with those of a wood-fueled three-stone fire. The Xunda stove burning peanut hull pellets shows the highest fuel energy-based mutagenicity-EF (revertants/megajoule$_{\text{thermal}}$). It is between than that of diesel exhaust, a known human carcinogen, and a natural-draft wood stove. Although the Mimi Moto burning hardwood pellets had the lowest fuel energy-based mutagenicity-EF, this value is between that of utility coal and utility wood boilers. This advanced stove/fuel combination has the potential to greatly reduce emissions in contrast to a traditional stove, but adequate ventilation is required to approach acceptable levels of indoor air quality.

8HA.9

Differential Toxicity of PM2.5 Emissions from Residential Wood Burning due to Varying Combustion Conditions.

MARCIA PEDROZA, Greg J. Evans, Arthur W. H. Chan, *SOCAAR, University of Toronto*

The contribution of residential wood combustion (RWC) to ambient fine particulate matter ($PM_{2.5}$) has been reported to be as high as 42% in some North American and European urban areas during the heating season. Wood combustion-generated $PM_{2.5}$ has been postulated to exert different toxic effects by causing oxidative stress via the generation of reactive oxygen species (referred to as the oxidative potential, OP), among other mechanisms. However, the effects of combustion conditions on the toxicity of the emissions are still poorly understood. In this work, we hypothesize that the toxicity of the $PM_{2.5}$ from wood burning is affected by varying combustion conditions, such as fuel, ventilation, and temperature. The developed methodology includes fuel combustion in a temperature-controlled quartz tube furnace coupled with online measurements of CO_2 and CO concentrations, followed by $PM_{2.5}$ offline analysis by thermal desorption/gas chromatography-mass spectrometry (TD/GC-MS), and thermo-optical organic carbon/elemental carbon (OC/EC) analysis. As a primary metric for toxicity, we measure the OP of the particles with the dithiothreitol assay (OP^{DTT}), which is especially sensitive to highly oxidized organics. As secondary metrics, we are using OC/EC ratios, and modified combustion efficiency (MCE). Our results do not show significant differences between the OP^{DTT} of the $PM_{2.5}$ of hardwood and softwood combustion. The OP^{DTT} was found to increase with decreased oxygen concentrations, but enhancing ventilation did not decrease OP^{DTT}, likely due to lower effective temperatures of combustion. There is a moderate positive correlation between the OP^{DTT} and the OC fraction (R^2=0.56); both show sharp increases under enhanced ventilation conditions and under oxygen-deficient combustion for all the types of wood tested. The highest OP^{DTT} was obtained under smoldering combustion temperatures. The results presented here will inform best practices of residential wood burning to limit health impacts.

8HA.10

Ambient Particulate Matter Oxidative Potential: Chemical Determinants, Associated Health Effects, and Strategies for Risk Management.

DONG GAO, Susannah Ripley, Scott Weichenthal, Krystal Godri Pollitt, *Yale University*

Exposure to ambient air pollution has an adverse influence on human health. There is increasing evidence that oxidative potential (OP), the capacity of airborne pollutants to oxidize target molecules by generating redox oxidizing species, is a plausible metric for particulate matter (PM) toxicity. Several acellular techniques have been used to measure OP (respiratory tract lining fluid, dithiothreitol, ascorbic acid, and electron paramagnetic resonance assays). We will present a meta-analysis of the PM chemical constituents that have been identified to drive the OP response. We further discuss the epidemiologic literature to identify studies that reported an association between exposure to ambient PM and a health outcome in a human population, and in which exposure was measured by both PM mass concentration and OP. Laboratory studies have shown that specific redox-active metals and quinones are able to contribute OP directly. However, interactions among PM species may alter the redox properties of PM components. In ambient PM measurements, all OP assays were found to be correlated with metals (Fe, Cu) and organic species (photochemically aged organics). Across the epidemiological studies reviewed, associations between fine PM (PM2.5) mass and cardio-respiratory outcomes were found to be stronger at elevated OP levels but findings varied across the different OP measurement techniques. Future work should aim to identify specific situations in which PM OP can improve air pollution exposure assessment and/or risk management. This may be particularly useful in countries with low PM2.5 mass concentrations over broad spatial scales where such information may greatly improve the efficiency of risk management activities.

8HA.11

3-D Surface Mesh Model to Predict Aerosolized Contaminant Fate and Transport in the Human Respiratory System.

JACKY ROSATI ROWE, Ray Burton, Rob McCauley, Wei Tang, *US EPA, ORD*

We have developed a comprehensive, three-dimensional surface mesh model of the human respiratory system. This novel, public model is an important advancement in the field of aerosolized contaminant transport, deposition, and clearance in the human respiratory system. The model addresses sex, age, and human physiology from the nares through the 9th generation of the lung. Algorithms that learn from the upper lung generation data (generations 0-9) are then used to develop the 10th-23rd generations needed to complete the lung. Multiple sets of human data were used to ensure the model is representative of the general population; previously identified surface or physiological anomalies due to scan inaccuracies, movement, resolution and/or human disease have been removed. The model allows for nasal or mouth breathing with a physiologically accurate mouth, tongue, gums and uvula. Additionally, the complete model physiology allows for expansion and contraction during the breathing process.

A user interface has been developed to allow researchers and the broader health community simplified access to this model and the associated data. The user inputs specifics such as sex, age, and the physical parameters they are investigating into the interface. A surface model is then generated that includes the nasal and oral cavities, pharynx, larynx, trachea, and three airway paths an average of 23 generations deep into each of the five lobes. This specific surface model is then exported to a standard stereolithography (STL) CAD file format. While available for use in many broad applications, current research is using this surface mesh model as the basis for computational fluid dynamics models to investigate respiratory drug delivery, PM based aerosol exposure/dose determinations, and respiratory flow visualization. The model is also being considered for use in respiratory surgery simulations.

8HA.13

Fate of Transition Metals in Acellular Phosphate -Based Assays for PM Toxicity: Equilibrium Modelling and Macroscopic Experimental Study.

JAYASHREE YALAMANCHILI, Christopher Hennigan, Brian Reed, *University of Maryland, Baltimore County*

Among the diverse chemical constituents that make up atmospheric aerosols, transition metals are hypothesized to possess an enhanced toxicity based on their ability to support electron exchange, and to catalyze and generate reactive oxygen species (ROS) in biological tissues. The toxicity of metals is related to the oxidative stress induced by the ROS that are generated. The most widely used acellular assays for ROS measurements in PM employ phosphate (PO4) buffers (pH = 7.4 and T = 37 °C) to simulate conditions in the human body. However, the high PO4 concentrations (typically 0.1 – 0.5 M) and pH can induce physical and chemical transformations of soluble transition metals. In this study, we show that precipitation of the transition metals Fe(II), Fe(III), Cu(II), and Mn(II) are thermodynamically favored in phosphate-based assays used to measure the oxidative potential (OP) of PM. Fe and Mn precipitation is likely to occur at extremely low metal concentrations (< 0.5 µM), levels that are imperceptible to the naked eye. Cu is the most soluble of the four metals, which may partly explain its heightened sensitivity in OP assays. Macroscopic experimental results at higher metal concentrations (> 100 µM) with visible precipitates provide quasi-validation of the thermodynamic modeling. At lower metal concentrations (< 10 µM) chemical analysis of dissolved metals and laser particle light scattering measurements confirm reductions in transition metal concentrations, precipitate formation and significant oxidation of Fe(II) to Fe(III) and Mn(II) to Mn(II). The current results suggest an artifact in acellular assays of aerosol OP that is likely widespread; the implications for studies of PM toxicity are discussed.

8HA.14

Evaluating the Accuracy of Optical Particle Counters for Estimating Size-Resolved Particulate Matter Mass Concentrations in Occupied Homes.

YICHENG ZENG, Insung Kang, Kari Abromitis, Parham Azimi, Brent Stephens, *Illinois Institute of Technology*

Optical particle counters (OPCs) are commonly used to characterize particle number concentrations in indoor environments and to estimate size-resolved mass-based concentrations of particulate matter (e.g., PM_1, $PM_{2.5}$, or PM_{10}) by assuming particle shape and density. To date, studies have compared the utility and accuracy of using research-grade aerosol instrumentation (such as scanning mobility particle sizers combined with aerodynamic particle sizers) as well as low-cost particle counters to estimate total and/or size-resolved PM mass concentrations, but there is limited data on the accuracy of mid-range OPCs (e.g. ~$2500 USD) for estimating mass-based PM concentrations. Here we present results from a sampling campaign in which time- and size-resolved indoor particle concentrations were measured using MetOne GT-526S OPCs in 41 occupied homes in Chicago, IL; co-located size-resolved gravimetric PM samples were also collected using Sioutas Personal Cascade Impactors deployed in a subset of home visits for comparison between instruments. Gravimetric samples have been collected in 21 home visits to date with a goal of 30 visits by 2020 (sampling is still ongoing). Preliminary results show reasonable correlations between the OPC estimates and actual size-resolved mass-based concentrations (e.g., $PM_{0.5}$, PM_1, and $PM_{2.5}$), but that correlations vary highly between home visits likely because of (i) differences in indoor particle density and/or shapes and/or (ii) the vast majority of PM mass was observed in the size bin smaller than 0.25 µm (which is below the detection limit of ~0.3 µm of the OPCs). These data are expected to provide useful insights into how accuracy mid-cost OPCs can (or cannot) be used to estimate PM mass concentrations.

8HA.15

Changing of Chemical Composition and Potential Exposure Risks of Aerosols from Electronic Nicotine Delivery Systems as a Function of E-Liquid Composition and Heating Power.

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Electronic nicotine delivery systems (ENDS) aerosolize a mix of chemicals in e-liquids, including main components, propylene glycol (PG), vegetable glycerin (VG), and additives, that is then inhaled. ENDS use has dramatically increased recently, especially in youth. While ENDS may be perceived as a less harmful alternative to traditional cigarettes due to the absence of inhalation of combustion byproducts, the health risks associated with inhalation of aerosolized PG/VG and their by-products are unknown. Thus, it is important to identify the complex mixture of chemical constituents that make up ENDS aerosols to further aid in evaluating systemic exposures and health risk assessments. This study systematically examines the chemical properties of e-liquids from a commercially available ENDS with a range of selected e-liquid compositions and operation settings. The e-liquids consisting of selected ratios of PG and VG were aerosolized with selected voltage settings that represent common usage. The ENDS aerosol was continuously sampled in real-time by an aerosol chemical speciation monitor (ACSM).

The mass spectral data collected by the ACSM describe the chemical composition of the ENDS aerosol changed depending on e-liquid composition and heating power of the ENDS. The particle phase of the ENDS aerosol plumes mostly consisted of VG due to its low vapor pressure. A higher heating power of the ENDS was directly correlated to a higher ratio of ions with high mass-to-charge ratios (m/z), indicating more oligomer formation with a higher coil temperature of ENDS. Given that some of the oligomers may be more toxic and difficult to decompose compared with PG and VG molecules, the findings of this study suggest that the behaviors and preferences of ENDS users could lead to differences in systemic exposures and potential health risks. This study also establishes a source apportionment method that can be used to identify the chemical composition of ENDS generated aerosols, which can be further used to inform tobacco-product control and real-time air monitoring.

8HA.16

Germicidal Ultraviolet Light Does Not Damage or Impede Performance of N95 Masks Upon Multiple Uses.

ZHE ZHAO, Zhaobo Zhang, Mariana Lanzarini-Lopes, Shahnawaz Sinha, Hojung Rho, Pierre Herckes, Paul Westerhoff, *Arizona State University*

The outbreak of COVID-19 pandemic is causing an increasing need of personal protection equipment (PPE) worldwide, including the demand for facial breathing masks used by healthcare workers. Disinfecting and reusing these masks may offer benefits in the short-term to meet urgent demand for healthcare workers. In this paper, based on previous study that 1J/cm^2 UV dose could achieve over 3-log reduction in recoverable virus, we demonstrated germicidal ultraviolet irradiation can be used to disinfect both N95-rated and non-rated surgical masks. Either 265nm LEDs or 254nm low pressure UV lamps at 1J/cm^2 and 10J/cm^2 had no significant influence on the masks' ability to remove aerosolized virus-sized particles. Additional testing on physical properties showed no change in polymer structure, surface functional groups, morphology and surface hydrophobicity for multiple layers in the mask before and after UV irradiation, and no change in pressure drop or tensile strength of mask materials. Results were similar when applying 254nm low-pressure UV lamps and 265nm light emitting diodes. Based on the findings and design feasibility considerations, a 254nm UV treatment system and operational manual were prepared to enable treatment and reuse of N95 facial masks. Findings from this study can not only provide short term strategies to reuse of PPE materials but also contribute to the basis of plans for long term practices and help to deal with the shortage of PPE materials during future unanticipated pandemics.

8HA.18

Environmentally Persistent Free Radicals and Reactive Oxygen Species Measurements in the Size-Segregated Ambient Particles Collected at the Highway and Urban Site.

BRIAN HWANG, Ting Fang, Randy Pham, Jinlai Wei, Heejung Jung, Manabu Shiraiwa, *University of California, Irvine*

Recent studies show people who live close to the highway has about 5 % higher chance of developing dementia and asthma. Although the exact mechanism in how emissions from the highway can cause these adverse health effects are poorly understood, previous studies suggest oxidative stress by reactive oxygen species (ROS) generated from the inhaled particles play an important role in the development of respiratory and neurological illness. Transition metals such as iron and copper which are found to be abundant in the tire/brake wear and road dust particulate matter (PM) can be a significant source of ROS. These transition metals can react with organic hydroperoxides emitted from the tailpipe or hydrogen peroxides in the lung fluid to generate ROS through Fenton-like reactions. Environmentally persistent free radicals (EPFRs) which are stable radicals with similar chemical characteristics as semiquinones are often found in combustion generated PM. EPFRs can also generate ROS through the redox reaction with iron and copper. The exact sources of EPFR and ROS and their abundance near or next to highway PM are hardly quantified.

In this study, PM2.5 and size-segregated ambient particles were collected at the near road sites and urban background location in the South Coast Air Basin using a high volume PM2.5 sampler and a micro-orifice uniform deposition impactors (MOUDI) respectively. EPFRs are directly measured from the particles on filters using an electron paramagnetic resonance (EPR) spectrometer. The preliminary results show EPFRs in the highway PM2.5 are 2 – 4 times higher than the urban background. At the highway site, EPFR concentrations are found to be highly correlated with CO and NO2 mixing ratios, suggesting that EPFRs may be mainly emitted from the tailpipe. Interestingly, negative correlation between EPFRs and O3 was observed, suggesting O3 or photolysis may play a role to quench EPFRs or inhibit their production. We also conducted ROS measurements to measure OH·, O2·, and organic radicals from particle water extracts using EPR combined with a spin-trapping technique.

8HA.19

Determining Real-Time Mass Deposition With a Quartz Crystal Microbalance in a Parallel-Flow, Electrostatic Air Liquid Interface Exposure System.

KAMALJEET KAUR, Dana Overacker, Hamid Ghandehari, Chris Reilly, Robert Paine, Kerry Kelly, *University of Utah*

Air-liquid interface (ALI) in vitro exposure systems are gaining interest as a more realistic strategy for in vitro particle exposure than submerged culture approaches. One of the persistent challenges in working with ALI systems is getting a good estimation of particle mass deposition, which defines the delivered dose to cells. Although a few commercially available ALI systems are equipped with online mass deposition monitoring, most studies use indirect methods to estimate mass doses. These different indirect methods may contribute to inconsistencies in the results from in vitro studies of aerosolized nanoparticles. This study explores the effectiveness of a commercially available Quartz Crystal Microbalance (QCM) system to estimate the real-time deposition of particle mass inside a parallel-flow, electrostatic ALI system. The QCM system required minor modifications including custom-designed and fabricated headers for the ALI chamber. Three QCM systems were simultaneously placed in three of the wells of a six-well plate in the ALI exposure chamber to evaluate the uniformity of particle deposition within the ALI. The measurements from fluorescein dosimetry and QCM revealed an uneven deposition between wells of the ALI exposure chamber. The performance of the QCM system was also evaluated using two different methods. First, using fluorescein deposition in one well, depositions in three other wells were estimated, which was then compared to the actual QCM readings placed inside the same wells. Second, using the QCM measured deposition in one well, the deposition in three other wells was estimated and compared to deposition measured by fluorescein dosimetry. For both methods, the comparison between the expected mass deposition and actual deposition yields a linear fit with the slope ~1. This good fit suggests that QCM systems can be used to measure real-time mass deposition in an electrostatic ALI system.

8HA.20

In-vitro Cytotoxicity of Lab-generated Tunable Soot: Insight into Military Burn Pit Contribution to Chronic Multisymptom Illnesses (CMI).

DHRUV MITROO, Durgesh Das, Benjamin Kumfer, Nathan Ravi, *Veterans Research and Education Foundation*

Whether released during unpredictable events, such as oil-well fires, or through routine activity, such as military burn pit operation, combustion emissions are problematic for the long-term health of military personnel. Deployed military preventive medicine units evaluating the presence of airborne toxins at forward operating bases (FOBs) have reported polycyclic aromatic hydrocarbons (PAHs) and dioxins, in both aerosol and gas-phase, originating from military burn pits. Importantly, cohort studies have associated burn pit emissions with chronic multisymptom illnesses (CMI); unsurprising given the pits' sustained use and proximity to barracks. Thus far, the molecular pathway through which burn pit emissions lead to CMI remains unclear, thwarting the exploration of therapeutic (or preventive) options. The problem is made more complicated by the wide variation in chemical composition and physical properties of carbonaceous particles generated in open and variable combustion systems. To address these issues, we utilized a bench-top soot generator comprising an ethylene tri-flow burner and a control panel, that uses different flame structures to produce carbonaceous aerosols with tunable properties. We tailored the combustion conditions, i.e., temperature, fuel and oxidizer mixtures, and flame type (premixed and non-premixed), to generate soot with varying properties, such as size, surface area, EC/OC, and PAH loading, characteristic of military burn pit emissions. Herein we present initial physical and chemical characterization results for produced aerosol (soot), measurements of its stability in solution, and descriptions of its cytotoxic effects on human cell lines. The cytotoxicity results illuminate how the aryl hydrocarbon receptor (AhR) may be involved in influencing the elimination or potentiating PAH's toxicity. While the work presented is centered on replicating military bun pit emissions, we note that our soot generator can be used to create standards of different types of soot geared towards understanding combustion aerosol pollution in general.

8HA.21

The Influence of the Water Activity Estimation Method on the Accuracy of the Hygroscopic Particle Growth Model.

PATRICK O'SHAUGHNESSY, Alessandra Pratt, *University of Iowa*

This research was motivated by the need to accurately determine deposition sites of pharmaceutical compounds that alleviate airway diseases with the use of computational fluid dynamic (CFD) modeling of the human lung. A fundamental aspect of the mathematical model developed to predict the hygroscopic growth of pharmaceutical particles is the relationship between the solute content of the droplet solution and its water activity – the ratio of the water vapor pressure near the surface of the droplet relative to the water vapor pressure in the atmosphere. A comparison between the use of Raoult's Law and the use of a polynomial expression to model water activity relative to solute solution mass percent based on direct measurements was conducted. A set of published coupled differential equations for predicting droplet growth and droplet temperature change were used to predict the growth of sodium chloride particles as the test substance. Differential equations were solved using a MATLAB ordinary differential equation solver function. Experimental validation of the model was accomplished with the novel use of video photography to measure the growth of a salt particle frame-by-frame on a microscope slide placed on a light microscope. The experimental data indicated an initial growth phase that is consistent with the model when adjusted to simulate the dissolution of the salt core. Application of the polynomial expression proved to be more accurate than when applying Raoult's Law for estimating water activity. Model accuracy during the initial growth phase is particularly important for particles entering the humid environment of the lung that are too large to reach equilibrium before entering the lower branches of the pulmonary system, which will therefore improve the accuracy of deposition site estimation within the lung. Future research will incorporate this added aspect of the hygroscopic growth model applied to more complex pharmaceutical compounds.

8HA.22

Evaluation of Low-Cost Optical Particle Counters for Agricultural Exposure Measurements. JUSTINE OLEGARIO, Swastika Regmi, Sinan Sousan, *East Carolina University*

Prolonged exposure to dust has been shown to have negative health effects in agricultural workers, primarily with the development of respiratory diseases. Low-cost sensors may be cost-effective tools for farmers to use in determining when they are exposed to harmful levels of dust during their workday. The purpose of this study is to identify low-cost sensors that may be reliably used in occupational settings to help workers and employers identify how much respirable particle matter is being inhaled. The study utilized two different low-cost optical particle counters (OPCs) to collect data on dust exposure which were worn on a belt by the participant: the OPC-N3 developed by Alphasense and the AirBeam2 developed by HabitatMap. Additionally, an AirChek TOUCH air sampling pump fit with a respirable dust aluminum cyclone allowed for collection of respirable particulate matter (PM4) to determine the true concentration of exposure. Results from data analysis suggests that the AirBeam2 may be greatly underestimating the amount of particulate matter that farmworkers are exposed to and therefore may not be suitable for occupational exposure measurements in comparison to the OPC-N3. Comparison of the PM4 measurements made by the OPC-N3 are similar to the gravimetrical filter measurement at concentrations of < 50 µg/m3.

8HA.23

Cyanobacterial Microcystin Production and Aerosolization Dynamics in the Chowan River-Albemarle Sound Estuarine Continuum, NC. HALEY E. PLAAS, Nathan S. Hall, Karen Rossignol, Karsten Baumann, Ryan Paerl, Kimberly Popendorf, Malcolm A. Barnard, Jill Paxson, Colleen Karl, Hans W. Paerl, *University of North Carolina at Chapel Hill*

The environmental health of the Chowan River-Albemarle Sound (CR-AS) estuarine continuum is threatened by the recent expansion of harmful cyanobacterial blooms (CyanoHABs), specifically the genus *Microcystis*, which produces a suite of toxins including microcystin, a hepatotoxin. Several studies have associated microcystin ingestion with adverse health outcomes, namely liver disease, but few have examined health risks from the inhalation of microcystin in spray aerosol (SA). As entrained air bubbles burst at the water surface due to wave action, film and jet drops are ejected into the air, aerosolizing toxigenic cyanobacteria and/or extracellular toxins. Spray aerosol formation has been characterized in the ocean (sea spray aerosol/ SSA) and large lake systems (lake spray aerosol/ LSA), but knowledge gaps remain regarding the physicochemical properties of spray aerosol produced in estuarine ecosystems, and more specifically during CyanoHAB episodes *in situ*. Thus, our field campaign elucidated the potential incorporation of microcystin into spray aerosol on the CR-AS. We collected $PM_{2.5}$ on filters using a high-volume Tisch sampler and measured real-time $PM_{2.5}$ mass concentrations with a high-resolution nephelometer. Wave activity and emission of SA was scaled by correlations of highly resolved wind speed and $PM_{2.5}$ measurements. Filters were respectively analyzed for airborne CyanoHAB species and microcystin concentrations via 16S rRNA and *mycA* gene amplicon sequencing and LC-MS/MS. Water samples were collected in parallel and analyzed to calculate the SA enrichment factors for CyanoHAB DNA and microcystin. Generalized linear models were used to examine environmental correlates of CyanoHAB incorporation into aerosol. All data were collected in collaboration with the NC Department of Environmental Quality (NCDEQ) and citizen scientists of the Chowan Edenton Environmental Group (CEEG). By exploring the intersection of CyanoHABs, water and air quality, and public health, this work serves to protect public welfare in the CR-AS region.

8HA.24

Development of a Semi-Automated Instrument to Measure the Cellular Reactive Oxygen Species (Ros) Activity of Ambient Particulate Matter.

SUDHEER SALANA, Vishal Verma, *University of Illinois Urbana-Champaign*

Several automated instruments exist today to measure the acellular oxidative potential of ambient particulate matter (PM). Moreover, a few online instruments have also been developed for the real time measurements of acellular reactive oxygen species (ROS) activity of the ambient particles. However, no such automated system exists for measuring the cellular ROS activity, which severely limits the comparison between two types of assays. Cellular assays provide a much better means of ROS assessment as they incorporate the biological processes involved in the PM-induced ROS generation. Considering this need, here we aim to develop a semi-automated instrument to conduct the macrophage ROS assay using rat alveolar cells (NR8383), which is a well-established and widely used cell line for the cellular oxidative potential measurements. The instrument uses dichlorofluorescein (DCFH) as a probe to detect the ROS activity of particulate matter. The instrument is capable of analyzing at least two ambient PM samples extracted in water, within a span of four hours, including both negative and positive controls. Preliminary experiments conducted on various standard metal solutions show a very good agreement between manual and automated results for the relative ROS response as compared to the negative control (slope = 0.74 and r^2=0.9). The instrument also has a very low limit of detection (<2.6 µg equivalents of Zymosan). The analysis of the time dependent ROS response, and measurement of the ROS activity of the PM-laden filter samples collected during field trials is currently underway, which will help to further evaluate the precision and accuracy of the system. Coupled with other acellular assays, this instrument would provide a comprehensive analysis of the cellular oxidative potential of particular matter samples.

8IA.1

Exposure to Long-range-transported Particulate Matter and Evaluation of Health Effects using MPPD model.

HYEON-JU OH, Yoonki Min, *Rutgers, The State University of New Jersey*

Exposure to particulate matters (PM) is known to cause cardiovascular disease and increase mortality and morbidity. Asian dust clouds are carried eastwards by prevailing westerly winds and these dust clouds were eventually transported for more than one full circuit around the globe in about 2 weeks in Korea. Here, we have characterized concentrations of PM and synoptic air flow trajectories were classified into four clusters by HYSPLIT model for Asian dusts in Jeju island for spring season. Also, we evaluated contribution of specific microenvironments to the exposure for different age groups and calculated inhaled PM doses and deposited mass/mass flux so as to evaluate health effects using Multiple-Path Particle Dosimetry (MPPD) model. The average outdoor PM_{10} concentrations ranged within 29.3 – 65.4 µg/m^3, while the concentrations of PM_{10} for the Asian dust were 127.0 – 342.0 µg/m^3. The concentrations of PM_{10} in indoors were within 26.32 - 43.5 µg/m^3. Air masses from cluster 1 and 2 were 24 % and 29 % (in 2017), cluster 2 and 3 were 24 % and 32 % (in 2018) and cluster 1 and 3 were 28 % and 26 % (in 2019), more frequent, respectively, for Asian dusts. The calculated inhaled PM10 doses from specific microenvironments (Home, working or school and transportation) were from 5.28 µg to 101.48 µg depending on age group and different microenvironments while the calculated PM10 inhaled doses for Asian dusts ranged within 67.92 µg - 769.27 µg. In the aerosol deposition based on MPPD model, the corresponding values for daily particle deposited mass for two age groups ranged from 8.64 $\times 10^{-5}$ (age 8) to 8.64 $\times 10^{-4}$ (age 21). Overall, the highest contributions were found to come from indoor working time (age 21) (male) and outdoor activity for Asian dust (age 21). This work shows human exposure to PM for Asian dust associated with health effects for a sustainability.

8IA.2

Characterizing Coffee Home Roasting and Grinding Emissions Using Low Cost Sensors.

ANIYA KHALILI1, Carmen Pacheco-Borden, Shelly Miller, *University of Colorado Boulder*

Coffee is one of the most universally consumed nonalcoholic beverages. In 2020, worldwide coffee revenue equaled US$363 billion (Shahbandeh, 2020). Diacetyl, 2,3-pentanedione, 2,3-hexanedione, particulate matter (PM), and volatile organic compounds (VOCs) produced during the roasting and grinding of coffee (Pengelly et al. 2019) can boost the development of respiratory diseases such as obliterative bronchiolitis (Kreiss et al., 2002). The growing micro roasting/grinding culture have increased concerns regarding potential respiratory health effects associated with consumer exposure to home roasting and grinding of coffee.

Roasting and grinding experiments were conducted in a residential apartment in Boulder, Colorado using two residential home roasting devices (none of the roasters had an air cleaning filter) and one residential grinding device. Two low-cost sensors were used to collect indoor air samples: the “Awair Element” and the “Airthinx”. In the roasting studies the influence of roast level (dark vs. light), whether windows were open or closed, and two different home coffee roasters were investigated. Similarly, in the grinding experiments the influence of grind size (fine), whether windows were open or closed has been investigated.

Roasting results indicated PM2.5 and VOC emissions are highest when the windows are closed. The average PM2.5 was in the unhealthy range (above 35 ug/m3): PM2.5 average range: 1.3-245.6 ug/m3). VOCs, were also elevated during roasting: the average range was 100.9-954.1 ppb. The results also show that dark roast produced more emissions than light roast with both open and closed windows. The results from grinding at home showed little-to-no emissions during grinding.

PM 2.5 is a major source of respiratory disease; therefore, home roasters must consider using proper exhaust fans and ventilation during roasting. Future research to investigate the effects of home roasting and grinding emissions on human health is recommended.

8IA.3

Indoor Mopping with a Terpene-Based Cleaner in the Presence of Ozone Initiates the Rapid Formation of Peroxy Radicals, Volatile Oxidation Products, and Secondary Organic Aerosols.

COLLEEN MARCIEL ROSALES, Jinglin Jiang, Ahmad Lahib, Vinay Kumar, Emily Reidy, Brandon Bottorff, Alexandre Tomas, Sebastien Dusanter, Antonios Tasoglou, Heinz Huber, Brandon E. Boor, Philip Stevens, *Indiana University*

Indoor air pollutants, in both gaseous and particle (aerosol) forms, may be either directly emitted or chemically generated (i.e. secondary formation) from common activities such as cleaning. Secondary formation of aerosols is less understood indoors compared to ambient air pollution. In addition, there have been few direct, real time measurements of intermediates, none of which precisely point to secondary formation of aerosols indoors. In the quickly emerging field of indoor chemistry, a complete understanding of the chemical mechanisms of secondary aerosol formation is critical in protecting human health indoors, especially for workers repeatedly exposed to cleaning agents at workplaces.

To aid in understanding secondary aerosol formation, various instruments that measure gas- and aerosol-phase species were deployed to the Indiana University Research and Teaching Preserve during the summer of 2019. Indoor cleaning activities were simulated by mopping and wiping surfaces in a sunlit room provided with outdoor air via a mechanical ventilation system. Application of a commonly used commercial household cleaner released a mixture of monoterpenes (e.g. limonene), monoterpenoids (e.g. citral), and monoterpene alcohols (e.g. terpineol), with monoterpene concentrations reaching ~250 to 400 ppb. Immediately thereafter, HO_2 and RO_2 radicals (peak: ~3×10^9 molecules cm^{-3}) and volatile monoterpene oxidation products, such as limononic acid, limonalic acid, and limononaldehyde, were observed, quickly followed by new particle formation and growth starting from ~1 nm (peak number concentration: ~10^5 cm^{-3} for particles below 100 nm). Radical and aerosol concentrations reached levels that are comparable to outdoor traffic-impacted areas, emulating “indoor smog” for a few minutes. It was found that aerosol formation indoors during these events are highly driven by the ozonolysis of the monoterpene mixtures found in cleaning products when indoor ozone levels are ~5 to 10 ppb. Current models for radicals and aerosol formation reasonably estimate the measured concentrations, albeit underestimating the measurements up to about a factor of 2, suggesting an incomplete understanding of the indoor oxidation mechanisms due to sources that were unaccounted for, e.g. surface films as reservoirs. These results lay the foundation for regulatory policies on issues such as permissible compositions of household cleaning products and residential and workplace building regulations for ventilation systems.

8IA.4

New Particle Formation (1-3nm) in Preschools in Nur-Sultan, Kazakhstan. MEHDI AMOUEI TORKMAHALLEH, Kamila Turganova, Tomiris Madiyarova, Zhuldyz Zhigulina, Enoch Adotey, Milad Malekipirbazari, *Dept Chem & Mat Engr, Sch Engr & Dig Sci, Nazarbayev Univ*

This study is the first report that provides evidence for the exposure to new particles in indoor environments with a focus on preschools, and demonstrates the major driving force for the formation of cluster mode particles (1-3nm). Cluster mode particles and ultraviolate absorbing particles (UVPM) were measured inside two modern preschools located in Nur-Sultan city of Kazakhstan from October 28 to November 27, 2019. Candle burning contributed to the emission of new particles as small as 2 nm. The major source of the new particle formation indoors was secondary organic aerosol (SOA) with particles below 2nm and concentrations above 10^7 particles/cm^3. New particle formation (NPF) events were observed at different time of the day and also continuously throughout the day depending on the concentrations of the VOCs and independent of the ozone concentration in the range of 20 to 60 ppb. Below 20 ppb ambient ozone no major NPF event was observed. The major sources of volatile organic carbon (VOC) sources for the SOA formation were cleaning detergents, painting and gluing materials in the two preschools. Additionally, VOCs from frequent smoking near the preschool II served as the precursor of NPF events in the form of SOA. The infiltration of smoking fumes into the preschool II was well associated with the elevation of the ultraviolet PM (UVPM at 375 nm) concentrations inside the preschool II. The UVPM concentration reached as high as 7µg/m^3 in one of the measurement days. Some changes in the training and cleaning programs may cause significant reductions in the exposure to the children to new particles. Such changes includes but are not limited to performing cleaning before and after the presence of the children in the preschools and conducting the art activities in the morning when the ozone concentration is lower compared to the afternoon.

8IA.5

Measuring Microbial Growth and MVOC Emissions in Carpet and Drywall Under Elevated Relative Humidity. SARAH R. HAINES, Emma C. Hall, Pawel K. Misztal, Allen Goldstein, Rachel I. Adams, Karen C. Dannemiller, *Ohio State University*

Microorganisms grow in carpet dust and on drywall at elevated relative humidity (RH) conditions (>80% and >90% RH, respectively). Growth may release microbial volatile organic compounds (MVOCs). However, it is unknown how microbial growth and MVOC emissions vary in various building materials under different RH conditions. The goal of this study is to characterize the microbial contribution to indoor chemistry under elevated relative humidity conditions and in different building materials. Dust was collected from San Francisco, CA, Columbus, OH and Gainesville, FL, embedded into unused nylon carpet. Samples of painted drywall were inoculated in homes in San Francisco, CA and Columbus, OH. Samples were incubated at either 50%, 65%, 70%, 75%, 80%, 85% or 95% equilibrium RH for 2 – 4 weeks depending on the experiment. A proton transfer reaction time-of-flight mass spectrometer (PTR-ToF-MS) was used to measure VOCs at 1s time resolution. Results indicated that location origin of the sample (CA, OH, FL) was most indicative of determining species composition (R2=0.21, p=0.001). Fungal communities in samples of CA dust embedded in carpet incubated at elevated RH for 4 weeks were found to cluster into three distinct groups based on equilibrium relative humidity, Low (50%-70% RH), Medium (75%-85% RH) and High (95% RH). *Aspergillus sydowii* (p=0.03, p=0.0002), *Penicillium chrysogenum* (p=0.02, p=0.002), and *Penicillium gladioli* (p=0.009, p=0.0003) were more associated with the High RH conditions than Low or Medium conditions, respectively. *Wallemia canadensis* (p=0.006), *Wallemia muriae* (p=0.02), *Wallemia sebi* (p=0.02) and *Wallemia tropicalis* (p=0.002) were more associated with the Medium RH condition when compared to the Low RH condition. Further work will examine relationships between MVOCs and the different groupings of relative humidity.

8IA.6

Assessment of Exposures to Ozone Due to the Use of Ionization-type Car Air Purifiers. TAEWON HAN, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Because of the growing public awareness of the health risks associated with air pollution, air purification indoors and in other enclosed spaces, e.g., cars, has gained widespread popularity in recent years, and a large variety of air purifiers are available for residential and commercial buildings, automobiles, and for personal protection. Air purifiers are typically based on three types of technologies: (1) filtration, (2) ionization, and (3) ozonolysis of air impurities. Ionization-based devices emit a steady stream of negative ions into the air, and these ions impart a charge on airborne particles, causing their deposition on surfaces. However, due to their ionization process, ozone (O_3) is produced, and its concentrations are often higher than 0.07 ppm National Ambient Air Quality Standard for ambient air. Thus, this emission of O_3 raises serious health concerns about the use of ionizers. This study determined O_3 exposure levels when using 15 commercially available ionization-type air purifiers (e.g., cigar jack socket type and portable type). We measured O_3 emissions and the number of ions near the exhaust face of each air purifier in a laboratory. We found that the ionizers emitted $0.003\text{-}169\times10^6$ ions/cm^3, and four air purifiers produced O_3 concentrations up to 0.7 ppm. These air purifiers were also pilot-tested when measuring O_3 emissions and particulate matter (PM) presence in a car during its regular operation. Surprisingly, O_3 concentration was very low (less than 3 ppb), most likely due to a larger space, but PM removal was also not efficient, less than 29%. In addition, these air purifiers were not well-suited for effective protection against ultrafine particles (e.g., virus). The results are based on a limited number of samplers, and thus we will investigate the ionizers more thoroughly at different car operating conditions (recirculation vs. fresh air mode).

8IA.7

Investigating Aerosol Emissions and Their Volatility from the Use of Different Cooking Oils. SUMIT SANKHYAN, Kayley Zabinski, Sameer Patel, Marina Vance, *University of Colorado Boulder*

Cooking is one of the main contributors to aerosol emissions in indoor environments. Heating oils at high temperatures emit aerosols in the fine and ultrafine size ranges. Cooking emissions have been associated with various respiratory and cardiovascular ailments [1]. Negative health effects of indoor cooking-related exposure are usually characterized by aerosol lung deposition which is a function of size and concentration. The volatility of aerosols may also influence their biological response once they deposit in the respiratory tract, which makes it an important factor to study in indoor microenvironments [2]. This study aims to bring indoor cooking measurements into perspective by isolating cooking oil emissions from other ingredients and potential sources.

Aerosol emission rates were calculated for a variety of popular cooking oils with a range of smoke points using an electric heat source at various temperatures (below and above their individual smoke points). Oils tested include canola, avocado, peanut, soybean, olive, refined and unrefined coconut, and lard. Aerosol size distributions were characterized using a Scanning Mobility Particle Sizer (TSI) and an Aerodynamic Particle Sizer (TSI). The volatility of oil-generated aerosols was investigated by analyzing their size distributions after thermal conditioning through a thermal denuder. Black carbon (BC) and brown carbon (BrC) concentrations were measured using a 5-wavelength aethalometer (Aethlabs). Preliminary results indicate that oils with higher smoke points, such as soybean oil emit more particles compared with lower smoke point oils, such as canola oil. At 180 ^{o}C, a common deep-frying temperature, coconut oil, and soybean oil had the highest emissions among all oils tested.

[1] Hoskins et al. (2003), Indoor and Built Environment, 12.6, 427-433.
[2] Buonanno et al. (2011), Aerosol Science and Technology, 45(9), 1069-1077.

8IA.8

Particle and Chemical Emissions from Fused Filament Fabrication 3D Printers Using Emerging Filaments Including Metals. QIAN ZHANG, Marilyn Black, Rodney J. Weber, *Underwriters Laboratories Inc.*

Studies have shown that fused filament fabrication (FFF) 3D printers that are widely used by the general public emit high levels of ultrafine and fine particles, as well as numerous volatile organic compounds (VOCs). Research has found the emission characteristics depend on print conditions like extrusion temperature, print material, printer and filament brands. As more new materials and filaments are becoming available in the market, this study aims at characterizing particle and VOC emissions from emerging filaments and comparing to previously studied ones to understand which print conditions are mostly linked to emissions. We measured particle and VOC emissions from multiple FFF 3D printers and filaments using an established standardized testing method in a specialized exposure chamber. The studied new filaments include thermoplastics, metals, and mixture of thermoplastics with metals, flame retardants, or carbon fibers. Particle concentration and size, and concentration and composition of VOCs emitted as a function of filament material, extrusion nozzle temperature and filament additives are investigated. Metal composition of emitted particles and raw filament materials will also be analyzed, and the potential health impacts associated with particles, metals and VOCs will be discussed.

8IA.9

Measurements of Particle Phase (PM2.5) Per- and Polyfluoroalkyl Substances (PFAS) in Indoor Air. NAOMI CHANG, Jiaqi Zhou, Karsten Baumann, Zhenfa Zhang, Wanda Bodnar, Glenn Morrison, Barbara Turpin, *UNC-Chapel Hill*

Per- and polyfluoroalkyl substances (PFAS) are found in heat-, stain-, and water-resistant products widely used indoors. Exposure to PFAS is associated with adverse health effects like hepatotoxicity, immunotoxicity, and thyroid disease. While ingestion is a dominant route of exposure for some PFAS, it is also important to understand the degree to which inhalation of indoor PFAS on respirable particulate matter ($PM_{2.5}$) may contribute to exposure. We measured particulate PFAS air concentrations in 3 homes and 1 university building under normal operation and in 3 offices and 1 classroom during high-pressure, high-temperature professional carpet cleaning. Window wipe samples were collected in 1 home. Air sampling intervals ranged from 4 hours to 7 days at 12 L/min on a quartz fiber filter downstream of a multi-jet 2.5 µm cut-point impactor. Samples were quantified by AB SCIEX Triple Quad™ 6500 LC/MS for 34 targeted PFAS with authentic mass-labeled standards. Eight PFAS were detected during carpet cleaning with the highest concentrations of PFOA, PFHxA, PFHpA, PFDS, and PFDoA (123.4 pg/m^3, 48.2 pg/m^3, 31.6 pg/m^3, 52.8 pg/m^3, 8.4 pg/m^3, respectively) found in the classroom, which was cleaned with the highest pressure and temperature device. One office contained PFTrA (5.9 pg/m^3) and PFNA (4.9 pg/m^3) and two offices contained PFUnA (1.4 pg/m^3 and 3.2 pg/m^3). Only the classroom contained PFDS. PFOA was detected in all homes (max 4.6 pg/m^3), PFHxA (8.1 pg/m^3) in 1 home, and PFDA (1.7 pg/m^3) in another. At least 6 PFAS were detected in each window wipe sample with PFOA, PFDA, PFDoA, PFTrA, and PFTA detected in all. The variation in PFAS between rooms and homes reflects the diversity of indoor sources of PFAS. Results suggest that carpet cleaning bears a potential occupational exposure health risk for maintenance workers. Notably, PFOA was commonly found despite U.S. production being halted around 2002.

8IA.10

Quantifying the Effect of Indoor Conditions on Exposure to Gas-Phase Bleach Products. PASCALE LAKEY, Youngbo Won, Atila Novoselac, Donghyun Rim, Manabu Shiraiwa, *University of California, Irvine*

Application of bleach indoors has previously been associated with many different health effects and respiratory symptoms such as wheezing, shortness of breath and non-allergenic asthma [1]. Bleach leads to the formation of many harmful and irritating products in the gas-phase including hypochlorous acid, chlorine gas, chloramines, nitryl chloride, and OH and Cl radicals [2]. A kinetic model was previously developed to investigate the reactions controlling gas-phase bleach products measured during the House Observations of Microbial and Environmental Chemistry (HOMEChem) campaign [2]. The model included reactions in the bleach and gas-phase as well as uptake to particles and wall losses. Air exchange was included in the model as well as mass transport through a boundary layer next to the bleach. Parameters in the model, such as rate coefficients were based on literature values whenever possible. In the current study, this kinetic model was used to investigate the impact of changing indoor conditions on gas-phase bleach product concentrations and to provide parameters to a computational fluid dynamics (CFD) model which can investigate spatial heterogeneity indoors.

Simulations suggested that air-exchange must be high (> 5 h-1) in order to compete with other indoor loss pathways and reduce concentrations of bleach products. Acidification of bleach on surfaces increases HOCl, Cl2 and ClNO2 significantly down to pH 7.5, but does not impact the total concentration of chloramines. Additionally, increasing the surface area or decreasing the room volume by a certain factor would increase concentrations of HOCl, Cl2 and ClNO2 by the same factor. Results from the CFD simulations suggested that there was a large spatial heterogeneity for many of the gas-phase bleach products.

References

[1] B. Matulonga et al., Resp. med. 117, 264-271 (2016).
[2] J. M. Mattila et al., Environ. Sci. Technol., 54, 1730–1739 (2020).

8IA.11

Aerosol Emissions from Biogas, LPG, and Wood Cooking in Nepal and the Impact of Fuel Mixes on Overall Pollution Burden. CHERYL WEYANT, Ryan Thompson, Nicholas Lam, Basudev Upadhyay, Prabin Shrestha, Shovana Maharjan, Kaushila Rai, Chija Adhikari, Amod Pokhrel, *University of Michigan*

Household air pollution from solid fuel cooking causes millions of deaths each year and contributes to climate change. The health burden can be reduced if households transition to cleaner cooking fuels such as LPG or biogas, yet emission measurements during household cooking is limited and the outcomes of using multiple fuels per household is poorly characterized. In this study, 20 households in Nepal were rigorously monitored over three seasons. Measurements included stove use monitoring on all stoves, fuel consumption assessments, and detailed emissions measurements from LPG, biogas, and wood stoves. Emission factors were reported for elemental carbon (EC), organic carbon (OC), particulate matter ($PM_{2.5}$), and carbon monoxide (CO). Biogas cooking emission factors were 7.4 ± 10.9 $mgMJ^{-1}$ for $PM_{2.5}$ and 0.2 ± 0.3 $mgMJ^{-1}$ for EC on a fuel energy basis, and were not significantly different from LPG stoves (9.5 ± 6.8 $mgMJ^{-1}$ for $PM_{2.5}$ and 0.3 ± 0.3 $mgMJ^{-1}$ for EC, $p > 0.05$). Wood stoves emitted 50 times more $PM_{2.5}$ than biogas on a fuel energy basis and 230 times more EC. EC emissions were about 3% of total particle emissions from biogas and LPG stoves. Most $PM_{2.5}$ emissions from gas stoves were attributed to food frying and stove ignition (90%), not the gas fuel (10%), implying that there is a limit to emission reductions that can be achieved with improved fuels. To assess the impact of using multiple fuels in a households, emission factors were integrated with fuel consumption and stove use data to estimate total household emission rates from cooking from all household stoves. This method allows the indoor emissions from different stove/fuel combinations to be quantified and compared. In addition, measurements were conducted to allow for assessments of seasonal trends in household emission rates.

8IA.12

Per- and Polyfluoroalkyl Substances (PFASs) in Fine Aerosols (PM2.5) during Floor Waxing. JIAQI ZHOU, Karsten Baumann, Naomi Chang, Jason Surratt, Wanda Bodnar, Zhenfa Zhang, Glenn Morrison, Joanna Atkin, Barbara Turpin, *UNC-Chapel Hill*

Per- and polyfluoroalkyl substances (PFASs), with their water- and heat-resistant properties, have been widely used in industrial and consumer products, including floor waxes and sealants. Studies have shown adverse health effects associated with PFASs exposure, e.g., increased risk of cancer and immunotoxicity. However, little is known about the extent to which PFASs are emitted during floor stripping/waxing, and the potential for occupational exposures and subsequent health risks. In our study, we measured PFASs concentrations in fine particles ($PM_{2.5}$) during floor stripping and waxing events performed in a university building and estimated the PFASs emission rates. $PM_{2.5}$ samples were collected on 37mm quartz fiber filters downstream of a multiple-jet 2.5 mm cut-point impactor before, during, and after floor stripping/waxing activities. Samples were analyzed for 34 targeted PFASs by LC-MS/MS on an AB SCIEX Triple Quad™ 6500 mass spectrometer system. In total, ten PFAS compounds were detected during floor waxing with concentrations ranging from 0.6-29.8 pg/m^3. Five of these were statistically significantly elevated in concentrations during stripping/waxing, specifically: perfluoro-2-methoxyacetic acid (PFMOAA), perfluoro-n-butanoic acid (PFBA), perfluoro-n-hexanoic acid (PFHxA), perfluoro-n-heptanoic acid (PFHpA), and sodium perfluoro-1-octanesulfonate (PFOS). Emission rates and exposure implications for workers will be discussed.

8ID.1

The Underappreciated Role of Indoor Deposition in Determining Person-to-Person Aerosol Transmission. TAMI BOND, Delphine K. Farmer, Paul Francisco, Shantanu Jathar, Jeffrey R. Pierce, *Colorado State University*

The COVID-19 pandemic demonstrated that the public health community would benefit from better information on the mechanisms of particle transport between individuals. In outdoor settings, transport between two people is driven by wind and its fluctuations, and deposition has little effect on transport between people except for the very largest particles (100 µm). In indoor settings, both dispersion and removal of contaminated air are slower, so particle sizes that might carry infectious agents (1 or 10 µm) have longer transit times between people than they do outdoors. These longer person-to-person transit times mean that deposition to indoor surfaces plays an important role in the prediction of transport. For 10 µm particles, deposition loss rates are of the same order as ventilation loss rates. Yet particle deposition velocities are not well understood, with established models predicting much lower deposition rates than the sparse existing measurements. Building-management strategies, such as increasing ventilation or filtration, can decrease exposure to airborne infectious agents. We simulate mitigation strategies in residential and commercial situations using a multi-zone process model, and show how uncertainties in deposition velocity might cloud the ability to predict the benefit of these strategies.

8ID.2

Using Insights from Aerosol Science to Investigate the Dynamic Interplay Between Social Distancing Duration and Intensity in Reducing COVID-19 US Hospitalizations.

Pai Liu, PAYTON BEELER, Rajan K. Chakrabarty,
Washington University in St. Louis

We uncover and highlight the importance of social distancing duration and intensity in lowering hospitalization demand-to-supply during the COVID-19 epidemic in the United States (US). We have developed an epidemic progression model which includes susceptible-exposed-infected-recovered (SEIR) dynamics, age-stratified disease transmissibility, and the possible large-scale undocumented transmission of COVID-19 taking place in the US. The model accurately predicts the disease reproduction ratio (R0), which is analogous to aerosol aggregation kernel encountered in aerosol science. Calibrating our model using epidemiological data from the early stage of the pandemic (March 19-28) enabled us to unbiasedly address the question “How long and with what intensity does the US need to implement social distancing intervention during the COVID-19 pandemic?”. For social distancing lasting less than two weeks, we find a near-linear decrease in hospital beds demand with increasing intensity (????) of social distancing. For social distancing lasting longer than two weeks, our findings highlight the diminishing marginal benefit of social distancing, characterized by a linear decrease in medical demands against an exponentially increasing social distancing duration. Long-term implementation of strict social distancing with ???? > 50% could lead to the emergence of a second wave of infections due to the large residual of susceptible population, which highlights the need for contact-tracing and isolation before re-opening of the economy. Finally, we investigate the scenario of intermittent social distancing, and find an optimal social-to-no-distancing duration ratio of 5:1 corresponding to a sustainable reduction in medical demands.

8ID.3

Alternative Facemask Materials for DIY Facemask in the Time of COVID-19. Jessica Mirrielees, BO CHEN, Michael Moreno, Sarah Brooks, *Texas A&M University*

The effective use of face masks is crucial in preventing the spread of respiratory diseases such as COVID-19. The World Health Organization and the Center for Disease Control suggested that homemade masks may have some protective benefits when there was a shortage of medical face masks. To determine the best material for making homemade masks, several commercially available filter materials: an allergen filter, a vacuum bag, a bandana, a heavy-duty tool wipe, an industrial composite filter, as well as an N95 particulate respirator and a surgical mask were tested against size-resolved nonbiological surrogate particles (sodium chloride). Percent penetration over a range of diameters from 25 to 500 nm was measured for each filter sample at three different face velocities that simulate human breathing. Pressure drop was also measured to calculate the filter quality factor. Amongst the samples, the allergen filter is the best at air filtration. The results show that the percent penetration of 300 nm particles at a face velocity of 13 cm s-1 for the allergen filter was approximately 5%, for the industrial composite filter was around 11%, for the heavy-duty tool wipe was approximately 26%, and for other samples were approximately 30% or higher. The pressure drop for all the samples met the NIOSH N95 standard at low face velocity but failed at a high face velocity. Based on filter quality, the allergen filter, industrial composite filter, and vacuum bag were the best homemade mask options tested in this study. This study can provide guidance for the public to consider while sourcing material to make masks.

8ID.4

New Tools for a New Virus. TIMOTHY GORDON, Patricia Keady, Dominick Heskett, Braden Stump, Brian Annis, Touzong Xiong, Mark R. Stolzenburg, *Aerosol Devices Inc.*

Although common sense suggests that aerosolized SARS-CoV-2 must be an important vector for the transmission of COVID-19, no public studies have yet shown that viable SARS-CoV-2 can be isolated from ambient aerosol, nor do we know typical size distributions of virus particles or the number of virions per particle. Aerosol Devices Inc is developing new instrumentation, based on condensation growth tube (CGT) technology, to enable researchers to answer basic questions currently hampering mitigation of the COVID-19 pandemic. We have used finite element analysis to model laminar flow, heat/mass transfer and condensation-driven droplet growth in our initial CGT design to minimize instrument footprint and impaction losses. Our model determines where condensation of supersaturated vapor begins along a particle's trajectory and then calculates the subsequent droplet growth, accounting for the Kelvin effect on the equilibrium vapor pressure over a curved surface and non-continuum regime transport of both vapor and latent heat from the droplet. In this presentation we discuss how we are using this model to guide the development of the CGT as a "front end" for a virus collection/detection platform. Components of the platform may be swapped out depending on the needs of the particular application. For example, we are currently collaborating with two universities to integrate into the platform two different virus detectors based on unrelated technologies. In collaboration with colleagues from several other universities, we are developing instruments from the same basic platform that do not directly detect viruses but preserve them either in viable form as a concentrated liquid suspension or inactivated on a solid genomic preservative for subsequent laboratory analysis.

8ID.5

Field Measurements Related to Potential Aerosol Transmission of COVID-19. Andrew Jeremijenko, Wasim Javed, Joel Malek, BING GUO, *Texas A&M University at Qatar*

Aerosol samples were collected with a high-efficiency bioaerosol sampler from multiple indoor facilities and tested for SARS-Cov-2 virus using real-time quantitative reverse-transcription polymerase chain reaction (PCR) assays. Surface swab samples were also collected from these facilities and tested for the virus with the same assays. The highest aerosol virus concentration was detected in a patient room, at a level similar to that reported by other researchers. Positive aerosol samples were also obtained from a moderately crowded patient waiting area, where surface swab samples were also positive. However, aerosol samples tested negative from several other places, including an intensive care unit, a medical laundry facility, a sparsely visited fever clinic, and a long-term care facility. The aerosol sampling results support the notions that face masks, high rate of ventilation, high-efficiency particulate air filtration are effective ways to suppress virus aerosol concentration. On the other hand, surface swab samples from an air handling unit (AHU) testing positive suggests that infection through air movement in the HVAC system is a possibility, if the AHU filters do not capture infectious particles with sufficient efficiency. Details of the results and discussion will be provided during the conference presentation.

8ID.6

Filtration Performances of Non-medical Materials as Candidates for Homemade Face Mask Filters. WEIXING HAO, Andrew Parasch, Stephen Williams, Jiayu Li, Hongyan Ma, Joel Burken, Yang Wang, *Missouri University of Science and Technology*

The recent outbreak of the coronavirus disease (COVID-19) is causing a shortage of personal protective equipment (PPE) in different countries of the world. Because the coronavirus can transmit through droplets and aerosols, face masks, especially N95 respirators that require complex certification, are urgently needed. Given the situation, the U.S. Centers for Disease Control and Prevention (CDC) recommends that “in settings where face masks are not available, healthcare personnel might use homemade masks (e.g., bandana, scarf) for the care of patients with COVID-19 as a last resort.” Although aerosols and droplets can be removed through the fibers of these fabrics through a series of filtration mechanisms, their filtration performances have not been evaluated in detail. Moreover, there are a series of non-medical materials available on the market, such as household air filters, coffee filters, and different types of fabrics, which may be useful when medical mask filters are not available. In this study, we comprehensively evaluated the overall and size-dependent filtration performances of non-medical materials. The experiments were conducted under different face velocities to consider the influence of the filtering area used by the wearer. The flow resistance across these filter materials is collected as an indicator of the breathability of the materials. Based on the results, multiple layers of household air filters are able to achieve similar filtration efficiencies compared to the N95 material without causing a significant increase in flow resistance. Considering that these air filters may shed micrometer fibers during the cutting and folding processes, it is recommended that these filters should be inserted in multiple layers of fabrics when manufacturing homemade face masks.

8ID.7

Application of the NanoAerosol Generator in Efficacy Evaluation of Facial Coverings. SIQIN HE, Derek Oberreit, Steve Kosier, *Kanomax FMT, Inc.*

The interest in filtration efficiency characterization tests of face masks and respirators has grown substantially in response to the worldwide spread of Covid-19 and the consequent demand increase of personal protective equipment (PPE) supplies. It is believed the particulate filtration efficiency of the filter material used for manufacturing PPEs primarily affects how effectively they can protect the user against health and safety risks from airborne particles. The characterization of filtration efficiency is therefore critically required to evaluate the protection level of a PPE product and guide the proper use of it. Despite the extra size classification step in their generation, monodisperse test particles are usually preferred for testing filters due to the fact that filtration efficiency is a parameter that is primarily size-dependent. Substantial information can get lost in the integral measurements of a polydisperse test, especially for the applications with a few sizes of interest in particular, e.g. the Covid-19 related studies. With smaller droplets (nominally 500 nm) than other aerosol generators, the Kanomax NanoAerosol Generator (NAG) 3250 can minimize the surfactant effect that makes it challenging to produce monodisperse aerosols from monodisperse particle standards.

In this work, the NAG 3250 was used as the particle generator to aerosolize 100 and 300 nm monodisperse polystyrene latex (PSL) particles in a filter testing rig designed based on the ASTM standards for surgical masks. These generated monodisperse PSL particles were subsequently used to evaluate the particulate filtration efficiency of more than 20 facial covering materials in comparison with a few commercial facial masks and respirators. The results were used to guide the selection of alternative facemasks.

8ID.8

Filtration Efficiency of Respirators and Masks – How You Test Matters. TIM JOHNSON, Justin Koczak, Andrea Tiwari, *TSI Incorporated*

Recent global health developments have highlighted that the particulate filtration efficiency testing standards and procedures covering respirators, masks, and their media are often written in very general terms. These methods can rely on guidance from other organizations to provide the rest of the necessary details. Testing of surgical facemasks in the United States, for example, can require understanding requirements put forth by the ASTM, NIOSH, and the FDA, depending on the mask classification. This creates confusion for producers and testing organizations.

Moreover, in response to high demand, non-standard fabric and homemade masks are being produced in increasing volumes. A lack of clear testing guidance for this new class of masks has resulted in a wide variety of methods being used that give conflicting results, which compounds the problem. This trickles down to the end user, who may not have an accurate understanding of how well their mask or respirator is protecting them.

This presentation seeks to help clarify some of this confusion. Its objective is to provide members of the filtration and aerosol science communities with a basic understanding of the key factors at play in filtration testing. This will enable these scientists and engineers to better understand the methods and standards they may be required to test in accordance with; and to help them make better-informed decisions when deciding how to test and do research on masks and respirators that may fall outside the purview of officially-published guidance or requirements.

To this end, this presentation will address some key filtration fundamentals, selected testing methods, and the standards, the instrumentation that they depend on - aerosol generators and their resulting particle size distributions, different detector types, etc. - and how these factors can affect the test results.

8ID.9

Numerical Investigation on Transport and Removal of Airborne Virus from a Hospital Room. SUNIL KUMAR, Maria King, *Texas A&M University*

The COVID-19 virus ability to spread from an infected person to a healthy person through cough and sneeze has made the situation more critical. The droplets generated in cough and sneeze has the ability to travel a significant distance before falling on the ground. However, the small droplets (< 50 µm) possibly containing coronavirus (known of size 60-80 nm) generated in the process gets suspended in the air and transported with the air currents. The isolation wards and hospital rooms used for keeping the patients for treatment is considered to be a highly unsafe zone. Controlling the spread of airborne infectious viruses including COVID-19 in a health care facility is a serious concern to patients, staff, and visitors. Most of the hospital rooms use ceiling-based exhaust air inlet/outlet ventilation. The ventilation air entering the room through the duct provides comfort to the occupants of the room. On the other hand, the ventilation air also transports and spreads the small size bacteria and airborne viruses in the room. To minimize the spread of airborne infections, the hospital rooms need to be designed in such a manner that the residence time of the airborne bacteria or virus is reduced to a minimum. In this paper, a detailed study has been presented to predict the spreading process of bacteria/viruses in a scaled NIH hospital room using Computational Fluid Dynamics (CFD). The study is focused on predicting the formation of different pockets of contaminated air with their dynamic locations at different times. The examination considers the installation of air-curtain and investigates their effect in limiting the spread of the virus with the removal of contaminated air. The paper incorporates CFD analysis of air movements in the room and recommends necessary changes in design for decreasing the residence time of contaminated air, which will help to protect the health care workers and visitors.

8ID.10

Association between Long-Term PM2.5 Exposure and COVID-19 Spread in the United States. PAI LIU, Payton Beeler, Rajan K. Chakrabarty, *Washington University in St. Louis*

The rampage of coronavirus disease 2019 (COVID-19) epidemic has spread across the United States (US) and killed more than a-hundred-thousand people. Latest epidemiology studies have identified long-term exposure to air pollution as a significant contributor to the COVID-19 mortality. However, the influence of various PM2.5 composition on COVID-19 progression – an essential information necessary for enforcing effective air pollution regulations – remains an unknown research question. Here we discuss the results on a statistical analysis investigating the relationship between the PM2.5 chemical composition and COVID-19 progression rate in the continental US between March 2 and April 29, 2020, during which the country was under the stay-at-home order. We collected state-level long-term (between 2000 and 2017) PM2.5 composition dataset produced by Van Donekelaar et al. (2019). This dataset is a fusion of three different sources: ground-based monitors, GEOS-CHEM model, and satellite observations. The derived PM2.5 composition data is next correlated with the corresponding state-wise basic reproduction ratio (R0) values of COVID-19, which were inferred from the time-evolution of epidemic size (between March 2 and April 29, 2020) with the well-established susceptible-exposed-infected-removed model. This presentation discusses a significant positive correlation between the PM2.5 composition and the R0 values of COVID-19.

8ID.11

Estimating Deposition of Viral, Bacterial and Fungal Aerosols in the Human Respiratory Tract: A Two Model Comparison. LYNN SECONDO, Jessica Sagona, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Modeling of the regional and total deposition of bioaerosols in the respiratory system might help in determining risk of disease development due to exposures. Computational models can provide estimates of particle deposition fractions for given breathing and particle parameters; however, most models have not focused on bioaerosols. We calculated deposition fractions in a reference adult with a recent bioaerosol-specific lung deposition model (BAIL) and with two multiple-path deposition models (MPPD) for three different breathing scenarios: “default” (subject sitting upright and breathing nasally), “light exercise”, and “mouth breathing”, keeping breathing parameters and bioaerosols characteristics the same for each scenario. The modeled species included: Bacillus anthracis spores and cells, Aspergillus clavatus and Stachybotrys chartarum fungal spores, and the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) as individual virus particles, virus as aerosol, and virus as respiratory droplets. BAIL generally calculated higher deposition fractions in the extrathoracic region and lower deposition fractions in the alveolar region than the MPPD. Deposition fractions in the tracheobronchial region were similar among the three models; total deposition fraction patterns tended to be driven by the extrathoracic deposition fraction, with BAIL resulting in higher deposition in some scenarios. The extent of difference between deposition fractions calculated by BAIL and other models depended on particle size, with BAIL generally indicating lower total deposition for bacteria-sized bioaerosols. We conclude that BAIL predicts somewhat lower deposition and, potentially, reduced risk of illness from smaller bioaerosols that cause illness due to deposition in the alveolar region. According to BAIL, 16% of the SARS-CoV-2 virus will deposit in the alveolar region. On the other hand, it suggests higher deposition in the extrathoracic region, especially for light exercise and mouth-breathing scenarios. Additional comparisons between the models for other breathing scenarios, people’s age, and different bioaerosol particles will help improve our understanding of bioaerosol deposition.

8ID.12

The Significant of Turbulence Stochastic Accuracy in Simulation of Aerosol Transmission. AMIR A. MOFAKHAM, Goodarz Ahmadi, *Clarkson University*

As a result of the ongoing COVID-19 pandemic, attention has been given to numerical simulation of aerosol transport and dispersion to assess the risk of human-to-human airborne virus transmission. The respiratory droplets emitted by an infected person via coughing, sneezing, talking, and breathing interact with ventilation airflows that are typically in the state of turbulent motion. To model particle-laden turbulent airflows, commonly a RANS turbulence model is used which requires using a turbulence stochastic model to include the turbulence dispersion effects on micro and nano-droplets. However, the default turbulence stochastic model of commercial CFD software is usually unable to correctly predict the turbulence fluctuating velocity field. A series of simulation results were presented where the results of the default turbulence stochastic model of commercial CFD software are compared with the improved Continuous Random Walk (CRW) and Discrete Random Walk (DRW) stochastic model. It was shown that the new improved CRW and DRW models correctly predict the aerosol dispersion and deposition in various passages, while the default model could lead to several orders of magnitude errors for certain size ranges. Therefore, the new model could be used to provide technical guidance on respiratory virus transmission such as SARS-CoV-2.

8ID.13

Numerical Simulation of Aerosol Transmission and Droplet Expulsion of COVID-19 by Speech. AMIR A. MOFAKHAM, Brian T. Helenbrook, Tanvir Ahmed, Byron D. Erath, Andrea Ferro, Deborah M. Brown, Goodarz Ahmadi, *Clarkson University*

The rapid spread of COVID-19 infection has raised questions regarding the potential routes of SARS-CoV-2 virus transmission among individuals. In the past, attention has been given to coughing and sneezing, but recent studies have shown that the number and size distributions of airborne droplets generating during speech are comparable to those of droplets emitted by coughing. However, droplet dynamics during speech are not fully understood. To address this need, a computational model was developed using ANSYS-Fluent with additional user-defined functions to track the motion and dispersion of droplets arising from specific speech utterances. Droplet evaporation and gravitational sedimentation effects were included in the analysis. Experimental airflow velocity and droplet size distributions at the mouth exit during the pronunciation of fricative consonants were used as the inlet boundary condition. Droplet dynamics in both unconfined and indoor environments were simulated. The simulations results were used to assess the risk of airborne human-to-human virus transmission from an infected person to other individuals in both the near and far-field. The effect of relative ambient humidity on droplet propagation was also examined. A series of simulations were performed, and the effects of the relative ambient humidity and the ventilation system on the droplet transmission were examined.

8ID.14

Air Quality Sensing-based Surveillance for Detection of Pathogens Causing Healthcare-associated Infections.

HEMA RAVINDRAN, Shantanu Sur, Suresh Dhaniyala, *Clarkson University*

As per Centers for Disease Control and Prevention (CDC), on any given day, 1 in 31 hospital patients suffer from at least one healthcare-associated infection (HAI). Microorganisms inhabiting hospital are distinct from those found in other indoor environments and are responsible for causing HAI and impacting patient recovery and outcome. Pathogens such as methicillin-resistant Staphylococcus aureus (MRSA), multi-drug resistant Gram-negative Bacilli, norovirus, Clostridium difficile, Acinetobacter baumannii, persist in the hospital environment for days and can predominantly disperse through air. The airborne transmission has gained attention recently with the SARS CoV-2 outbreak, where droplets and aerosol are thought to play a major role for the spread of infection, and hospitals are particularly vulnerable due to the congregation of COVID-19 patients.

To obtain a community-level understanding of airborne pathogens in a hospital environment, we characterized the airborne bacterial, fungal, and viral population over the course of 1 year in a local hospital. We used a low cost, portable air-quality monitoring and bioaerosol sampling device, 'TracB' (Trace Aerosol sensor and Collector for Bio-particles; Potsdam Sensors Corp), for this study. The devices are deployed in five critical zones of a hospital to monitor air quality in real time and analyze airborne pathogens offline. We observed a positive correlation (R2 = 0.67) between particle concentration and microbial load in the air. The contribution of outdoor air infiltration and human activities in the indoor aerosol concentration was evaluated. For the collected bioaerosol samples, metagenomics was used to characterize the microbial diversity and quantitative PCR for a targeted detection of HAI pathogens. Spatial correlation analyses revealed a communal behavior of pathogens with the naive microorganisms in hospital air. We will present details of the sampler, air monitoring, and pathogen characterization procedures, and the results from our ongoing work.

8ID.15

Investigating Filtration Efficiencies of Non-standard Fabric Filters.

SUMIT SANKHYAN, Hannah Teed, Teresa Barnes, Peter Ciesielski, Karen Heinselman, Sameer Patel, Marina Vance, *University of Colorado Boulder*

As a public health response to control the coronavirus disease (COVID-19) global pandemic, there is an urgent need to manufacture, test, and supply respirators and masks to healthcare providers, essential workers, and to the general population. This novel need is accompanied by a necessity to test the filtration efficiency and inhalation resistance of masks using non-standard materials as filters. It is essential to study the effects of factors such as mask fit, length of usage, and degradability due to repetitive use on filtration behavior of non-standard and "do it yourself" (DIY) masks in order to achieve optimum filtration performance and to put forth recommendations among the general public for mask usage.

In this study, overall and size-resolved filtration efficiencies were calculated for different mask prototypes and filter materials. A Scanning Mobility Particle Sizer (TSI) and an Aerodynamic Particle Sizer (TSI) were used to characterize the filtration efficiency of particles in the 12 nm- 10 µm size range. We tested various mask prototypes such as DIY cloth masks, surgical masks, N95 masks, BFE99 filters, and KN95 4-ply face masks. Preliminary results show that overall filtration efficiencies ranged from 30% to 100% for different mask prototypes. The inhalation resistance values for these masks ranged between 2-20 mm water column. Secondary investigations included studying the effect of degradability of the fabric filter material due to washing and drying on their filtration performance. We also investigated the potential of novel filter materials such as cellulose nanofibrils (CNF) coated fabric material as a substitute for DIY masks.

8ID.16

Properties of Materials Considered for Improvised Masks. STEVEN ROGAK, Timothy Sipkens, Hamed Nikookar, Mark Gunn, Jing Jane Wang, *University of British Columbia*

SARS-CoV-2, the virus responsible for COVID-19, was deemed a pandemic by the World Health Organization in 2020, with global reach and killing half a million people by the beginning of July 2020. The pandemic saw a surge in demand for surgical masks and N95 respirators by healthcare practitioners, which made it impossible for the general public to obtain adequate respiratory protection. This was convolved with confusing messaging from officials about whether mask use by the general public was advisable. In response, people started using common household materials, such as cloth masks, with little understanding of the factors controlling mask effectiveness. This work reconsiders a range of these materials and presents size-resolved penetration curves and pressure drop, which gives a measure of breathability, for each material. A sodium chloride challenge aerosol is generated using an ultrasonic mesh nebulizer, before being charge neutralized and passed through a portion of the candidate mask material, and finally characterized using an optical particle sizer (OPS). For thin materials, multiple layers were also considered. Gauze, dried baby wipes, and a knit jersey material were found to perform relatively well, while silk and spandex performed relatively poorly.

8ID.17

A Flexible Particle Filtration Efficiency Measurement System (PFEMS) for N95 Respirators, Surgical Masks, and Novel Filter Media. GREGORY SMALLWOOD, Joel Corbin, Fengshan Liu, Jalal Norooz Oliaee, Ian Leroux, Prem Lobo, *National Research Council Canada*

Shortages of N95 respirators, surgical masks, and related filter media (collectively referred to as filtration samples) during the COVID-19 pandemic has led to a rush of filtration sample production, including those from many companies new to the field. These filtration samples have been tested using a number of protocols, including NIOSH TEB-APR-STP-0059 (developed for certifying the industrially-targeted N95 respirator), ASTM F2100/F2299 (required for US FDA Particle Filtration Efficiency (PFE)), GB 2626 (China), and other related tests. While all of these protocols may be described as using particles with count median diameter of approximately 100 nm, differences in the face velocity and test particle properties (including size and material density) as well as aerosol neutralization may lead to different results obtained for the same filtration samples when tested in accordance with these different protocols.

In order to rapidly provide filtration efficiency data compatible with all of the above testing protocols, the National Research Council of Canada (NRC) has developed a flexible measurement system to evaluate the performance of filtration samples (particle filtration efficiency measurement system; PFEMS). PFEMS is based on pairs of condensation particle counters (CPCs) and scanning mobility particle sizers (SMPSs), and was initially designed as a modification of the NIOSH protocol. Using NaCl and polystyrene latex (PSL) aerosols, and utilizing a variable face velocity, we demonstrate that PFEMS is a highly flexible and rigorously validated system for simultaneously measuring the flow resistance (pressure drop), number-based filtration efficiency (NFE) and size-resolved filtration efficiency (SRFE), as well as determining mass-based filtration efficiency (MFE), of filter media, surgical and other masks, and respirators using aerosol research instrumentation.

An overview of filtration efficiency testing, the capabilities of the NRC PFEMS, and the physical causes of inconsistent results between the protocols are discussed.

8ID.18

Performance of a No-Sew Origami Mask for Improvised Respiratory Protection. JAMES SMITH, Jonathan Realmuto, Terence Sanger, Michael Kleinman, Michael J. Lawler, *University of California, Irvine*

The commercial supply of surgical masks and N95 respirators has become severely strained during the ongoing coronavirus disease 2019 (COVID-19) pandemic, requiring the use of improvised respiratory protection for front-line workers and at-risk public. However, many improvised face masks do not provide adequate filtration properties, are constructed using specialized fabrication techniques, or fail to provide a sufficient face seal. We have designed a mask fabrication technique that makes use of a folding procedure (origami) to transform a filtration base material into a mask. The design can provide a range of filtration efficiencies based on material choice, can be easily scaled to accommodate different facial sizes, and can be fabricated by non-experts. Using a mannequin-based fit test simulator, we experimentally explore the trade-off between filtration efficiency and flow resistance for different base materials and explore other key features such as carbon dioxide retention and inhalation from expired breath. We observed that masks constructed with higher filtration efficiency materials often exhibited a large range of expected efficiencies, implying that high efficiency media typically corresponds to high pressure drops, and ultimately higher leakage. Our results provide an improved understanding of the impacts of pressure drop on leakage and, in addition, provide a more reliable indicator of the expected performance of a mask design. This research can provide evidence-based guidance on the selection of materials and the design of improvised masks to enable non-experts the ability to rapidly produce respiratory protection on-demand.

8ID.19

Assessing Potential Airborne Virus Transmission in University Classrooms. KATHRYN VAN VALKINBURGH, Nigel Kaye, Ehsan Mousavi, Vincent Blouin, Ali Nafchi, Andrew Metcalf, *Clemson University*

As a result of the coronavirus outbreak, many educational institutions and universities have faced questions and uncertainties concerning the safety of hosting on-campus, in-person classes. Airborne transmission is a major concern for many infectious pathogens, including the novel coronavirus. Even with sufficient social distancing and surface disinfection measures taken, there is still risk of exposure through airborne transmission. Ventilation is the principle engineering method used to control airborne health hazards. In a classroom setting, the design of the ventilation system will affect factors such as the direction of airflow throughout the room, the rate of air exchange, and the exhaust point or recirculation pattern. The goal of this study is to evaluate such airborne transmission risk by first examining the ventilation systems of actual classrooms and evaluating the potential for viral transmission between indoor occupants in the same classroom or adjacent rooms in the same building.

This talk will discuss the results of ventilation testing of several different classrooms on Clemson University’s main campus. The classrooms represent a variety of sizes, layouts, building ages, and ventilation types. In each classroom, a particle atomizer was used to release a large number of aerosol particles ranging from 0.2 µm to 10 µm in diameter into the air. Seven different particle counters were placed strategically around each classroom. The particle counters tracked concentration over time to assess how quickly the particles were removed by the ventilation system. The experiment aims to evaluate the personal exposure risk of the various classroom ventilation systems in order to mitigate potential health impacts as it relates to the spreading of a viral pathogen.

8ID.20

Viable Virus Transport in Ventilation Airflow.

TATIANA BAIG, Maria King, *Texas A&M University*

Currently little is known on how SARS-CoV-2 spreads indoors and its infectability. The objective of this study is to gain more knowledge on the effect of environmental factors on the spread and infectivity of virus aerosols in the built environment. Understanding how the virus transmits indoors would allow for early detection of viral particles in room sized spaces. Bovine coronavirus (BCoV), was used as virus simulant in laboratory experiments conducted in a controlled humidity cabinet at Biosafety Level 2. An air-jet nebulizer was used to disseminate known numbers of BCoV. Particle tracking velocimetry with shadowgraphy techniques was used to monitor the effect of environmental conditions (temperature and relative humidity) on the size distribution and velocity of the virus particles. After aerosolization, the surface in the cabinet was sampled at regular time intervals to assess the number of particles impacted. The samples were quantified using quantitative polymerase chain reaction (qPCR). The virus aerosols that remained suspended in the air were collected using the portable viable bioaerosol collector (VBAC) with a reference air sampler and quantitated by qPCR. To monitor the effect of the ventilation on the virus movement, BCoV aerosols were also disseminated in a ¾ scale ventilated hospital model chamber equipped with several VBAC units operated at 100 L/min. The spatial-temporal distributions of the collected viral aerosols were enumerated using qPCR. Based on air property measurements, aerosol collections and the mechanical blueprint of the model chamber, a computational flow model was created to visualize the entrainment and movement of the virus in the ventilation airflow. Mitigation measures to reduce the spread of the virus were designed and modeled.

8ID.21

Agent Based Simulations of Human Interactions in Mixed Use Academic Buildings.

Sheryl Ehrman, ANUSHA SHETTY, Isaac Espinoza, Jochen Albrecht, Laxmi Ramasubramanian, *San José State University*

Transmission of COVID-19 occurs via respiratory droplets and aerosols emitted by infected persons which directly make contact with mucous membranes of the susceptible persons, or via droplet contamination of surfaces, which are touched by susceptible persons, who then touch mucous membranes. This surface route is currently thought to be less important than the direct droplet/aerosol route. Preliminary results from studies of outbreaks suggest indoor transmission is more likely than transmission outdoors [1]. To reduce transmission in occupational settings, an emphasis is placed on social distancing and on reducing the density of people in a room. For educational settings, people may be on campus for less than 8 hours.

Reducing risk in the workplace is challenging because people move throughout the day. Here, we present a simple agent-based simulation approach using the open source software GAMA. Rule sets based upon class schedules, research and administrative activities, and numbers of participants in each category, are used to model human movement. Through a Lagrangian framework, nearest neighbor interactions for an ensemble of agents can be quantified, resulting in an assessment of risk to individuals of contracting SARS-CoV-2, and also a quantification of the scope of contact tracing that would be required. Using an Eulerian framework, density of people can be tracked for specific locations. The results of this analysis can be used to identify hot spots, where schedule adjustments can be used to reduce risk in campus settings. Furthermore, these simulations could be used to generate inputs to SEIR models, enabling more realistic simulation outcomes. The model covers only exposure on campus and does not consider off-campus interactions. It also assumes rational and law-abiding behavior, which related research on our campus has shown to be an oversimplification of actual human behavior.

[1] Leclerc QJ, Fuller NM, Knight LE et al. What settings have been linked to SARS-CoV-2 transmission clusters? [version 2; peer review: 1 approved]. Wellcome Open Res 2020, 5:83 (https://doi.org/10.12688/wellcomeopenres.15889.2).

8ID.22

Evaluation of Aerosol Containment of Barrier Devices Used for Airway Management: Methodological Development and Efficacy Studies. CHRISTOPHER NIEDEK, Richard Fidler, Jan Hirsch, David Robinowitz, Qi Zhang, *University of California, Davis*

There is mounting evidence for SARS-CoV-2 transmission via bioaerosols emitted by infected individuals. This has prompted the use of barrier devices for bioaerosol containment in hospital settings. These devices are commonly named “aerosol boxes” despite the lack of empirical evidence demonstrating that such devices can effectively contain aerosols. Our group has designed a methodology for evaluating the aerosol containment capability of barrier devices and have performed testing on several designs.

Aerosols are generated from a solution of known composition and low instrumental background. The aerosols are then directed into a simulation manikin’s airway and ejected out of the manikin’s mouth, simulating respiration. For comparison, the barrier devices are placed over the head of the manikin. Using concurrent measurements from a high-resolution time-of-flight aerosol mass spectrometer and a condensation particle counter, aerosol leaks outside of barrier devices can be qualitatively and quantitatively compared at pre-defined positions.

The results suggest aerosols can leak through incompletely sealed arm holes and edges of the barrier devices. Unsealed arm holes may inadvertently direct aerosols towards the healthcare worker using the device for protection, in particular if the foot end of the barrier device is sealed. Moreover, a plume of aerosol may be released when removing the barrier devices. This can be avoided if care is taken to evacuate particulate matter from the device prior to removal with a suction device.

The methodology described here demonstrates the feasibility of determining aerosol containment efficacy of barrier devices. This study utilized inorganic aerosols and thus potential infection from exposure to leaked aerosols was not explored. However, preliminary data indicates the need for caution when employing barrier devices for bioaerosol containment. Our results demonstrate that barrier devices cannot replace other types of personal protective equipment when performing airway management in potentially infective patients.

8ID.23

HOME-FIT: HOmemade Masks for Everyone Fit and Improvement Testing. CANDICE SIRMOLLO, Karl Haro von Mogel, Don Collins, Mikeal Roose, *University of California, Riverside*

Homemade masks are commonly used to protect the general public from the spread of infectious respiratory diseases such as COVID-19 when surgical masks and N95 respirators are in short supply or are limited to healthcare workers. The usage of masks is recognized to play an integral role in reducing droplet transmission from the wearer to others, but can also reduce airborne transmission from the surrounding environment to the wearer. Airborne transmission via virus-containing particles can be an important form of transmission for many types of infectious diseases and its mechanisms should be considered when selecting a mask. Mask designs and materials vary significantly, resulting in a wide range of particle filtration and breathability levels. Several recent studies have investigated the filtration efficiency of particles through mask materials alone, providing the public with better informed guidance on what materials to select for a mask. However, very little is understood concerning different mask designs and the fit of the masks on different face shapes and sizes. To investigate this critical knowledge gap, testing has been conducted with human volunteers to evaluate different mask designs. Tests were conducted while various exercises are performed that are representative of real-world activities including normal breathing, deep breathing, turning head side to side, raising head up and down, talking out loud, grimacing, and bending over. Common mask designs have been tested for different face shapes and sizes, as well as variations of mask sizes, nose bridges, elastic vs. tie options, and fabric types. The size dependence of the filtration efficiency of particles between 0.01 and 1 µm that are able to leak inside of different mask designs are investigated. The results of this testing have guided the development of improved mask designs to provide optimal protection from the transmission of airborne respiratory diseases.

8ID.24

Infection Risk Assessment of COVID-19 through Aerosol Transmission: A Case Study of South China Seafood Market.

Xiaole Zhang, Zheng Ji, Yang Yue, Huan Liu, JING WANG, *ETH Zurich/Empa*

The Corona Virus Disease 2019 (COVID-19) is rapidly spreading throughout the world. Aerosol is a potential transmission route. We conducted the quantitative microbial risk assessment (QMRA) to evaluate the aerosol transmission risk by using the South China Seafood Market as an example. The key processes were integrated, including the viral shedding, dispersion, deposition in air, biologic decay, lung deposition and the infection risk based on the dose-response model. The available hospital bed for COVID-19 treatment per capita (1.17×10^{-3}) in Wuhan was adopted as a reference for manageable risk. The median risk of a customer to acquire SARS-CoV-2 infection via the aerosol route after one hour of exposure in the market with one infected shopkeeper was about 2.23×10^{-5} (95% confidence interval: 1.90×10^{-6} to 2.34×10^{-4}). The upper bound could increase and become close to the manageable risk with multiple infected shopkeepers. More detailed risk assessment should be conducted in poorly ventilated markets with multiple infected cases. The uncertainties were mainly due to the limited information of the dose-response relation and the viral shedding which need further studies. The risk rapidly decreased outside the market due to the dilution by ambient air, and became below 10^{-6} at 5 m away from the exit.

8JS.1

Qishen Huang - Seeking for Postdoctoral Research Position.

QISHEN HUANG, *Virginia Tech*

My name is Qishen Huang, a fifth-year Ph.D. student in Dr. Peter Vikesland group at Virginia Tech. I plan to graduate in the summer in 2021 and am trying to find a postdoctoral position in the field of aerosol chemistry and aerosol physics. I worked on the pH and chemical moiety characterization of micron-size droplets; thus I'm particularly interested in the characterization of air-water interface and mixing-states of atmospheric aerosols. Other than that, I'm also interested in the study of ice/cloud nucleation.

I was a chemist by training during undergraduate study and further studied in physical chemistry for my master degree. I joined Dr. Vikesland's lab in 2016 and started projects of designing functionalized gold nanoparticles (AuNPs) for analyte detection using surface-enhanced Raman spectroscopy (SERS). As time moved on, my research focus was shifted to the application of functionalized AuNPs in aerosol pH characterization. I found the realm of aerosol science very intriguing and is a field where my physical chemistry background fits in well. During my recent studies, I have studied the pH of different micro-size droplets, droplet evaporation behaviors as well as the crystallization properties of droplets. Some of the works are still on-going at this point.

I'm familiar with various instruments including UV-Vis, Raman spectroscopy, dynamic light scattering, contact-angle goniometer, and scanning electron-microscope etc. Moreover, I believe I can familiarize myself with new instruments in a short period after knowing the fundamentals of it. I also developed my skills in spectral and image data processing during my Ph.D. study using Mathematica and python, which I believe can be migrated onto different contexts shortly.

If you are interested in my recent studies and wanted to talk more, welcome to meet me at the meeting or email me directly at qishenh@vt.edu. Thank you.

8JS.2

Kumar Sarang (Marie Curie PH.D. Fellow), Seeking for Postdoc Position in the Field of Atmospheric Chemistry.

KUMAR SARANG, *ICHF PAS, Warsaw, Poland*

Presently, I am working as a research assistant and Marie Curie Ph.D. Fellow (NaMeS project) under the supervision of Prof Rafal Szmigielski at the ICHF PAS, Warsaw, Poland. The main aim of the research is to study the kinetics of the aqueous phase reactions of selected plant volatiles and investigate the secondary organic aerosol (SOA) products through the application of hyphenated mass spectrometry techniques. The significant fraction of PM2.5 in the atmosphere comes from SOA, which is a major concern for both the environment and human health. I currently have two peer-reviewed co-authored publications in ACS journals. So far, during my Ph.D. I worked on highly sophisticated laboratory techniques such as laser flash photolysis and GC-MS or LC-MS. I am also skilled in working on quantum calculations (ORCA) and reaction pathway simulation and modeling using COPASI.

Professional Experience:
Before the beginning of my Ph.D. in 2017, I worked on the smoke and trend analysis of tobacco and tobacco products (~ three years), where my main job was to analyze TPM, CO, and NOx in tobacco products (regular, HNB and electronic). I also worked for a short duration on resin production at Asian Paints Ltd. as a Product officer in 2014.

Research Interests:
I am interested in continuing my research career on understanding the aerosol formation and transformation processes, along with their impact on the environment and human health. Therefore, I am looking for opportunities where I can apply and expand my knowledge of understanding complex aerosol chemistry with the application of new experimental and modeling techniques to help and contribute to resolving uncertainty of its impact on the environment and human health.

Tentative availability:
I am supposed to defend my Ph.D. between August-October 2021, and presently, I hold no location preferences for future jobs.

8JS.3

Zhonghua Zheng, Ph.D. Candidate in Environmental Engineering and Science (UIUC), Faculty / Research Scientist / Postdoc.

ZHONGHUA ZHENG, *University of Illinois at Urbana-Champaign*

Introduction:
I am currently a Ph.D. candidate in **Environmental Engineering and Science** with a concentration in **Computational Science and Engineering** at the University of Illinois at Urbana-Champaign (UIUC), supervised by Prof. Nicole Riemer.

I have been a Data Scientist Intern at the industry and a Research Intern at the United States Department of Energy national laboratory for about three years.

Objective:
I am seeking for a Faculty / Research Scientist / Postdoc position.

Dissertation Research:
My **interdisciplinary dissertation research** investigates the integration of large-scale Earth system modeling and high-detail numerical model simulations via Data Science (Machine Learning). My research projects include but not limited to:

(1) **Built** computationally efficient **surrogate models** to predict aerosol mixing state at the global scale using a **supervised learning** approach
(2) **Quantified** error in aerosol mixing state induced by aerosol representation assumptions
(3) **Regionalized** the global aerosol mixing state using an **unsupervised learning** approach

Future Research:
My future research centers on integrating physics and chemistry, multi-source multi-sensor data, and a data-driven approach to improve the **modeling and engineering of complex urban environment systems** (e.g., project the effectiveness of air pollution mitigation measures).

Availability:
Tentative starting time is in Spring 2021 or Fall 2021.

Web: http://go.illinois.edu/zhonghua
Email: zzheng25@illinois.edu

8JS.4

Environmental Health Scientist: Exploring a Position to make Earth an Inhalable Place for Future Generations.

FARIA KHAN, *ICHF, PAS, Warsaw, Poland*

"*A scientist in his laboratory is not a mere technician: he is also a child confronting natural phenomena that impress him as though they were fairy tales*" ~ Marie Skłodowska Curie

After completing my BS (hons) in Applied Biosciences (2014) and MS in Industrial Biotechnology (2016), I started on my "fairytale journey" through a Ph.D. in Chemical Sciences from ICHF PAS, Warsaw, Poland in 2017 as a Marie Curie Early Stage Researcher. It is a co-funded position under the supervision of Prof. Rafal Szmigielski, co-supervised by Prof Jason D. Surratt from UNC, Chapel Hill. My research focus is on the **Toxicological Screening of Atmospheric Pollutants.**

My dissertation topic encompasses the *in vitro* toxicity testing of three important secondary organic aerosol (SOA) systems: a-Pinene SOA, Biomass Burning Aerosol and Isoprene derived SOA. It involves studying post-exposure perturbations in lung cells through high throughput screening and functional analysis. This has equipped me in handling instruments including spectrophotometers, fluorescent microscope, confocal microscope, and flow cytometer. At present, I am in a research secondment at UNC, Chapel Hill, USA, working on the final part of project and writing manuscripts for former two systems.

I have co-authored five peer-review research publications (three as first author) in nano-biotechnology domain from my BS and MS research and contributed to writing book chapters, systematic review, and a review article. Overall, I have a six years research experience in various scientific disciplines. I aspire young scientists through mentoring platforms such as CSIH Mentornet and NYAS platforms. During my MS, I was actively involved in science entrepreneurism trainings and university-based start-ups.

My future goals are to emerge as a scientific leader in environmental health and nanotechnology safety domain. I am exploring research scientist/ post-doctorate or industrial position. Will finally decide on what motivates me about the prospective position and how it will add to my knowledge and learning.A scientific research position related to policy-making shall be a dream job for me. I will finish my Ph.D in May 2021 and be available to join from June 2021. My geographical preference shall be an engaging position across US or E.U.

8JS.5

Joseph V. Puthussery, Ph.D. Candidate in Environmental Engineering and Science (UIUC), Looking for Postdoc Position in Instrument Development and Sampling Health-Related Aerosols.

JOSEPH V PUTHUSSERY, *University of Illinois Urbana-Champaign*

Introduction:
I am Joseph V. Puthussery a fourth-year Ph.D. student in Dr. Vishal Verma's "Illinois Lab for Aerosol Research" at the University of Illinois Urbana Champaign. My Ph.D. thesis is on the development of a comprehensive online oxidative potential (OP) measurement system to measure the real-time OP of ambient particulate matter (PM) using multiple acellular endpoints. My Ph.D. thesis objective is to collect highly time-resolved PM OP data and couple it with real-time PM chemical speciation data to provide a better mechanistic understanding of the redox properties of ambient PM.

Job interest: Post Doc

Research Experience:
(i) Real-time PM OP measurement system development and laboratory automation, (ii) participated in two long-term (> 3 months) field campaigns in Illinois, USA and New Delhi, India, (iii) source apportionment analysis, (iv) testing and development of a system for measuring the particle filtration efficiency of N95 respirators.

Research interests:
I am interested to work in the field of aerosol chemistry, instrument development, and health-related aerosols. I am also interested in working on developing more comprehensive real-time instruments to measure OP and various other chemical and biological (e.g. viruses) components in PM.

Anticipated availability: After May 2021

Geographical preferences: None

Contact: jvp3@illinois.edu

8JS.6

Sahil Bhandari, Final Year PhD in ChemE (UT Austin), Looking for Post-Doc Positions. SAHIL BHANDARI, *University of Texas at Austin*

Over the past four years of field measurements, air quality modeling, and high time resolution data mining in Igor, MATLAB, and R, 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 currently building a package in R to process the Positive Matrix Factorization results of the EPA PMF tool. Parallelly, 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 the 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 six second-author publications from my research.

Anticipated Availability: Beginning Spring 2021

Geographic Preference: California and Massachusetts

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. 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.

8JS.7

Meet the Job Seekers - Kayane Dingilian. KAYANE DINGILIAN, *The Ohio State University*

My name is Kayane Dingilian, and I am a Ph.D. candidate at The Ohio State University in the Department of Chemical and Biomolecular Engineering. I will be graduating at the end of December 2020 and will be available for a career position in January 2021.

I am seeking an academic position where I will be working primarily with undergraduates, whether in the capacity of faculty with research, as a lecturer, or as a postdoctoral scholar to further develop my teaching and research skills. During my graduate career, I developed senior-level coursework and lectured students in various levels of chemical engineering courses, with very positive results and feedback. I would like to continue with the same demographic in a full time career because of my ability to explain complex engineering concepts.

My primary research focus is aerosol physics with phase transitions and droplet freezing, even though I would also like to continue exploring aerosol chemistry. I excel at working as an experimentalist due to my characterization skills that facilitate connecting observed phenomena with theory and simulation. I enjoy employing techniques such as spectroscopy, scattering, and particle classifiers. I have also designed and built novel equipment for collecting quantitative data across various branches of the aerosol sciences. My interpersonal experiences in the laboratory include training graduate students, mentoring undergraduates, and collaborating with researchers across the U.S. and Europe.

I have ample experience using my communication skills to successfully deliver presentations at professional society conferences, within university-led symposia and competitions, and through outreach programs both on and off campus. I have been heavily involved in faculty-student development programs as well as laboratory safety program development and training.

I have experience living and researching on the West Coast, the East Coast and the Midwest, and I enjoyed those endeavors equally.

8JS.9

Li Li Ph.D. (Mechanical Engineering) Desired for a Post-Doctoral Research Position.

LI LI, *The University of Memphis*

I'm pursuing Ph.D. at The University of Memphis, advised by Dr. Ranga Gopalakrishnan and expected to graduate by April 2021. I have authored one article (J. Aerosol Sci. 140: 105481) comparing the predictions of Langevin dynamics simulations-based collision kernel models for diffusion charging of spherical aerosol particles to published experimental data. I have also extended this model to describe the charging of arbitrary shaped particles and validated the same by comparing with available experimental data. This work is currently being written up for publication and I will be happy to share the manuscript draft. Another facet of my current work involves the examination of ion-ion mutual recombination reactions that are mediated by interactions with neutral gas molecules. Lastly, using high length-to-diameter (>100) ratio cylindrical nanoparticles, I'm working on bipolar charging experiments to provide 1) unambiguous datasets for high aspect ratio cylinders that is currently unavailable in the literature and 2) test the charging model for nonspherical particles that I have developed.

In addition to these projects, I have also collaborated with my fellow graduate students and have been a co-author on two published articles. I am proficient in characterization techniques such as SEM, EDX, Raman and XRD and have ample experience in using aerosol experimental techniques such as electrospray aerosol generation, differential mobility analysis (DMA and Kanomax CPC) and aerosol spray coating processes. I have also mastered a variety of computational tools such as commercial CFD packages (ANSYS, COMSOL), Langevin Dynamics methods, Gaussian® computational chemistry package and molecular dynamics methods.

I'm interested in pursuing postdoctoral research with an intent to pursue a career in academia. Combining my background in materials science and aerosol physics, I am looking for opportunities that would allow me to contribute effectively and learn new experimental and computational tools.

8JS.10

Ying Li, Project Scientist: Seeking Faculty or Research Scientist Position.

YING LI, *University of California, Irvine*

I am a project scientist at the University of California Irvine (UCI). My interests focus on physicochemical properties of organic aerosols (OA) and kinetic simulations. Volatility and viscosity are important OA properties, both of which affect important aerosol processes. During my post-doctoral studies previously at the Max Planck Institute for Chemistry and currently at UCI, I developed one parameterization for volatility estimation based on molecular composition which can be applied to high-resolution mass spectrometry measurements. I also developed three parameterizations for glass transition temperature (T_g) estimation, based on molecular composition or volatility and those have been applied to volatility basis set and thermodynamic / chemical transport models to estimate OA viscosity. I also used the kinetic multi-layer model to simulate gas-particle partitioning of organic compounds and the water diffusion into viscous organic particles. My current main project is to fully couple the kinetic flux model with a thermodynamic model for the description of complex multi-component organic-inorganic-water systems. I am also familiar with chemical transport models and able to customize model codes. During my PhD I incorporated heterogeneous reactions on aerosol surfaces into the Weather Research and Forecasting/Chemistry model to study the effects of HONO sources on ozone and fine particulate matter formation.

I received the student presentation award at the International Conference on Fog, Fog collection and Dew in 2013. I was qualified to participate in the Lindau Nobel Laureate Meeting (Chemistry) in 2013 and was awarded the Lindau Fellowship (€30K) in 2015 to study volatility and phase state of OA and the application in chemical transport models. I have collaborated with researchers in Asia, Europe and US through my experiences studying in China, Germany, Japan and US. I have assisted advising several PhD students in China and US. My professional activities also included service as a reviewer for various manuscripts and scholarship applications. Please reach me at yingl47@uci.edu.

8JS.11

Jessica L. Amorim, MSc.in Analytical Chemistry, Analytical Chemist / Research Scientist. JESSICA LIMA AMORIM, *University of Alberta*

My name is Jessica Lima Amorim and I am currently in my second year of the master's program in analytical chemistry at the University of Alberta in Edmonton, Canada. I completed my B.S. in Chemistry in 2017 at Universidade Federal do Espírito Santo in Brazil. During my undergraduate studies, I investigated the properties of petroleum when exposed to weathering processes, focusing on the behavior of asphaltenes present in the oil. In 2014-2015 I had an opportunity to study at University of South Carolina as an exchange student for 1 year and, after an amazing experience at USC, I decided to pursue grad school in North America. In 2018 I was offered an opportunity for a master's degree at UofAlberta under supervision of Dr. Ran Zhao. My current research focuses on the fundamental understanding of the aqueous-phase processing of water-soluble organic compounds taking place in clouds and fogs. As I finish my master's degree I will be looking for job opportunities in analytical chemistry industries, considering my knowledge and experience with analytical techniques. I am particularly interested in the chemistry of aerosol emissions from vaping products. With the recent and ongoing legalization of cannabis in Canada and the United States, cannabis product manufacturing has been increasing and with that the emission of aerosol particles. These particles are associated not only with the solvents used by employees during the harvesting and processing of cannabis, but also with e-cigarette emissions. I believe this area is currently under-researched considering the environmental, occupational and public health impacts these particles pose. I will be available for full-time positions starting January, 2021 for companies located within North America.

8JS.12

Kanan Patel, PhD candidate at the University of Texas at Austin, Seeking Internship Opportunity at National Lab/Air Quality Consultancy/Regulatory Agency. KANAN PATEL, *University of Texas at Austin*

My name is Kanan Patel and I am a third year PhD student in Chemical Engineering at the University of Texas at Austin. My research focuses on understanding factors influencing ambient particulate matter concentration and composition by taking ambient measurements using mass spectrometers and integrating the data with a suite of modelling tools including source apportionment models such as Positive Matrix Factorization, thermodynamic models such as E-AIM and back trajectory analysis using HYSPLIT to understand the influence of sources vs meteorology on ambient PM composition and concentration. I have participated in several field campaigns – indoors and outdoors, in different parts of the world – including Austin, TX and Delhi, India. I am going to lead a field campaign in the coming academic year in Eagle Ford Shale, TX, to investigate the effects of oil and gas activities on ambient air quality in the region.

My expertise in terms of instrumentation include – operation/calibration of aerosol chemical speciation monitor, scanning electrical mobility spectrometer and chemical ionization mass spectrometer. I am also adept in tools such as positive matrix factorization, principal component and advanced statistical analysis and software such as Igor Pro, matlab, R and Python. I have published my findings from the field campaign in Austin (https://pubs.acs.org/doi/10.1021/acsearthspacechem.0c00016) and I am working on the manuscript on my work in Delhi. In addition, I have co-authored several other papers. Further details about my research can be found on my website (https://sites.google.com/view/kanan-patel).

Prior to joining graduate school, I worked with Royal Dutch Shell in India and Singapore, in the oil movements and product quality domain, leading small to medium scale brown field projects in the division.

I am looking for internship opportunities with an air quality consultancy/national lab/regulatory agency which I believe would help be combine my expertise in the field of air quality with my experience in the industry.

8JS.13

Pradeep Prathibha, PHD Candidate Pursuing Postdoctoral or Governmental Positions in Air Quality and Exposure Assessment with Particular Interest in Work That Informs Science Policy (SU/FA 2021, Any Location). PRADEEP S. PRATHIBHA, *Washington University in St. Louis*

My research characterizes community-level exposure to air pollution, particularly to inform health and clinical studies. My work, under the guidance of Dr. Jay R. Turner, consists of evaluating the impact of engineered vegetative buffers on near-road air quality, characterizing intra-urban ambient air quality through fixed- and mobile-platform measurements, and evaluating biomarkers of exposure to ambient air toxic metals. My experience encompasses:

Field work
1. Managing long-term, recurring passive sampling and active monitoring deployments
2. Conducting multiple week-long mobile-platform and stationary campaigns to characterize intra-urban spatiotemporal variations in gas- and particle-phase pollutants
3. Recruiting participants for outdoor residential air quality measurements through door-to-door canvassing and sharing research outcomes with stakeholders in plain language

Lab
1. Analyzing metallic content in various matrices (PM2.5, biomarkers such as toenail, hair, blood serum) through Inductively Coupled Plasma-Mass Spectrometry and ionic content through Ion Chromatography to meet EPA instrument performance and quality assurance guidelines
2. Developing lab safety protocols and training graduate research assistants to use IC/ICP-MS

Data Analysis and Modeling
1. Assessing environmental and instrumental parameters affecting inter- and intra-deployment agreements
2. Analyzing hyperlocal to urban-scale spatiotemporal data obtained from multi-year deployments to investigate the effects of the built environment on air pollution exposure of area residents using techniques like landuse regression modeling in ArcGIS and R.

I am a vehement proponent on adapting research to make informed public health and policy decisions. Drawing on science when weighing policy decisions should not be a matter of convenience, but rather a routine and intentional practice of relying on rigorously scrutinized data—often developed using federal or public funds. To this end, scientists and researchers, including myself, have the obligation to be persistent in the development and dissemination of science.

8JS.14

Colleen Marciel F. Rosales, PhD Candidate at Indiana University, Seeking Technical Applications Scientist or Indoor Air Quality Consultancy Jobs. COLLEEN MARCIEL ROSALES, *Indiana University*

I am Colleen Marciel F. Rosales, a 4th year PhD candidate at Indiana University. I work on the measurement and modeling of hydroxyl, hydroperoxy and peroxy radicals using a laser-induced fluorescence technique using our home-built instrument. I have participated in three field campaigns (ambient and indoor, including HOMEChem) and this summer, I am on my fourth field campaign, working on ambient radical chemistry.

Previously, I was a project officer for a wind tunnel fabrication, and I have had internships at a non-government organization (Clean Air Asia) and a government research institute (Philippine Nuclear Research Institute). I was also an instructor of record for chemistry four years at the University of the Philippines.

Because of my experience in chemical instrumentation (laser and vacuum systems, detection of radicals using fluorescence, detection of gases using spectrophotometric techniques), I am seeking job types like Technical Applications Scientist or Instrumentation Design Scientist. I would like to provide technical support to researchers that use advanced technologies. Because of my recent work in indoor air quality, I am also very interested in air quality consulting jobs such as Air Quality Scientist or Consultant. I believe my experience in modeling and simulations as well as various programming languages (Mathematica, MATLAB) also make me fit for jobs that require air quality modeling, such as regulatory or nonprofit work. I am open to Research Scientist or Project Scientist jobs that mostly focus on air quality, most especially secondary atmospheric and indoor chemistry. I am also be open to postdoctoral fellowships.

My anticipated job availability is Fall 2021 onwards. I am open to work in the Midwest area, most preferably in Indiana. I am also open to remote work.

8JS.15

Yixiang Wang, Current Position/PhD Candidate and Desired Position/Postdoc in PM2.5 Toxicology.

YIXIANG WANG, *University of Illinois Urbana-Champaign*

My name is Yixiang Wang, and I have seven years of experience in toxicology. During my master's period at Tsinghua University, I assessed the toxicity of nano TiO2 on marine microalgae (Phaeodactylum tricornutum). The results indicate that when particles don't express any oxidative potential (OP), and physical damage dominates the toxic mechanism, the algal cell population will be recovered with time. Currently, I am doing my Ph.D. in UIUC under the guidance of Vishal Verma. My topic is to use the mammalian cell line-based assays to understand the relationship between PM2.5 OP and cellular toxicity. In my first finished project, I provided the biological relevance to the chemical OP assays. We collected several PM2.5 samples from a campus site and tested the cytotoxicity, OP, and chemical composition. All chemical OP assays were correlated significantly with the cytotoxicity, but the •OH generation-based assays have higher correlations than antioxidant consumption assay. We hypothesized that the synergistic interactions among the organic compounds and metals on the ROS generation might account for better correlations. In my second project, I further tested the interactions of PM components on cytotoxicity. I concluded that while estimating the PM2.5 net toxicity, the interactions among different PM fractions can't be neglected. My third ongoing research is to explore the PM OP emission sources in the Midwest of the USA by a cellular OP assay. My research interest is to build the connection among the PM chemical composition, acellular OP assays, cellular OP assay, cytotoxicity, and epidemiological data. I expect that I will graduate from UIUC around June 2021. After graduation, I want to find a postdoc position in North America, China, or Europe.

8JS.16

Haoran Yu, Ph.D. Candidate, Post-doctoral Research Position in Aerosol Toxicology/Public Health.

HAORAN YU, *University of Illinois Urbana-Champaign*

Oxidative potential (OP) of fine particulate matter ($PM_{2.5}$) has been associated with many health outcomes. Various chemical endpoints have been developed for assessing the oxidative potential of ambient $PM_{2.5}$, yet no consensus has been reached for selecting the best endpoint as different endpoints are linked with different ROS-generation mechanism. My doctoral project is to investigate the health relevance of different chemical endpoints, and connect the OP activities with intrinsic mechanism towards various redox-active substances in PM.

The first topic of this project was to study the interactions among different PM components on the most commonly used endpoint, DTT activity. Synergistic/antagonistic interactions among organic species and transition metals were observed, indicating that simple summation of individual OP activities might lead to highly biased total activity due to interactions. To understand different ROS generation pathways catalyzed by different redox-active PM constituents, a multiple endpoint analyzing protocol was developed and automated for the second topic. Both DTT-based assays and surrogate lung fluid (SLF) based assays were integrated into the semi-automated multi-endpont ROS-activity analyzer (SAMERA) system. This system is currently employed for a spatiotemporal variability assessment on ambient $PM_{2.5}$ in Midwest U.S, which serves as the third topic.

I am Haoran Yu, a fourth-year Ph.D. candidate in Dr. Vishal Verma’s research group in University of Illinois at Urbana-Champaign. My anticipated graduation is in May 2021. I will be seeking a post-doctoral research position after graduation from my doctoral program in aerosol toxicology research associated with public health discipline. My research focus is the health relevance of the oxidative potential from different chemical mechanisms, and my special interest is on the connection of chemical identification of organic species in ambient $PM_{2.5}$ with the health outcomes from these species. I have no geographical preferences.

8JS.17

Job Interest: Industry Research Scientist (instrumentation or instrumentation development), or Aerosol Chemistry Postdoc. SABRINA CHEE, *University of California, Irvine*

My PhD research has focused on understanding the mechanism and contribution of acid-base reactive uptake on the formation and growth of nanoparticles (<30 nm). I have authored one first-author paper (three first-authors expected by graduation), and four other papers where I am coauthor. I have measured the composition of salt particles from 8 - 30 nm, where two trends have surfaced: one where the size-resolved acid:base ratio does not reflect expected stoichiometric values (e.g., 1 sulfuric acid per 2 bases), and one where they do. These properties of salt nanoparticles are important because their pH will affect downstream particle-phase and surface reactions in these young particles. My goal by the end of my PhD is to provide some level of prediction for models for whether a particle with given acid/base constituents will follow one of these two trends.

I am looking for a hands-on job where I can apply my instrumentation skills to a research problem, or develop an instrument for a research problem. I am experienced with troubleshooting and fixing aerosol characterization equipment, including quadrupole-CIMS, vacuum pumps, electrical mobility particle classifiers (APS, DMA, CPC), LC-MS (reverse-phase and normal phase), aerosol impaction collectors (S3, MOUDI), and ion chromatograph conductivity detection. I have written >15 data analysis functions in Igor Pro to streamline pulling data from files, averaging size distributions, normalizing mass spectra, and other applications. I can read LabView and Python code but am not fluent. I really enjoy working with instrumentation and am happy to learn new tools, techniques, and data analysis!

Current Position: PhD Candidate
Expected Graduation: June 2021
Geographic Region: CA or WA, preferably Bay Area, CA
Contact Info: schee@uci.edu,
www.linkedin.com/in/skychee

8JS.18

Sarah Toth, PhD Candidate, Environmental Engineering. SARAH TOTH, *University of Colorado Boulder*

NSF Graduate Fellowship Runner-Up
Denver, Colorado

Ambient particulate matter in urban environments is dynamic and heterogeneous, so understanding photovoltaic (PV) energy loss due to soiling is challenging. We deployed silicon reference cells in an urban-industrial area in Colorado for one year, co-located with measurements of ambient particulate matter concentrations. We developed a model that quantified the relationships between ambient air quality and PV soiling, and showed that urban air pollution can significantly reduce the performance of PV panels. In our next year of work we will deploy similar monitoring stations in the Los Angeles basin and leverage the large amount of historical air quality and PV performance measurements in the area in order to model air pollution and PV performance across the whole region.

Experience:
I have worked at the National Renewable Energy Lab (NREL) in the PV Reliability group since January 2017 and began my graduate degree at the University of Colorado at Boulder (CU Boulder) in August 2017. Since then I have been researching and publishing jointly with scientists at NREL and CU Boulder. I have primarily worked in Python and Solidworks.

Research Interests:
Low-cost air quality sensors, big data analysis, renewable energy.

Tentative availability:
PhD dissertation defense slated for May 2021.
Preference to stay in Colorado; willing to work-from-home full-time.

sarah.toth@colorado.edu

8JS.19

Rebecca Tanzer Gruener, PhD Candidate in Mechanical Engineering Seeking Research Positions in Academia, Government, or Industry. REBECCA TANZER GRUENER, *Carnegie Mellon University*

Thanks for reading my abstract! I'm a very ambitious, soon to be PhD grad from Carnegie Mellon University's CAPS (Center for Atmospheric Particle Studies) lab. I'd love to talk with you about potential job opportunities continuing research at either another university (post-doc), a national lab (as a research scientist or post-doc) or maybe even in industry (in your R&D group). Over the course of my PhD I've spent time involved with both field and lab work and would love to continue working in a lab setting. In terms of field work I have calibrated (using machine learning), deployed, and analyzed data from a large network of low-cost air quality sensors (40+ sensors throughout the city of Pittsburgh). I have used that data to evaluate changes in pollutants over space and time. Most recently I've utilized the sensor network to understand and quantify how the COVID-19 related closures have impacted our air quality. In the lab I've been working on identifying and quantifying emissions and SOA formation potential of common volatile chemical products. I have experience with various instruments in the lab setting (GC-MS, GC-FID, PTR-MS, gas monitors, etc.) and would love to further my experimental skills. I'm looking for a position conducting research in a lab, solving an "interesting" problem. If you think you have one, lets chat!

Publications

- **Tanzer-Gruener, Rebecca**; Li, J.; Eilenberg, S. R.; Robinson, A. L.; Presto, A. A. Impact of Modifiable Factors on Ambient Air Pollution: A Case Study of COVID-19 Shutdowns. Environ. Sci. Technol. Lett., **2020**, Article ASAP 10.1021/acs.estlett.0c00365.
- **Tanzer (Gruener), Rebecca.**; Malings, C.; Hauryliuk, A.; Subramanian, R.; Presto, A. A. Demonstration of a Low-Cost Multi-Pollutant Network to Quantify Intra-Urban Spatial Variations in Air Pollutant Source Impacts and to Evaluate Environmental Justice. International Journal of Environmental Research and Public Health., **2019**, 16(14), 2523.
- Malings, C.; **Tanzer, R.**; Hauryliuk, A.; Saha, P.K.; Robinson, A. L.; Presto, A. A.; Subramanian, R. Fine particle mass monitoring with low-cost sensors: Corrections and long-term performance evaluation, Aerosol Science and Technology, **2020**, 54:2, 160-174, DOI: 10.1080/02786826.2019.1623863.
- Malings, C., **Tanzer, R.**, Hauryliuk, A., Kumar, S. P. N., Zimmerman, N., Kara, L. B., Presto, A. A., and R. Subramanian: Development of a general calibration model and long-term performance evaluation of low-cost sensors for air pollutant gas monitoring, Atmos. Meas. Tech., **2019**, 12, 903–920, https://doi.org/10.5194/amt-12-903-2019.
- Subramanian, R.; Ellis, A.; Torres-Delgado, E.; **Tanzer, R.**; Malings, C.; Rivera, F.; Morales, M.; Baumgardner, D.; Presto, A. A.; Mayol-Bracero, O.L.; ACS Earth and Space Chemistry **2018** 2 (11), 1179-1186 DOI: 10.1021/acsearthspacechem.8b00079.

9AC.1

A Near-Explicit Mechanistic Evaluation of Isoprene Photochemical Secondary Organic Aerosol Formation and Evolution. JOEL A. THORNTON, John Shilling, ManishKumar Shrivastava, Emma D'Ambro, Maria Zawadowicz, Jiumeng Liu, *University of Washington, Seattle, WA*

Experimentally determined yields of secondary organic aerosol (SOA) from the photochemical oxidation of isoprene in the absence of aqueous acidic aerosol vary substantially, both within a given experiment and across different environmental chamber conditions. The underlying mechanisms driving this variation remain poorly evaluated, leading to significant uncertainty in how to extrapolate laboratory chamber results to the atmosphere. Herein, we compare SOA predictions from a near-explicit gas-phase chemical mechanism of isoprene oxidation by the hydroxyl radical (OH) in the presence and absence of nitrogen oxide radicals (NOx), to multiple chamber experiments on non-aqueous isoprene photochemical SOA (ipSOA) conducted by different groups in different chambers. SOA is predicted by volatility-driven gas-particle partitioning of hundreds of individual reaction products. The mechanism includes simplified descriptions of particle-phase organic chemistry, including organic hydroperoxide photolysis, and organic nitrate hydrolysis and accretion reactions. The model has good skill (mean normalized bias typically within 25%) at predicting the observed formation and evolution of ipSOA across a range of chambers and conditions at low NOx. The model has much less skill at describing the observed non-linear response of ipSOA to elevated NOx. Organic nitrate hydrolysis is unable to explain significant ipSOA at high NOx, whereas particle-phase accretion reactions of tertiary nitrates may play a role. Uncertainties in the chamber radical environment and fate of key organic peroxy radicals (RO_2) remain as or even more important than vapor losses to chamber walls in determining how best to extrapolate chamber-based yields to the atmosphere. Implications for likely atmospheric yields of ipSOA and recommendations for future chamber experiments are discussed.

9AC.2

Product Formation and Kinetics of Heterogeneous Hydroxyl Radical (OH) Oxidation of IEPOX-Derived SOA. JIN YAN, Yue Zhang, Yuzhi Chen, N. Cazimir Armstrong, Marc Webb, Zhenfa Zhang, Avram Gold, Andrew Lambe, Andrew Ault, Jason Surratt, *University of North Carolina at Chapel Hill*

Isoprene is the most abundant non-methane volatile organic compound emitted globally. Isoprene epoxydiols (IEPOX), key photooxidation products of isoprene under low-nitric oxide (NO) conditions, can form secondary organic aerosols (SOA) through acid-enhanced multiphase chemical reactions with inorganic sulfate particles ($Sulf_{inorg}$). Through converting $Sulf_{inorg}$ to organosulfates (OSs), this reaction changes physicochemical properties (e.g., thickness of organic shell and viscosity) of pre-existing aerosols over time. Our recent study demonstrated that heterogeneous hydroxyl radical (OH) oxidation of the major IEPOX-derived SOA components, 2-methyltetrol sulfates, generates more oxygenated OSs. To accurately describe the evolution of IEPOX-derived SOA in the atmosphere, this study explores the impacts of aerosol acidity and physicochemical properties on the heterogeneous oxidation rate of IEPOX-derived SOA so as to incorporate the results into a chemical kinetic model.

In this study, IEPOX will be reacted with $Sulf_{inorg}$ in a flow tube reactor to form IEPOX-derived SOA with different acidities and physicochemical properties by altering $Sulf_{inorg}$ acidity and its reaction time with IEPOX. The fresh SOA will be subsequently aged in an oxidation flow reactor at varying ambient-relevant OH exposures under low-NO conditions. The aged SOA will be sampled by an online aerosol chemical speciation monitor (ACSM) and collected onto Teflon filters for molecular-level analyses by a recently developed hydrophilic liquid interaction chromatography method interfaced to high-resolution quadrupole time-of-flight mass spectrometry equipped with electrospray ionization (HILIC/ESI-HR-QTOFMS). Measured chemical composition will facilitate developing a kinetic model for the oxidation of fresh IEPOX-derived SOA parameterized by OH exposure and a set of parameters describing properties of IEPOX-derived SOA. To further separate and group oxidation products based on reaction pathways, a positive matrix factorization (PMF) technique will be applied to cross-compare with the kinetic model.

9AC.3

Unexpected pH-Dependent Stereochemistry in Organosulfate Formation in Aerosol. MADELINE COOKE, Yuzhi Chen, Yue Zhang, Ziying Lei, Isabel Ledskey, Jamy Lee, Nicolas Aliaga Buchenau, Andrew Lambe, Jason Surratt, Andrew Ault, *University of Michigan*

Understanding the chemical reaction mechanisms that drive the formation of atmospheric fine aerosols is critical to predicting air quality and climate, particularly for low-volatility organic species formed from the oxidation of abundant volatile organic compounds (e.g. isoprene) known as secondary organic aerosol (SOA). Organosulfate formation from multiphase chemistry of isoprene-derived epoxides is a primary formation pathway for SOA, but our ability to predict product yields is limited due to a lack of mechanistic understanding. Herein, we find that the epoxide-ring opening mechanisms in atmospheric aerosol can occur via two pathways: S_N1 or S_N2. These mechanistic pathways are pH-dependent, with the S_N2 mechanism increasing at higher pH and the S_N1 mechanism increasing at lower pH. Both mechanisms of organosulfate formation are possible under typical ambient aerosol acidity ranges of pH 0 to 5. Our results indicate that organosulfate formation is maximized under the most acidic conditions where sulfate is still present in high concentrations (pH = 1.5). Surprisingly, both S_N1 and S_N2 sulfate additions lead to greater formation of specific diastereomer products as measured with hydrophilic interaction liquid chromatography (HILIC) interfaced to electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (QTOFMS). The stereochemical enhancement of organosulfate compounds has important implications for the formation of SOA and degradation of air quality.

9CA.1

Measurements and Modeling of the Temperature and Humidity Dependent Viscosity Between -30 and 30 Degree Celsius. SABIN KASPAROGLU, Markus Petters, Ying Li, Manabu Shiraiwa, *North Carolina State University*

Atmospheric aerosols can assume amorphous semi-solid or glassy phase states whose viscosity depends on atmospheric temperature and relative humidity. New measurements characterizing viscosity of sub-100 nm particles from the dimer relaxation method are provided to construct the phase state diagram of citric acid between -30 and 30 degrees Celsius. These measurements of citric acid particles extend the available data of temperature and humidity dependent viscosity to -30 degrees Celsius. The measurements are also tested against the model which predicts the viscosity of the compound applying the water-organic binary mixing rule as a function of the glass transition temperature, a glass transition temperature scaled viscosity fragility, and water uptake parameterization. The proposed function is also compiled from literature data and able to use the fragility parameterization to predict the viscosity. Predicted relationships agree well with observations and with measured isopleths of constant viscosity at $\sim 10^7$ Pa s even at cold temperatures. In addition, simulations of the kinetic multi-layer model of gas-particle interactions (KM-GAP) are performed to explore the isopleths of equilibrium time scales, at different temperature and relative humidity values. KM-GAP model simulations showed that the equilibrium limitations of citric acid are below the coalescence time of this study’s experiments at all studied temperature ranges. However, there are some discrepancies for sucrose at colder temperatures, which can be attributed to kinetic limitations of water uptake at the time scales of the dimer relaxation experiments.

9CA.2

Humidity Dependent Absorption Enhancements for Brown Carbon Surrogates. KYLE GORKOWSKI, James D. Lee, Christian Carrico, Tyler Capek, Claudio Mazzoleni, Allison Aiken, Manvendra Dubey, *Los Alamos National Lab*

Large uncertainties remain with aerosol optical properties and their relative humidity (RH) dependence that impact atmospheric radiative transfer significantly. These uncertainties are especially challenging for the humidity dependence of light absorption by brown carbon aerosols. To address these challenges, we report on laboratory optical measurements of surrogate brown carbon species as a function RH and a model framework to interpret them.

We used an RH-controlled single scattering albedometer to measure in-situ aerosol light extinction and scattering. This custom instrument was built utilizing a cavity-attenuated phase shift-single scattering albedo PM monitor (CAPS-PMSSA, Aerodyne, Inc.) at 450nm. We sampled three brown carbon surrogates (Sunset Yellow, Sodium Fluorescein, and Para Red); each was aerosolized and size selected, comprised of a single molecular species, and had a different hygroscopicity. For each species, we performed a combined optical and hygroscopic closure analysis. We compared the resulting hygroscopic responses to available thermodynamic models. The protocols established in this laboratory work will be applied during the 2021 DOE-ARM TRACER field campaign in Houston, Texas, to examine the effects of humidity on convectively processed absorbing aerosols.

9CA.3

Model for Competitive Condensation of Supersaturated Vapor on a Soot Aggregate. ELLA IVANOVA, Alexei Khalizov, Gennady Gor, *New Jersey Institute of Technology*

Atmospheric soot is a major pollutant for the environment. It is the second most significant factor behind global warming, after the greenhouse effect of carbon dioxide. Also, soot has a negative impact on human health. In order to assess these negative impacts of soot on both climate and human health one has to know the microstructure of soot aggregates, which are influenced on their optical properties.

Soot is made of small particles, which are fractal aggregates. However, experiments show that the condensation of vapors on aggregates often causes their restructuring to globules. It was showed that restructuring can be induced by a very small amount of condensate, if the coating material is not distributed uniformly over the aggregate surface of monomers, but located in the gap between them.

In this work, we consider the model for competitive condensation of supersaturated vapor on a soot nanoparticle aggregate: condensation of liquid between monomers or on their surface. Previously, it was shown that it is possible to predict the condensation outcome based on a single dimensionless parameter chi. This parameter chi contains information about the diameter of monomer spheres in the aggregate, the supersaturation of condensing vapor, and also the molar volume and surface tension of the condensate. The main goal of this work to consider different profiles of the condensed liquid between monomers and estimate how does it affect the model for competitive condensation of supersaturated vapor on a soot aggregate. All calculations were numerical. Also, this work is the basis for the process of modeling the restructuring of soot aggregates.

9IA.1

Oxidized Primary Organic Aerosol and Secondary Organic Aerosol Formation Initiated by Chlorine Oxidation of Indoor Pollutants during Bleach Cleaning.

ANITA AVERY, Francesca Majluf, Jordan Krechmer, Nirvan Bhattacharyya, Lea Hildebrandt Ruiz, Maddy Reed, William Brune, Manjula Canagaratna, Andrew Lambe, *Aerodyne Research, Inc.*

Bleach cleaning activities, which are becoming increasingly prevalent in response to the SARS-CoV-2 pandemic, emit reactive halogen species, including molecular chlorine (Cl_2) and hypochlorous acid (HOCl), that participate in complex, multiphase chemistry. These chlorinated compounds are detrimental to human health. Additionally, reactions between indoor air pollutants (IAPs) and chlorine atoms (Cl) plus hydroxyl radicals (OH) that are generated from photolysis of Cl_2 and/or HOCl generate oxidized primary organic aerosol (OPOA) and/or secondary organic aerosol (SOA) species, which are also associated with adverse health effects. However, the mechanisms leading to OPOA and SOA formation during bleach cleaning are poorly understood. To investigate SOA/OPOA generated during indoor bleach cleaning activities, a prototype halogen oxidation flow reactor (OFR) equipped with low-pressure mercury lamps (λ= 254 or $\lambda > 350$ nm emission output) was developed. The halogen OFR can generate elevated OH and Cl concentrations that are available for reaction with surrogate IAPs in several minutes' exposure time. In different experiments, the oxidants employed were switched between Cl, Cl + OH, HOCl and Cl_2 by varying the precursor halogen species and the OFR photochemical conditions. α-pinene, squalene, and oleic acid (representative of passive indoor, human, and cooking sources, respectively) were used as SOA/OPOA precursors. SOA/OPOA generated from these reactions were characterized with several state-of-the-art mass spectrometry techniques, including AMS, CIMS, and PTR-MS. Our measurements can be used to identify molecular tracers for chlorine-initiated oxidation chemistry during bleach cleaning. These results emphasize the importance of secondary chemistry during and after bleach cleaning activity.

9IA.2

Deposited Particulate Matter from Cigarette Smoke Is a Major, Dynamic, and Chemically-Diverse Reservoir of Thirdhand Smoke.

ROGER SHEU, Tori Hass-Mitchell, Akima Ringsdorf, Achim Edtbauer, Thomas Klüpfel, Jonathan Williams, Drew Gentner, *Yale University*

Thirdhand smoke (THS) refers to the contamination and subsequent off-gassing of hazardous organic compounds following smoke exposure. Recently, thirdhand smoke, comprised of nicotine and other known co-emitted hazardous (e.g. carcinogenic) compounds, was shown to be transported by previously-exposed people into clean, non-smoking environments via unexplored reservoirs and processes. For the first time, through laboratory experiments simultaneously employing detailed online and offline high-resolution mass spectrometry, we expand the volatility and functionality range of identified gas- and aerosol-phase compounds in smoke and particulate matter (PM). We demonstrate that primary PM is a substantial, long-lasting, and chemically diverse reservoir for reactive volatile, intermediate volatility, and semi-volatile organic compounds. PM can deposit onto common indoor (e.g. clothes, furnishings, building interiors) and human (e.g. skin, hair, airways) surfaces, where they can off-gas appreciable amounts over long timescales (e.g. over three days in this study). This work showcases a major underlying repository for THS, along with associated mechanisms for persistent THS contamination and transport, which act alongside adsorption and desorption of gases by clothing, furnishings, and other surfaces. In non-smoking environments, the off-gassed compounds will be available to partition to other surfaces or other indoor particles, increasing their persistence and pathways for human exposure. The results and analysis from tobacco smoke are applicable to similar organic aerosol sources (e.g. biomass burning and cooking), and the methods demonstrated can be applied to other dynamic gas-phase complex mixtures.

9IA.3

Emissions from Essential Oil Diffusers. BOWEN DU, Heather Schwartz-Narbonne, Jeffrey Siegel, *University of Toronto*

Essential oils are becoming increasingly popular as scents and antibiotics as well as broadly used in aromatherapy. Many types of oils have been claimed to have positive health impacts. Evidence suggests essential oils may also affect the central nervous systems and alter mood, cognitive function, and behavior. However, the constitution of aerosols emitted by essential oils is poorly understood. We characterized the VOC (α-pinene, β-pinene, eucalyptol, linalool, linalyl acetate, limonene) and particle (10 – 300 nm) emissions from four types of essential oils (lemon, eucalyptus, lavender, and grapeseed) vaporized by an ultrasonic diffuser using deionized water. Both types of emissions were found to vary considerably between oils. Eucalyptus and lemon oils had overall higher VOC emission rates, with eucalyptol and limonene being the predominant VOC species emitting at a rate of over 10 mg/h. Limonene was also detected in the emissions of other oils, varying from 0.8 – 4 mg/h. The PM_1 emission rate was the highest for grapeseed oil (1 – 1.5 mg/h), followed by lemon oil at 0.8 – 1 mg/h. In contrast, eucalyptus and lavender oils had PM_1 emission rates below 0.1 mg/h. The particle size distribution measured suggested that the particles emitted were mostly smaller than 100 nm in size except for grapeseed oil where the predominant size was above 300 nm. Particle emissions from the eucalyptus oil were elevated by a factor of 4 – 5 when tap water was used as would commonly be used. The overall high emission rates, as well as the potential for secondary aerosol formation with the emitted VOCs, suggests caution in the use of these devices, particularly in poorly ventilated indoor environments.

9ID.1

Assessing the Effectiveness of Using Face Coverings to Mitigate the Transport of Particles Generated from Coughing. LIQIAO LI, Muchuan Niu, Yifang Zhu, *University of California, Los Angeles*

Respiratory droplets produced by coughing within a close range of about 6 feet is one of the main routes of human to human transmission of SARS-CoV-2 virus during the COVID-19 pandemic. This work investigated the effectiveness of different face coverings to mitigate cough particles at 1ft, 3ft, and 6ft away from the coughing source in a 138 m^3 laboratory room. We measured particle number concentration (PNC) and particle size distribution under ten conditions: (1) no face covering; (2) white cotton mask; (3) black cloth mask; (4) surgical mask; (5) N95 mask; (6) face shield; (7) face shield + white cotton mask; (8) face shield + black cloth mask; (9) face shield + surgical mask; (10) KN95 mask. Without any face covering, the average of the background-subtracted peak PNC measured during coughing could reach 123 ± 90 #/cm^3 at 1 ft and decrease to a near-background level within 2-4 seconds. At 1 ft, black cloth mask and face shield reduced the PNC to 29% and 68%, respectively, of those without face coverings. When the sampling location moved from 1 ft to 3 ft, the PNC was reduced to 27% without face coverings, 16% with black cloth mask, and 21% with face shield only, respectively. At all other conditions, the PNC was reduced to < 15% of what was measured at 1 ft without face coverings. About 99% of the cough droplets were less than 2.46 µm. The average mode size was 0.59±0.06 µm. Surgical mask, N95 mask, and KN95 mask by itself offer good protection and substantially reduced the cough particles to < 7%. Face shield and black cloth mask by itself does not offer sufficient protection. Nevertheless, wearing any type of face masks would help reduce the transport of cough particles.

9ID.2

Evaluation of Particle Filtration Efficiency of Commercially Available Materials for Homemade Face Mask Usage. TAEKYU JOO, Masayuki Takeuchi, Joy Barr, Emily Blum, Eric Parker, John Tipton, Julia Vernedoe, Nga Lee Ng, *Georgia Institute of Technology*

The COVID-19 pandemic has resulted in a severe shortage of personal protective equipment, including N95 respirators. Organizations such as CDC and WHO recommend using homemade masks as a protection for individuals and to reduce the transmission of the virus. Here, we evaluate size-dependent filtration efficiency of sub-micron particles of commercially available materials (N = 24) using sodium chloride aerosols. Specifically, single layer of woven fabrics such as cotton and polyester, blended fabrics, non-woven fabrics, cellulose-based materials, materials used in hospitals, and various filter materials are tested. Different combinations of woven, non-woven, and blended fabrics are also evaluated. The particle filtration efficiency of all materials tested are compared with commercial N95 respirators and surgical masks. Filter materials such as HEPA, MERV 13, and coffee filter report efficient filtration (94-99%, 58-89%, and 31-93%, respectively) compared to the other tested samples. However, we do not recommend using HEPA and MERV 13 filters on their own unless they are certified to be fiberglass-free. The coffee filter exhibits potential breathability issues as indicated by the large pressure drop. Other than these filter materials, we find that Halyard sterilization wrap, tightly woven fabric, and double reinforced crepe show good filtration efficiency (54-85%, 29-63%, and 23-64%, respectively). We observe an improvement in particle filtration efficiency when multiple layers of materials are used. Results from this study provide guidelines for individuals to make better decisions on what materials to use for homemade masks to increase protection against the disease.

9ID.3

The Use of Common Material to Alternative Masks for General Public: Fractional Filtration Efficiency and Breathability Perspective. CHENXING PEI, Qisheng Ou, Seong Chan Kim, Sheng-Chieh Chen, David Y. H. Pui, *University of Minnesota*

As COVID-19 pandemic has caused more than 8 million confirmed cases globally (as of Jun 18th, 2020), it is critical to slow down the spreading of SARS-CoV-2 to protect the healthcare system from overload. Wearing a respirator or a mask has been proven as an effective method to protect both wearer and others, but commercially available respirators and masks should be reserved for healthcare workers under currently desperate shortage. The use of the alternative material becomes an option for general public to make the DIY masks, with their efficacy seldom reported. In this study, we tested commercial respirators and masks, furnace filters, vacuum cleaner filters, and common household materials. We evaluated materials' fractional filtration efficiency and breathing resistance, which are primary factors affecting the respiratory protection. To compare the efficiency-resistance tradeoff, figure of merit of each tested common material was also calculated. Media with electrostatic charge (electret) is recommended due to its high efficiency with low flow resistance; multiple-layer household fabrics and sterilization wraps are acceptable materials; coffee filter is inadvisable due to its low efficiency. The outcome of this study can not only offer guidance for general public under current pandemic, but also suggest the appropriate alternative respiratory protection materials under heavy air pollution episode.

9IM.1

Improvement on Differential Mobility Analyzer Method for Estimation of the Enthalpy of Vaporization Using an Algorithm to Derive Particle Size Changes from Full-Size Distribution.

CHIRANJIVI BHATTARAI, Andrey Khlystov, *Desert Research Institute*

One of the most popular methods for studying the volatility properties of an aerosol is the tendem differential mobility analyzer (TDMA) technique. In the TDMA method, a narrow size range of particles is selected by a front differential mobility analyzer (DMA) and is exposed to an elevated temperature in a thermodenuder causing particles to evaporate. The size distribution of the evaporated aerosols is then measured with a second DMA and the mean or mode size is used to derive aerosol thermodynamic properties. The TDMA method usually takes a relatively long time to acquire sufficient data, as several sizes at several temperatures need to be measured consecutively. Here, we report a more efficient approach for determination of enthalpy of vaporization of single component aerosols using the TDMA method. In this method, size changes of all particles transmitted by the front DMA are measured at an elevated temperature point (45 oC). An inversion algorithm is then applied to the original and evaporated size distributions to derive size changes at individual aerosol size bins. The algorithm was developed by Heisler and co-workers in 1976 and is based on the preservation of particle number concentration. We performed a detailed theoretical and numerical analysis of the uncertainties associated with the inversion algorithm and verified it experimentally using an adipic acid aerosol. The algorithm applied to broad size distribution measurements provided results that are within 10 % of the TDMA measurements. We will describe the theoretical basis for derivation of the enthalpy of vaporization from measurements of size changes at several size bins without assumptions on the evaporation coefficient. Enthalpy of vaporization for adipic acid and pimelic acids determined with this method is 117 and 100 kJ/mol, respectively. This compares well with the available literature data (95 --154 and 80 --162 kJ/mol, respectively).

9IM.2

Design and Characterization of an Advanced Thermal Denuder.

MARTIN IRWIN, Jacob Swanson, Adam M Boies, *Catalytic Instruments*

Aerosols are comprised of solid and semi-volatile particles suspended in a gas. The semi-volatile fraction comprises tens of thousands of organic compounds. By precisely changing the temperature of an aerosol sample, semi-volatile constituents can be selectively partitions based on their volatility, which is the basis of the thermal denuder. In this device, particles typically pass through a heated section of tube wherein semi-volatile material evaporates. The “dried” particles and evaporated vapor then pass into a cooled section where the vapor adsorbs to activated carbon. The “dried” particles pass out the device to be measured.

One issue with this technique is the transition from the hot section to the cooled section typically creates two undesired effects: 1) the vapors nucleate and form additional particles rather than adsorb to the activated or 2) the vapors adsorb to the existing particles rather than the activated carbon. One solution to these problems can be found in addressing the heating and/or cooling rates, transitions, etc. Secondary to these problems of a fundamental nature is that the geometry described typically results in a “large” device. Due to the size (and thermal mass) of the device, the temperature cannot be changed rapidly, which limits the number of temperature setpoints typically achievable.

In the Advanced Thermal Denuder, the problematic transition from the heating section to the cooled section has been eliminated because there is just a single section that is heated. Energy flows from the inside to the outside. This results in the adsorption section being cooler than the aerosol heating section. The direction of heat flow maximizes adsorption capacity near the exterior of the device where the adsorbent is located. We present data characterizing the design and performance of this new Adavanced Thermal Denuder operating at 1 LPM in the temperature range of 20ºC to 400ºC.

9IM.3

Performance Characteristics of a Dual Stage Porous Tube Thermodiluter. AARON AVENIDO, Justin Koczak, Modi Chen, Francisco Romay, Russell Graze, Noah Bock, Darrick Zarling, *TSI Incorporated*

When measuring aerosols from combustion and other high-temperature sources, it is necessary to dilute and condition the sample gas to reduce its temperature, dew point, and particle concentration while minimizing losses. To address this need, TSI has developed the Model 3098 Porous Tube Thermodiluter (PTT), a new accessory that integrates with the Model 3090 Engine Exhaust Particle Sizer spectrometer^{TM} (EEPS^{TM}) for a complete fast particle measurement solution.

The PTT consists of two independently-controlled dilution stages with a catalytic stripper positioned between them to remove volatile particles. Each dilution stage consists of a mass flow controller (MFC) and a porous tube diluter. The dilution air flows radially inward through the walls of the porous tubes, reducing losses. A third MFC controls the amount of flow removed between the dilution stages to keep the flow rate through the main section of the PTT constant regardless of dilution factor. This maintains constant residence time, thereby keeping particle losses consistent. The three MFCs allow the system to independently and dynamically control the primary and secondary dilution factors, and provide a stable and accurate total dilution factor from as low as 10:1 to as high as 500:1. The PTT control system is built into the TSI EEPS^{TM} software, which provides a single user-interface for both dilution parameters and particle spectrometer control.

System performance of the PTT is presented, including accuracy of dilution factor across the full control range, and size-dependent system particle penetration and resulting particle loss correction function, which is included in the data processing algorithm. Additionally, particle size distribution and total solid particle number concentration of engine exhaust collected using the system are compared to those collected with EEPS^{TM}, Scanning Mobility Particle Sizer^{TM} (SMPS^{TM}), and condensation particle counter (CPC), using conventional ejector diluters and a catalytic stripper.

9SD.1

Improving Estimates of PM2.5 Concentration and Chemical Composition by Application of High Spectral Resolution Lidar. BETHANY SUTHERLAND, Nicholas Meskhidze, *NC State University*

Remote sensing is an effective means of monitoring aerosol mass loadings. Retrievals of aerosol optical depth (AOD) have been used to improve model simulations of PM2.5 concentration and to infer ground-level PM2.5. However, recent advances in active remote-sensing techniques (e.g., HSRL -High Spectral Resolution Lidar) and algorithm development (e.g., CATCH- Creating Aerosol Types from Chemistry) allow for retrievals of both aerosol PM2.5 mass concentrations and chemical composition.

In this presentation, we offer two new methodologies that combine the products of the CATCH algorithm with HSRL-retrieved AOD and aerosol types to derive the mass concentration and chemical composition of PM2.5. The methods are validated against the data from the NASA DISCOVER-AQ BWC Campaign (2011) and ground measurements from EPA's Air Quality System network. In Method 1, the CATCH-HSRL combination is used to improve the regional air-quality model-predicted PM2.5 concentrations and chemical composition. In Method 2, PM2.5 concentrations and chemical composition are derived using the CATCH-HSRL combination alone.

Results show good agreement for both methods with the ground measurements. Method 1 and 2 yield r2 values of 0.61 and 0.69 and RMSE of 6.1 µg/m3 and 6.8 µg/m3, respectively. By comparison, the unconstrained CMAQ simulations produced r2=0.30 and RMSE=4.0 µg/m3. The estimates of PM2.5 chemical composition by both methods were similar (or better) compared to CMAQ simulations.

9SD.2

Ensemble-Based Deep Learning for Estimating PM2.5 over California with Multi-Source Big Data Including Wildfire Smoke.

Lianfa Li, Mariam Girguis, Frederick Lurmann, Nathan Pavlovic, Crystal McClure, Meredith Franklin, Jun Wu, Luke Oman, Carrie Breton, Frank Gilliland, RIMA HABRE, *University of Southern California*

Introduction: Estimating $PM_{2.5}$ concentrations and their prediction uncertainties at a high spatiotemporal resolution is important for air pollution health effect studies. This is particularly challenging for California, with highly variable natural and anthropogenic emissions, meteorology, topography and land use.

Methods: Using ensemble-based deep learning with big data fused from multiple sources we developed a $PM_{2.5}$ prediction model with uncertainty estimates at a high spatial (1km x 1km) and temporal (weekly) resolution for a 10-year time span (2008-2017). Data sources included remote sensing data (MAIAC aerosol optical depth (AOD), normalized difference vegetation index, impervious surface), MERRA-2 GMI Replay Simulation (M2GMI) output, wildfire smoke plume dispersion estimates (HYSPLIT and MODIS fire radiative power), meteorology, land cover, traffic, elevation, and spatiotemporal trends (geo-coordinates, temporal basis functions, time index). Missing MAIAC AOD observations were imputed and adjusted for relative humidity and vertical distribution.
Results: Ensemble deep learning to predict $PM_{2.5}$ achieved an overall mean training RMSE of 1.54 µg/m3 (R^2: 0.94) and test RMSE of 2.29 µg/m3 (R^2: 0.87). The top predictors included M2GMI carbon monoxide mixing ratio in the bottom layer, temporal basis functions, spatial location, air temperature, MAIAC AOD, and $PM_{2.5}$ sea salt mass concentration. In an independent test using three long-term AQS sites and one short-term non-AQS site, our model achieved a high correlation (>0.8) and a low RMSE (<3 µg/m3). Statewide predictions indicated that our model can capture the spatial distribution and temporal peaks in wildfire-related $PM_{2.5}$. The coefficient of variation indicated highest uncertainty over deciduous and mixed forests and open water land covers.

Conclusion: Our method can be generalized to other similarly complex regions. Prediction uncertainty estimates can also inform further model development and measurement error evaluations in exposure and health studies.

9SD.3

Examining Neighborhood Scale Variability of Co-incident PM2.5 and AOD Measurements: Results from Citizen Enabled Aerosol Measurements for Satellites (CEAMS).

MICHAEL CHEESEMAN, Bonne Ford, John Volckens, Jeffrey R. Pierce, Eric Wendt, Casey Quinn, Christian L'Orange, John Mehaffy, Shantanu Jathar, Marilee Long, Zoey Rosen, *Colorado State University, Fort Collins, CO*

Exposure to ambient fine particulate matter ($PM_{2.5}$) is associated with adverse health impacts. Studies have generally relied on surface monitoring networks to quantify population exposure to $PM_{2.5}$ but these estimates are uncertain due to large spatial gaps between monitors. Satellite observations of aerosol optical depth (AOD), a column-integrated measure of light extinction due to aerosols, have been increasingly used to estimate surface $PM_{2.5}$ and fill the spatial gaps of monitoring networks. However, satellite-derived $PM_{2.5}$ estimates have large uncertainties due, in part, to a lack of information on the ratio of $PM_{2.5}$ and AOD. More co-incident $PM_{2.5}$ and AOD measurements are needed to reduce the uncertainties in satellite-derived $PM_{2.5}$. Thus, we present concurrent $PM_{2.5}$ and AOD measurements from a high density network of low-cost samplers developed by the Citizen-Enabled Aerosol Measurements for Satellites (CEAMS) project. The sampler used, called the Aerosol Mass and Optical Depth (AMOD) sampler, is a low-cost, portable instrument capable of taking autonomous, high-quality measurements of AOD and $PM_{2.5}$ simultaneously. The AMOD includes a set of four optically filtered photodiodes for multi-wavelength (440, 500, 675, and 870 nm) AOD, a Plantower PMS5003 sensor for time-resolved optical PM measurements, and a pump and cyclone system for time-integrated gravimetric filter measurements of particle mass. The AMOD uses autonomous sun alignment to provide semi-continuous AOD measurements. We present validation results using co-located AMOD and standard monitoring measurements (i.e. AERONET sun photometers and Federal Equivalent Method $PM_{2.5}$). We also present data from pilot campaigns in Colorado that captured both winter and summer conditions, stagnation events, and wildfire smoke events. We quantify the bias of satellite-derived $PM_{2.5}$ due to its reliance on AOD only captured during satellite-overpass times. And, finally, we investigate (1) neighborhood scale differences in nighttime $PM_{2.5}$ and (2) the role of elevation and overnight pooling of pollution.

10AC.1

Rapid Formation of Sulfate Aerosols through Aqueous Aerosol Oxidation by Isoprene Hydroxy Hydroperoxides (ISOPOOH). YUE ZHANG, Jin Yan, Yuzhi Chen, N. Cazimir Armstrong, Zhenfa Zhang, Avram Gold, Barbara Turpin, Jason Surratt, *University of North Carolina at Chapel Hill*

Isoprene is the most abundant non-methane volatile organic compound (VOC) emitted globally. Isomeric isoprene hydroxy hydroperoxides (ISOPOOH), key photooxidation products of isoprene, likely comprise the second most abundant class of peroxides in the atmosphere, following hydrogen peroxide. Studies have shown that hydrogen peroxide plays important roles in the formation of inorganic sulfates in cloud water mimics. However, the potential for ISOPOOH to play a role in sulfate formation in wet aerosol oxidation from reduced sulfur species (such as inorganic sulfite) is not well understood. This study systematically investigates the reaction kinetics and products of ISOPOOH reacting with particle phase inorganic sulfite and discusses implications to the sulfate aerosol budget.

In order to examine the reaction kinetics of ISOPOOH with aqueous sulfite, ammonium bisulfite particles were injected into the UNC indoor environmental chamber under dark conditions with 70% RH. After the inorganic sulfite concentrations stabilized, selected concentrations of gas-phase 1,2-ISOPOOH was injected into the chamber to initiate the multiphase reaction. The gas-phase ISOPOOH and particle-phase species were sampled with online instruments, including a chemical ionization mass spectrometer (CIMS), an aerosol chemical speciation monitor (ACSM), and a particle-into-liquid sampler (PILS), and also collected by Teflon filters for offline molecular-level analyses by an ultra-performance liquid chromatography coupled to an electrospray ionization high resolution quadrupole time-of-flight mass spectrometry (UPLC-ESI-HR-QTOFMS). Results show that a significant amount of inorganic sulfite was converted to inorganic sulfate and organosulfates in the particle phase at relatively fast reaction rates, altering the chemical and physical properties of the particles including phase state, pH, reactivity, and composition. Given the high abundance and water solubility of ISOPOOH in the ambient environment, the multiphase reactions examined in our study indicate significant impacts of ISOPOOH on the atmospheric lifecycle of sulfur and the physicochemical properties of ambient particles.

10AC.2

Enhanced Sulfate Production by Nitrate Photolysis in the Presence of Halide Ions in Atmospheric Particles. RUIFENG ZHANG, Masao Gen, Dandan Huang, Yongjie Li, Chak K. Chan, *City University of Hong Kong*

Heterogeneous oxidation of SO_2 is an effective production pathway of sulfate in the atmosphere. We recently reported a novel pathway for the heterogeneous oxidation of SO_2 by in-particle oxidants (OH, NO_2 and NO_2^-/HNO_2) produced from particulate nitrate photolysis (*Environ. Sci. Technol.* 2019, 53, 8757-8766). Particulate nitrate is often found to coexist with chloride and other halide ions, especially in aged sea-salt aerosols and combustion aerosols. Reactive uptake experiments of SO_2 with UV-irradiated nitrate particles showed that sulfate production rates were enhanced by a factor of 1.4, 1.3, and 2.0 in the presence of Cl^-, Br^-, and I^-, respectively, compared to those in the absence of halide ions. The larger sulfate production was attributed to enhanced nitrate photolysis promoted by the increased incomplete solvation of nitrate at the air-particle interface due to the presence of surface-active halide ions. Modeling results based on the experimental data show that the nitrate photolysis rate constants increase by a factor of 2.0, 1.7, and 3.7 in the presence of Cl^-, Br^-, and I^-, respectively. A linear relation was found between the nitrate photolysis rate constant, j_{NO3-}, and the initial molar ratio of Cl^- to NO_3^-, $[Cl^-]_0/[NO_3^-]_0$, as $j_{NO3-} = 9.7\times10^{-5}[Cl^-]_0/[NO_3^-]_0 + 1.9\times10^{-5}$ at $[Cl^-]_0/[NO_3^-]_0$ below 0.2. The present study demonstrates that the presence of halide ions enhances sulfate production produced during particulate nitrate photolysis and provides insights into the enhanced formation of in-particle oxidants that may increase atmospheric oxidative capacity.

10AC.3

Contribution of Particulate Nitrate Photolysis to Heterogeneous Sulfate Formation for Winter Haze in China. HAOTIAN ZHENG, Shaojie Song, Golam Sarwar, Masao Gen, Shuxiao Wang, Dian Ding, Xing Chang, Shuping Zhang, Jia Xing, Yele Sun, Dongsheng Ji, Chak K. Chan, Jian Gao, Michael McElroy, *Tsinghua University*

Nitrate and sulfate are two key components of airborne particulate matter (PM). While multiple formation mechanisms have been proposed for sulfate, current air quality models commonly underestimate its concentrations and mass fractions during northern China winter haze events. On the other hand, current models usually overestimate the mass fractions of nitrate. Very recently, laboratory studies have proposed that nitrous acid (N(III)) produced by particulate nitrate photolysis can oxidize sulfur dioxide to produce sulfate. Here, for the first time, we parameterize this heterogeneous mechanism into the state-of-the-art Community Multi-scale Air Quality (CMAQ) model and quantify its contributions to sulfate formation. We find that the significance of this mechanism mainly depends on the enhancement effects (by 1–3 orders of magnitude as suggested by the available experimental studies) of nitrate photolysis rate constant (JNO_3) in aerosol liquid water compared to that in the gas phase. Comparisons between model simulations and in-situ observations in Beijing suggest that this pathway can explain about 15% (assuming an enhancement factor (EF) of 10) to 65% (assuming EF = 100) of the model–observation gaps in sulfate concentrations during winter haze. Our study strongly calls for future research on reducing the uncertainty in EF.

10CC.1

Characterization of Black Carbon Aerosol and Its Impacts on Aerosol-Cloud Interactions in the Marine Environment. NILIMA SARWAR, Armin Sorooshian, Haflidi Jonsson, Richard Flagan, John Seinfeld, Andrew Metcalf, *Clemson University*

Ambient data on atmospheric black carbon (BC) aerosol was collected near Monterey, California in an aircraft-based field campaign named the Marine Aerosol Cloud and Wildfire Study (MACAWS) in June and July of 2018. A Single-Particle Soot Photometer (SP2) was used to measure BC aerosol and its mixing state. During the collaborative field project, data were collected on BC and other aerosol particles from different types of sources, including emissions from open biomass burning, marine combustion engines, on-road diesel engines, and aerosol from long-range transport. Recent studies have found that despite the various sources of BC aerosol, the marine environment is affected both directly and indirectly by the BC particles.

In this talk, the mass concentration, size distribution, and mixing state of BC aerosol particles are used to evaluate the differences between BC emitted from marine activities and BC emitted from wildfires. The influence of BC aerosol on the formation and properties of the marine boundary layer are assessed as a function of their emission sources from both nearby and far-off sources. The 2018 MACAWS dataset includes a comprehensive characterization of aerosol and cloud properties as measured in situ by aircraft, and this study will characterize the aerosol-cloud interactions and evaluate its impacts on the marine atmosphere.

10CC.2

Impact of African Dust, Biomass Burning, and Other Air Mass Types on Cloud Condensation Nuclei Concentrations at a Coastal Location in the Southeastern United States. EVA-LOU EDWARDS, Andrea F Corral, Hossein Dadashazar, Paquita Zuidema, Cassandra Gaston, Anne Barkley, Armin Sorooshian, *University of Arizona*

This study investigates the influence of different air mass types, including African dust and biomass burning (BB), on cloud condensation nuclei (CCN) concentrations at 0.2% ($CCN_{0.2\%}$) and 1.0% ($CCN_{1.0\%}$) supersaturation (SS) in Miami, Florida. Based on ground site measurements, $CCN_{0.2\%}$ and $CCN_{1.0\%}$ concentrations were 373 ± 200 cm^{-3} and 584 ± 323 cm^{-3}, respectively, on days with minimal presence of African dust and BB (i.e., background days). In contrast, CCN concentrations were not elevated on days with highest influence of African dust (289 ± 104 cm^{-3} [0.2% SS] and 591 ± 302 cm^{-3} [1.0% SS]). However, CCN concentrations were substantially enhanced on days with the greatest impact from BB (1408± 976 cm^{-3} [0.2% SS] and 3337 ± 1252 cm^{-3} [1.0% SS]). Ratios of $CCN_{0.2\%}$: $CCN_{1.0\%}$ were used to compare the hygroscopicity of the aerosol associated with African dust, BB, and background days. Average ratios were similar for days impacted by African dust and BB (0.54 ± 0.17 and 0.55 ± 0.17, respectively). A much higher average ratio was observed on background days (0.71 ± 0.14), owing in part to a strong presence of sea salt and reduced presence of more hydrophobic species such as those of a carbonaceous nature. Finally, periods of heavy rainfall were shown to effectively decrease both $CCN_{0.2\%}$ and $CCN_{1.0\%}$ concentrations, although the rate at which such concentrations increased after the rain varied. This work contributes knowledge on the nucleating ability of African dust and BB after varying periods of atmospheric transport (days to weeks), which can lead to improvements in model predictions for CCN concentrations in comparable situations.

10CC.3

Improved Estimates of Preindustrial Biomass Burning Reduce the Magnitude of Aerosol Climate Forcing in the Southern Hemisphere. PENGFEI LIU, Jed Kaplan, Loretta Mickley, Yang Li, Nathan Chellman, Monica Arienzo, Jack Kodros, Jeffrey R. Pierce, Michael Sigl, Johannes Freitag, Robert Mulvaney, Mark Curran, Joseph McConnell, *Harvard University*

Fire plays a pivotal role in shaping terrestrial ecosystems and the chemical composition of the atmosphere, and thus influences Earth's climate. Although contemporary patterns and causes of wildfire are well understood, the trend and magnitude of fire activity over the last few centuries are controversial. This uncertainty in past fire-related aerosol emissions hinders understanding of preindustrial to present-day aerosol radiative forcing because the aerosol baseline largely depends on estimates of preindustrial biomass burning. Here we present new evidence from a broad array of 14 Antarctic ice cores and 1 central Andean ice core, suggesting that historical fire emissions in the Southern Hemisphere (SH) significantly exceeded present-day levels. To understand this observation, we use a global fire model to show that overall SH fire emissions could have declined by 30% over the 20th century, possibly because of the rapid expansion of land use for agriculture and animal production. Results from atmospheric chemistry transport and deposition model simulations using our new scenario of declining fire emissions show significantly improved agreement with the ice-core records, compared to similar model results obtained with widely used emission estimates that suggest SH fire increased over the last century. We further show that the decreasing trend in fire emissions largely compensates for the cooling effect of increasing aerosols from other anthropogenic sources. The estimated magnitude of total aerosol forcing in the SH since the 1750s is 42% less than that based on an emission inventory widely used in climate models.

10IA.1

Use of Low-cost Air Quality Sensors to Quantify Human Activity Pattern Based PM2.5 Exposures.

JIAYU LI, Aliaksei Hauryliuk, Krystal Suero, Shifali Kerudi, Megan Henriksen, Albert A. Presto, *Carnegie Mellon University*

People spend 87% of their time in buildings. However, epidemiological studies usually interpret the harmful effects of $PM_{2.5}$ based on outdoor concentrations. This compromise is mainly due to the lack of affordable and accurate measurement techniques to sample air pollutants with a high spatiotemporal resolution. This study focused on characterizing air pollution profiles of indoor and outdoor environments, utilizing multiple real-time multi-pollutant sensors (RAMPs). The measured results were coupled with human activity patterns (HAP), detailing whereabouts of people, to estimate HAP-based personal exposures. The HAP-based exposure was compared with that solely determined based on outdoor measurement.

We sampled over 20 indoor environments and 10 representative outdoor environments with RAMPs for $PM_{2.5}$, CO, and, O_3 concentrations. The 20 indoor environments can be characterized as three major categories (residential buildings, common spaces, and restaurants). The 10 outdoor sites represent urban environments. The diurnal patterns of $PM_{2.5}$, CO, and O_3 concentrations from each category are significantly different. In residential buildings, $PM_{2.5}$ and CO emissions related to cooking dominate during the mealtimes, especially for families with gas stoves. The common spaces, including offices, classrooms, gyms, and libraries, show a lower concentration due to better ventilation conditions. By coupling these diurnal patterns with HAP, we used the Monte Carlo Simulation to estimate the HAP-based personal exposure. The simulation indicated that personal exposure is highly dependent on residential environments. The HAP-based $PM_{2.5}$ exposure is 5-10% lower than the exposure solely based on outdoor concentrations, while the HAP-based CO and O_3 exposures 150-200 % higher and 30-50 % lower than those estimated solely from outdoor measurements.

10IA.2

Using a Particle Sensor Network to Characterize Indoor and Outdoor Air Quality of Buildings in Areas Prone to Wildfires.

HEIDI VREELAND, Amara Holder, Sarah Coefield, Ben Schmidt, Tom Javins, Curtis Noonan, Brian McCaughey, Gayle Hagler, *U.S. EPA*

When wildfire events increase outdoor particulate matter concentrations to unsafe levels, a common recommendation for mitigating smoke exposure is to spend time indoors. However, effectively reducing smoke exposure and maintaining clean air indoors depends on a variety of building characteristics and occupant behavioral factors. To gain insights into the indoor/outdoor relationships of $PM_{2.5}$ across buildings, this study utilizes low-cost sensors (PurpleAir PA-II-SD) to characterize indoor and outdoor $PM_{2.5}$ at public and commercial buildings in two locations impacted by wildfire events in recent years: Missoula, Montana and Hoopa, California. Sensors were stationed inside and outside of 18 buildings across Missoula during summer 2019 (July–Sept) to coincide with peak fire season, and 11 buildings across Hoopa during winter (Nov 2019 – Feb 2020) when woodstove heating dominates outdoor emissions. Preliminary results suggest that indoor reductions ranged from 6% to 44% (26±11%) in Missoula, and 19% to 69% (51±16%) in Hoopa. The smaller reductions in Missoula are largely attributed to frequent door openings for ventilation during summer. In Missoula, indoor reductions were similar during smoke-impacted and typical (non-smoke) periods indicating that measurements taken outside of fire season are informative and may be useful for improving smoke preparedness. Although the only smoke events that occurred in Missoula during summer 2019 were moderate and associated with prescribed burns, this work provides valuable insights into the variance among indoor/outdoor $PM_{2.5}$. This work also demonstrates the utility of low-cost sensor networks for residents and public health agencies to better understand where clean indoor spaces exist and, potentially, to offer guidance on reducing indoor concentrations before smoke events occur.

The views expressed in this abstract are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

10IA.3

Investigation of Heatwave Effect on PM2.5 Levels Indoors using Consumer-grade Air Quality Sensors.

RUIKANG HE, Ioanna Tsoulou, Sanjeevi Thirumurugesan, Brian Morgan, Stephania Gonzalez, Deborah Plotnik, Jennifer Senick, Gediminas Mainelis, Clinton J. Andrews, *Rutgers, The State University of New Jersey*

Heatwaves have negative health effects on vulnerable populations due to thermal stress. At the same time, the effect of heatwaves (t > 90F) on indoor air quality is largely unknown. To start filling this data gap, we recruited 24 seniors from 3 sites in Elizabeth, NJ, to participate in a study during which we deployed consumer-grade sensors in their apartments to monitor particulate matter ($PM_{2.5)}$, air temperature, relative humidity, CO_2, and air conditioner (AC) use. Additionally, one empty apartment that was used as a control and one outdoor station were set up with the same type of sensors. Measurements were performed from July to September of 2017.

We found that indoor $PM_{2.5}$ levels varied among apartments. Still, heatwave had similar effects on indoor $PM_{2.5}$ levels for all apartments, regardless of the building sites and individual behaviors of seniors, such as smoking and the financial ability to use AC. For each site, the $PM_{2.5}$ levels during heatwaves days were higher than during non-heatwaves days for both smokers and non-smokers. Moreover, since human activity is a large contributor to indoor $PM_{2.5}$, we separated the data into an active period (6:00 am to 9:00 pm) and the rest period (10:00 pm to next day 5:00 am), and found that the observation above was valid for both active and rest periods: during both time periods indoor $PM_{2.5}$ levels were higher during heatwave days than during regular days.

Overall, our data suggest that long-term resident-to-building-to-neighborhood evaluation can be helpful for studies on how climate change affects human life. Our experience also demonstrated the utility and usability of consumer-grade air quality sensors to study factors affecting indoor air pollution. This research was funded by NSF grant AGS-1645786.

10ID.1

Evaluation of Decontamination Methods for Commercial and Alternative Respirator and Mask Materials -- View from Filtration Aspect.

QISHENG OU, Chenxing Pei, Seong Chan Kim, Elizabeth Abell, David Y. H. Pui, *University of Minnesota*

This study aims to evaluate the filtration performance of three commercially available (3M 8210 respirator, Halyard 48207 surgical mask, and 3M 1820 procedure mask) and two alternative face mask and respirator materials (Halyard H600 sterilization wrap and Cummins EX101) after selected decontamination treatments, including isopropanol (IPA) treatments (soaking or spraying), ultraviolet germicidal irradiation (UVGI), and heat treatments (dry heat at 77oC or steam heat). Both IPA soaking and spraying removed most electrostatic charges on all four electret materials (three commercial and one alternative), causing significant deterioration of filtration efficiency to unacceptable level. The other non-electret alternative material sustained its N95-grade performance after both IPA soaking and spraying treatments, demonstrating the possible application of IPA disinfection for non-electret alternative respirator/mask materials. UVGI preserved the filtration of all three commercially available respirator/mask materials after up to 10 treatments, suggesting it can be a possible decontamination method for hospital and clinic use without compromising respirator/mask performance. The considerations of the practical implementation of this method was discussed. Between the two heat treatment methods tested, dry heat showed better compatibility with electret material by sustaining both filtration efficiency and fit (tested on commercial respirator only), although adding moisture was reported in favor of virus inactivation. Heat treatment is easily accessible method for general publics to implement at home, while it is recommended to maintain the moisture level below saturation. Comparing to size-integrated method, the size-resolved fractional efficiency measurement technique, although more time consuming, proved to be a better method for evaluating respirator/mask filtration performance after decontaminations by providing more sensitive detection of performance degradation and the capability of distinguishing charge loss to other mechanisms causing efficiency deterioration. Detailed descriptions are provided in methodology part to emphasize the cares needed for an appropriate efficiency evaluation. The limited results in this study on worn masks made of alternative sterilization wrap indicated possible performance degradation of electret material caused by normal human wearing activities, suggesting the need of assessing respirator/mask decontamination strategy by testing practically worn-and-decontaminated/reused samples instead of unworn only-decontaminated counterparts.

10ID.2

Filtration Efficiencies of Nanoscale Aerosol by Cloth Mask Materials Used to Slow the Spread of SARS CoV-2. CHRISTOPHER ZANGMEISTER, James Radney, Edward Vicenzi, Jamie Weaver, *National Institute of Standards and Technology*

Filtration efficiency (FE), differential pressure (ΔP), quality factor (QF) and construction parameters were measured for 32 cloth materials (14 cotton, 1 wool, 9 synthetic, 4 synthetic blends, and 4 synthetic/cotton blends) used in cloth masks intended for protection from the SARS CoV-2 virus (diameter 100 ± 10 nm). Seven polypropylene-based fiber filter materials were also measured, including surgical masks and N95 respirators. Additional measurements were performed on both multi-layered and mixed-material samples of natural, synthetic, or natural-synthetic blends to mimic cloth mask construction methods. Materials were micro-imaged and tested against size selected NaCl aerosol with particle mobility diameters between 50 nm and 825 nm. Three of the top five best performing samples were woven 100% cotton with high to moderate yarn counts and the other two were woven synthetics of moderate yarn counts. In contrast to recently published studies, samples utilizing mixed materials did not exhibit a significant difference in the measured FE when compared to the product of the individual FE for the components. The FE and ΔP increased monotonically with the number of cloth layers for a lightweight flannel, suggesting that multi-layered cloth masks may offer increased protection from nanometer-sized aerosol with a maximum FE dictated by breathability (i.e. ΔP).

10ID.3

Decontamination and Re-Use of Surgical Masks and N95 Respirators during the COVID-19 Pandemic: Effect of Autoclave Sterilization and Ethanol Treatment on Filter Efficiency and Breathability. SERGEY A. GRINSHPUN, Michael Yermakov, Marat Khodoun, *University of Cincinnati*

An extraordinary demand for disposable filtering facepieces (surgical masks and N95 respirators) has substantially exceeded their supply during the COVID-19 pandemic. While disposable devices are generally not approved for routine decontamination and re-use, their decontamination and re-use widely occurred “as a crisis capacity strategy to ensure continued availability,” according the US Centers for Disease Control and Prevention, with a very limited testing conducted on how decontamination may affect the performance of a mask or respirator. We evaluated surgical masks and N95 respirators commonly used in healthcare environments with respect to their performance changes resulting from sterilization by autoclaving and treatment with 70% ethanol (alcohol). These decontamination methods are frequently utilized when filtering facepieces are being re-used in hospitals. We determined experimentally the changes in collection efficiency (filter protection factor) and pressure drop (breathability) for surgical masks and N95 filtering facepieces after applying the above disinfection treatments. The collection efficiency testing was focused on particle sizes approximately from 37 to 3,200 nm measured with an Electrical Low Pressure Impactor (ELPI) to represent the aerosolized single viruses, their agglomerates, bacteria and larger particle-carriers. It was concluded that the protection level and breathability originally offered by the tested devices may be significantly compromised by autoclaving and alcohol treatment. Quantitatively, the changes were found to depend on a respiratory protective device (type and model), particle size, breathing flow rate, type of treatment and other factors. Additionally, physical damages were observed in some models of N95 respirators after autoclaving, including a notable detachment of the nose foam, partial disintegration of the filter material around the nose clip, loss of strap elasticity and others.

10IM.1

Comparison of Inversion Schemes for Retrieving Black Carbon Mixing State Distributions using CPMA-SP2 Measurements. Naseri Arash, Timothy Sipkens, Una Trivanovic, Mohsen Kazemimanesh, Olanrewaju Wasiu Bello, Allan Bertram, Steven Rogak, JASON S. OLFERT, *University of Alberta*

Black carbon (BC) is one of the main contributors to the anthropogenic radiative forcing that causes climate change. The short life cycle of BC and its presence in complex forms (e.g., mixed with or coated by other inorganic and organic materials) results in large uncertainties in BC contribution to radiative forcing. To lower these uncertainties, robust measurements of the distribution of refractory BC mass and non-refractory (e.g. organic) coatings of atmospheric particles is required. Often, these measurements use simplified assumptions for data analysis, e.g. irregular morphology of BC is often represented as an equivalent sphere and described with an effective density. Recently, Broda et al. (2018) proposed a novel method by employing the Twomey-Markowski inversion scheme with a CPMA-SP2 system to attain the two-dimensional refractory BC mass-total particle mass distribution, indicating the distribution of the mixing state. This study improves this method by implementing a novel Bayesian approach that combines data with an exponential distance prior that naturally correlates counts for particles that are expected to share characteristics. To start, both inversion methods are tested with some fabricated data (i.e. ‘phantoms’). Results indicated that the exponential distance method can improve the accuracy of reconstructions of narrow and broad distributions by ~60% and ~20%, respectively. Both methods were then implemented on a set of experimental data generated by injecting sodium chloride solutions, using an ultrasonic atomizer, into a turbulent diffusion flame. This resulted in particles that can be composed of sodium chloride and soot. Solutions of 0.03% and 3% salt in deionized water, which produced sharp and diffuse black carbon mixing state distributions, respectively, were used to demonstrate how the exponential distance prior can improve the description of the mixing state for each case.

10IM.2

Online Shape and Density Measurement of Single Black Carbon Aerosol Particles. Shurong Wang, Kaili Zhou, JianMin Chen, Kimberly Prather, Xin Yang, XIAOFEI WANG, *Fudan University*

Black carbon (BC) aerosols play crucial roles in affecting air quality, climate, and human health. Density and morphology reflect chemical composition, mixing state and aging pathway of BC particles. A novel method, which mainly consists of an aerodynamic aerosol classifier, a differential mobility analyzer and a single-particle soot photometer, was developed to calculate shape factor and density of single BC particle by measuring its aerodynamic diameter (D_a), electrical mobility diameters (D_m) and BC mass content (m_{BC}). Ambient BC aerosols with different D_a (200 nm, 350 nm, 500 nm) were studied by this method. BC-dominated particles were only observed in particles with 200nm D_a and 135nm D_m, which accounted for ~75.6% of particles with 200nm D_a in the winter sampling days. Surprisingly, morphology of BC-dominated particles was near-spherical, indicating just a few absorbed substances on BC particles could change their morphology from irregular to near-spherical. Aerosols of Mode(D_a =350nm, D_m=259.5nm) and of Mode(D_a =500nm, D_m=358.7nm) constituted up to ~73.6% and ~81.9% of ambient aerosols with 350nm D_a and 500nm D_a. Most BC particles in these two modes was internally mixed with secondary substances, and their morphology was likely to be spherical. Ammonium sulfate and ammonium nitrate were the main secondary substances of BC particles in these two modes, consistent with their measured densities (1.62 g/cm3 and 1.77g/cm3 respectively) and average single particle mass spectra. Generally, the new online system can investigate both morphology and density of each single BC particle, which can help identify the formation and aging pathway of BC aerosols.

10IM.3

Elemental Analysis of Oxygenated Organic Coatings on Black Carbon Particles using a Soot-Particle Aerosol Mass Spectrometer. MUTIAN MA, Laura-Helena Rivellini, Yuxi Cui, Megan Willis, Rio Wilkie, Jonathan Abbatt, Manjula Canagaratna, Junfeng Wang, Xinlei Ge, Alex Lee, *National University of Singapore*

Chemical characterization of organic coatings is important to advance our understanding of the physio-chemical properties and environmental fate of black carbon (BC). Soot-particle aerosol mass spectrometer (SP-AMS) has been utilized for this purpose in field studies. The laser vaporization (LV) scheme of SP-AMS can heat up BC cores gradually until they are completely vaporized, during which organic coatings can be vaporized at temperatures lower than that of thermal vaporizer (TV) used in a standard high-resolution aerosol mass spectrometer (HR-AMS).

This work investigates the effects of vaporization schemes on fragmentation and elemental analysis of oxygenated organic species (30 in total) using three SP-AMS. We show that LV can reduce the fragmentation of organic molecules. Substantial enhancement of $C_2H_3O^+/CO_2^+$ and $C_2H_4O_2^+$ signals were observed for most species vaporized by the LV scheme, suggesting that the observational frameworks developed based on HR-AMS field data may not be directly applicable for evaluating the chemical evolution of oxygenated organic aerosol (OOA) coated on ambient BC. The uncertainties of H:C and O:C determined by the improved-ambient (I-A) method for both LV and TV approaches were similar, and scaling factors of 1.10 for H:C and 0.89 for O:C were determined to facilitate more direct comparisons between observations from the two vaporization schemes. Applying the scaling factors to ambient data, we found that even the time series of OOA components determined by LV and TV scheme are strongly correlated at the same location, OOA coatings were likely less oxygenated compared to those externally mixed with BC. Lastly, the I-A method was updated based on the multilinear regression model for the LV scheme measurements, which can reduce the relative errors of O:C from -26% to 6%, and the relative errors of H:C remain similar.

10SD.1

Developing a Framework for Refining Ammonia Emissions Estimates with Satellite-based Observations with Air Quality Modeling. CONGMENG LYU, Mahmoudreza Momeni, Shannon Capps, Matthew Lombardo, Mark Shephard, Amir Hakami, Daven Henze, Steven Thomas, Peter Rayner, *Drexel University*

The Community Multiscale Air Quality (CMAQ) model calculates the impact of emission on atmospheric composition, including inorganic aerosols, while considering the transport and reactions of chemical constituents. Adjusting emissions by comparing modeled concentrations with observations is possible when the science processes are well understood as is the case for inorganic species such as ammonia (NH3). Four-dimensional variational data assimilation leverages differences in simulated and actual observations to revise estimates of emissions with spatial specificity. In this study, we evaluate the capacity of a CMAQ-based data assimilation system to improve NH3 emissions, which are relatively uncertain given the diversity of emissions processes in the agricultural sector. To do so, a Python-based four-dimensional variational framework (py4dvar) is integrated with CMAQ and its adjoint to constrain NH3 emissions with observations from the satellite-based Cross-track Infrared Sounder (CrIS). The framework, including the adjoint of CMAQ and the CrIS observation operator, are evaluated. Additionally, the py4dvar implementation is tested. Specifically, pseudo-observation tests are conducted with the CrIS observation operator to evaluate the extent to which emissions are expected to be recovered with the assimilation.

10SD.2

A Novel Single-scattering Property Database of Irregular Aerosol Particles for Satellite-based Aerosol Remote Sensing. MASANORI SAITO, Ping Yang, Xu Liu, *Department of Atmospheric Sciences, Texas A&M University*

Atmospheric aerosol particles associated with air pollution, dust storms, and volcanic eruptions have substantial impacts on Earth's environment and human health. Satellite observations have been used to monitor the global distributions of aerosol particle characteristics such as aerosol optical depth (AOD). Recent studies have focused on the abundance of fine particles with a diameter less than 2.5 µm, which emphasizes the importance of size characterizations of aerosol particles. However, the complexity of aerosol optical and microphysical properties poses a significant challenge for a better understanding of the aerosol characteristics based on spaceborne observations. Aerosol optical properties such as the refractive index, which typical satellite-based aerosol retrieval approaches assumes to be constant, may have significant spatial and temporal variations. Majority of aerosol particles, in particular intermediate-to-large size particles, are non-spherical. To reliably monitor the global distribution of aerosol particles with satellite measurements, it is necessary to know the spectral single-scattering properties of various aerosol particles including their particle sizes, refractive indices, and shapes. This presentation reports on a single-scattering property database of various dust aerosol particles by using the physical-geometric optics method (PGOM) for large particle size domain and the invariant-imbedding T-matrix (II-TM) method for small to intermediate particle size domain. These two computational methods can compute reliable single-scattering properties including the values in the backscattering direction. Comparisons of the scattering properties between laboratory measurements and the present simulations show reasonable consistency. Furthermore, we apply the dust aerosol scattering properties to simulate various spaceborne satellite observations, including multiangle polarimetric observations, thermal infrared observations, and lidar observations. In this presentation, we will demonstrate the capability of current satellite observations with the scattering property database to infer aerosol optical properties including particle size and AOD.

10SD.3

Retrieving Low-cost Air Quality Sensor Network by Integrating Fixed and Satellite Monitoring Systems for a Northern China City. HUANG ZHANG, Chun-Ying Chao, Melanie Hammer, Randall Martin, Pratim Biswas, *Washington University in St Louis*

North China Plain (NCP) is one of the most particle matter (PM) polluted area in the world. Integrating measured values from satellite remote sensing, fixed monitoring stations, and a low-cost PM sensor network could enhance the spatial and temporal resolution of ground-level PM2.5 measurements[1]. This study examines the performance of fixed monitoring stations, a low-cost PM sensor network, and satellite aerosol optical depth (AOD) from multiple satellite products (MAIAC, MODIS, and Himawari-8) to improve the spatiotemporal resolution of PM2.5 concentration for a typical city, named Xinxiang city, in the NCP during 2017. First, measured values of low-cost PM sensors are retrieved by fixed monitoring sites. The low-cost sensor datasets demonstrate high linearity against those of fixed monitoring stations with R^2 value of 0.84. Second, the retrieval PM2.5 concentrations between the AOD datasets and the fixed monitoring stations demonstrate a moderate correlation coefficient with R^2 value of 0.52. Third, to evaluate the impact of human activities on air quality, four traditional Chinese festivals in 2017, Chinese New Year, Tomb Sweeping Day, Ghost Festival, and Moon Festival, are chosen to analyze the spatial and temporal distribution of ground-level PM2.5 concentration by creating heat maps over Xinxiang city. The results show that low-cost PM sensor networks and AOD datasets can be incorporated with traditional measurement methods to substantially improve the resolution of pollution maps.

[1] Li, J., Zhang, H., Chao, C.Y., Chien, C.H., Wu, C.Y., Luo, C.H., Chen, L.J. and Biswas, P., 2020. Integrating low-cost air quality sensor networks with fixed and satellite monitoring systems to study ground-level PM2. 5. Atmospheric Environment, 223, p.117293.

11AC.1

Particle- and Gas-phase Chamber Measurements of Dimethyl Sulfide Oxidation. MATTHEW GOSS, Qing Ye, Gabriel Isaacman-VanWertz, Jesse Kroll, *MIT*

Dimethyl sulfide (DMS) is the largest natural source of sulfur and an important source of non-sea salt aerosol over the oceans, however its complete oxidative pathway and ultimate fate are still not fully understood. The recent discovery of hydroperoxymethyl thioformate has highlighted major uncertainties in the DMS oxidation mechanism, particularly under low-NO conditions. Here, we perform high- and low-NOx chamber experiments to examine the formation and transformation of a variety of products from DMS oxidation in the presence of seed particles. Aerosol particles are characterized by an Aerosol Mass Spectrometer (AMS) and complemented by gas-phase mass spectrometric measurements to capture the full distribution of sulfur-containing oxidation products. Specific results include the measurements of multi-generational gas- and particle-phase chemistry, characterization of previously unidentified species in the gas- and particle-phases, and analysis of particle size evolution.

11AC.2

Global Modeling of Heterogeneous Hydroxymethanesulfonate Chemistry. SHAOJIE SONG, *Harvard University*

Hydroxymethanesulfonate (HMS) has recently been identified as an abundant organosulfur compound in aerosols during winter haze episodes in northern China. It has also been detected in other regions, although the concentrations are low. Because of the sparse field measurements, the global significance of HMS and its spatial and seasonal patterns remain unclear. Here, we implement HMS chemistry into the GEOS-Chem chemical transport model and conduct multiple global simulations. The developed model accounts for cloud entrainment and gas–aqueous mass transfer within the rate expressions for heterogeneous sulfur chemistry. Our simulations can generally reproduce the available HMS observations, and show that East Asia has the highest HMS concentration, followed by Europe and North America. The simulated HMS shows a seasonal pattern with higher values in the colder period. Photochemical oxidizing capacity affects the competition of formaldehyde with oxidants (such as ozone and hydrogen peroxide) for sulfur dioxide and is a key factor influencing the seasonality of HMS. The highest average HMS concentration (1–3 $\mu g\ m^{-3}$) and HMS/sulfate molar ratio (0.1–0.2) are found in northern China winter. The simulations suggest that aqueous clouds act as the major medium for HMS chemistry while aerosol liquid water may play a role if its rate constant for HMS formation is greatly enhanced compared to cloud water.

11AC.3

Inorganic PM2.5 Composition in Fairbanks Alaska Winter: Large Contributions from HMS. MICHAEL BATTAGLIA JR., Rime El Asmar, James Campbell, Meeta Cesler-Maloney, William Simpson, Jingqiu Mao, Athanasios Nenes, Rodney J. Weber, *Georgia Institute of Technology*

Fairbanks, Alaska, is a near-Arctic, in-land city known to experience intense winter-time atmospheric inversions with high concentrations of PM2.5 mass that often exceed air quality standards. In preparation for the Sustainably Navigating Arctic Pollution -- Through Engaging Communities (SNAP-TEC) field study planned for 2022, we characterized ambient wintertime aerosols in Fairbanks during January-March 2020. An Aerodyne ASCM configured for PM2.5 sampling was deployed to begin the first year-long continuous speciated PM2.5 mass-spectrometer measurement in Alaska. A particle-into-liquid sampler coupled to ion chromatograph (PILS-IC) utilizing Metrohm columns and eluents was used to characterize water-soluble anions from Jan-March, with a specific interest in separately measuring hydroxymethanesulfonate (HMS) and inorganic sulfate. Daily filter samples were analyzed by anion and cation ICs for comparisons with online instruments. Additionally, MOUDIs continuously sampled for 3-5 days were deployed and used to develop size distributions of anions and cations. ACSM analysis revealed that fine aerosols in Fairbanks were dominated by organic species, typically comprising about 60% of the PM2.5 mass. During periods of intense inversions and extreme cold, HMS was found at concentrations similar to those of inorganic sulfate, both at times reaching concentrations over 10 ug per cubic meter. The source of the HMS is being investigated, factors include high emissions, higher gas-to-particle conversion, and possibly other formation mechanisms that are enhanced at lower temperatures. Delineating the HMS and inorganic sulfate may provide improved methods for reducing the high levels of PM2.5 found in Fairbanks during winter months.

11CC.1

Direct Comparison of the Submicron Aerosol Hygroscopicity of Water-Soluble Sugars and Ammonium Sulfate-Organic Mixtures. PATRICIA RAZAFINDRAMBININA, Joseph Nelson Dawson, Kotiba A. Malek, Tim Raymond, Dabrina Dutcher, Akua Asa-Awuku, Miriam Freedman, *University of Maryland*

Water-soluble organic compounds (WSOC) can exist in the atmosphere as aerosol particles. Both man-made and naturally occurring WSOC aerosol particles can readily uptake water and form droplets that can affect the particle’s overall effect on climate forcing. Understanding the water uptake ability of such particles is key to improving current climate models. In this study, we examine the validity and reliability of three water uptake measurement methods by investigating the hygroscopicity and cloud condensation nuclei (CCN) activity of four atmospherically relevant sugars: sucrose, levoglucosan, trehalose, and raffinose. In addition to small sugars, we present the water uptake of select WSOC as internal and external mixtures with ammonium sulfate at sub and supersaturated conditions. At subsaturated conditions, the optical growth factor (f_{RH}) obtained from cavity ring-down spectroscopy measurements and the geometric growth factor (G_{f}) from humidified tandem differential mobility analyses was converted to the single parameter hygroscopicity, κ. κ allows subsaturated hygroscopic properties to be compared to supersaturated measurements made by the cloud condensation nuclei counter (CCNC), as measured critical activation diameters (d_{p50}) can be directly converted into κ. Values reported in this work show that the single parameter hygroscopicity term for the selected WSOC is molecular weight dependent. κ-values obtained from the three methods were comparable in precision, with systematic deviations in the average mean for each method.

11CC.2

Temperature Dependent Entropy Driven Water Uptake in Phase Separated Aerosol Particles. MARIA LBADAOUI-DARVAS, Satoshi Takahama, Athanasios Nenes, *LAPI, EPFL (Switzerland)*

Cloud droplets activation and growth are related to water uptake by aerosol particles. Interfacial mass transfer— that governs water uptake if mean free path is comparable to particle size — is quantified by the mass accommodation coefficient (α), probability that a molecule hitting the surface of a particle is absorbed. Mass accommodation coefficients below 0.1 lead to increased supersaturation development and larger droplet number in clouds – with important implications for aerosol-cloud interactions. Reduced α values are observed if a hydrophobic film covers the particle; and are unlikely to be representative of global values. In ambient particles, especially at high humidity, surface tension reductions can still have a significant impact on droplet formation. Liquid-liquid phase separation (LLPS), which occurs in organic aerosol if the O:C ratio is below ~0.8, yields particles having complex organic coating. LLPS is suspected to contribute to the discrepancies between measured a modeled CCN activities, but its exact role is to date unclear.

We perform steered molecular dynamics simulations to reconstruct the free energy profile of water uptake across a vapor/hydroxy cis-pinonic acid/water double interface at 300 K and 200 K. Free energy profiles are used to estimate a range of effective accommodation coefficients. Near-unity α values are observed for the lower temperature, whereas at room temperature $0.05<\alpha<0.38$, which can impart a mild direct effect on supersaturation and cloud droplet development. The free energy minimum near the organic/water interface — which originates from locally increased conformational entropy from local mixing—at 300 K results in a water concentration gradient in the organic phase, which helps to maintain LLPS and low surface tension at very high RHs. The effect diminishes at 200 K. These results highlight the need to consider a temperature dependent parametrization of α in parcel model simulations.

11CC.3

Using Model Particle Systems to Constrain Atmospheric Particle "Glassiness" and Mixing Limitations. LUKE HABIB, Neil Donahue, *Carnegie Mellon University*

Atmospheric aerosols have highly uncertain and poorly understood effects on climate change and human health. That uncertainty is in part due to uncertainty surrounding the mixing state of aerosol populations, which is commonly assumed to be well internally mixed, especially for atmospheric models. If atmospheric aerosol particles are not internal mixtures, it could be much more difficult to understand their health and climate effects. When distinct aerosol populations come in contact with each other, mixing should happen on a time scale of a few hours in order to support the internal mixing assumption. For semi-volatile organics, gas-phase exchange between aerosol populations via condensation and evaporation ("Marcolli mixing") can be a major source of mixing between accumulation-mode particles with slow coagulation. However, the existence of viscous, semi-solid, or "glassy" particles may impede this by posing potential diffusion limitations to Marcolli mixing. Here we describe experiments on carefully prepared particle populations representing "glassy" aged organic particles (glucose particles with ammonium sulfate seeds) and fresh biomass burning organic aerosol particles (erythritol particles with black carbon seeds) to develop a model phase space for organic aerosol systems and better understand when particle "glassiness" impedes gas-phase exchange of semi-volatile organics. The mixing state of these particle populations is quantified using an Aerosol Mass Spectrometer (AMS) in the Event Trigger (ET) and Soot Particle (SP) modes simultaneously. The ET mode of the AMS records single particle mass spectral data based on "triggering" data acquisition at desired mass-to-charge ratios and the SP mode allows for refractory black carbon particles to be characterized. Preliminary results and previous studies suggest that at some relative humidity threshold, glassy particles will plasticize and diffusive mixing limitations will break down; we expect the relative humidity of the glass transition to increase with decreasing temperature.

11HA.1

Chemical and Toxicological Characterization of Vaping Emission Products from Commonly Used Vape Juice Diluents. HUANHUAN JIANG, C.M. Sabbir Ahmed, Thomas Martin, Alexa Canchola, Iain Oswald, Jose Garcia, Jin Chen, Kevin Koby, Anthony Buchanan, Zixu Zhao, Haofei Zhang, Kunpeng Chen, Ying-Hsuan Lin, *University of California, Riverside*

There have been an increasing number of reports on the detrimental vaping-related incidents, such as lung injury, lipid pneumonia, and the occurrence of seizures, which illicit a great health concern regarding the usage of vaping products including e-cigarettes and cannabis. The prevalence of vaping among adolescents has increased dramatically within the past decade for the reduced consumption of nicotine and lack of combustion needed to consume the product during vaping. The major components of vape juices and e-liquids are the viscosity enhancers, the percentage of which can reach up to 100%. Previous studies have reported that the thermal degradation and oxidation of commonly used viscosity enhancers (e.g., propylene glycol) can produce a large amount of highly toxic aldehydes (e.g., formaldehyde and acetaldehyde). Recently, a variety of new juice diluents have been introduced into the market. However, to date, the chemical compositions and toxicological characterization of vaping products from these juice diluents are largely unknown. This pilot study aims to provide a molecular and toxicological characterization of e-cigarette vaping products from seven commonly used viscosity enhancers, including propylene glycol, glycerin, medium-chain triglyceride (MCT) oil, triethyl citrate, squalane, vitamin E (tocopherol), and vitamin E acetate (tocopheryl acetate). The vaping products in both gas and particle phase were collected into two tandem impingers. Samples collected in isopropyl alcohol and o-(2,3,4,5,6-pentafluorobenzyl)hydroxylamine hydrochloride (PFBHA) aqueous solution were applied to GC-MS and LC-MS for chemical analysis. Samples collected in LHC-9 cell culture media were applied for cell proliferation and cytotoxicity evaluation in human epithelial lung cells (BEAS-2B). Our study demonstrates that during vaping processes, changes in chemical composition of several commonly used vape juice diluents (also known as cutting agents) lead to the formation of toxic byproducts, including quinones, carbonyls, esters and alkyl alcohols. The resulting vaping emission condensates cause inhibited cell proliferation and enhanced cytotoxicity in human airway epithelial cells. In particular, we observed a high yield of duroquinone and durohydroquinone from the vaping of vitamin E and vitamin E acetate. This might help explain the recent outbreak of e-cigarette or vaping product use-associated lung injury that was linked to the vaping of e-liquid containing vitamin E acetate. These findings highlight the significant role of toxic byproducts in vaping-associated health effects.

11HA.2

Accretion Reactions Characterized in Unflavored Electronic Nicotine Delivery System (ENDS) Aerosols by Hydrophilic Interaction Liquid Chromatography Coupled to High-Resolution Quadrupole Time-of-Flight Mass Spectrometry (HILIC/QTOF-MS). SARAH SUDA PETTERS, Yue Zhang, Jin Yan, Caz Nichols, Timothy Fennell, Michelle McCombs, Kamau Peters, Jonathan Thornburg, Jason Surratt, *University of North Carolina at Chapel Hill*

Electronic nicotine delivery systems (ENDS), including electronic cigarettes (e-cigs), are an emerging health concern due to the relatively unknown health consequences of long-term use. Large differences in aerosol generation, due to a variety of factors such as coil temperature, e-liquid content, and nicotine carrier, result in large and often uncharacterized variabilities in e-cig aerosol composition. Recent studies reveal that thermal breakdown of ENDS carrier liquids (humectants including propylene glycol and glycerol) and added flavors yield volatile aldehydes and decomposition products. Many ENDS aerosol characterization studies focus on volatile compounds and the development of gas-phase chemical characterization methods and have potentially missed oligomerization reactions occurring in heated e-liquid mixtures. Here we use hydrophilic interaction liquid chromatography coupled with electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (HILIC/ESI-HR-QTOFMS) to demonstrate that accretion reactions forming C-O-C bonds can occur in unflavored e-cig aerosols. We identify ether, acetal, and heterocycle formation from humectants and first-generation thermal decomposition products. Additional chemical characterization, including comparison to authentic standards and MS/MS fragmentation spectra, were used to confirm the identities of some of the measured compounds. These oligomerization reactions alter the vapor pressure, solubility, reactivity, and other physicochemical properties of the aerosol by raising the molecular weight and altering functional group composition. In contrast to the heated gas chromatography methods preferred for the detection of volatile and semi-volatile humectants, flavors, nicotine and aldehydes in prior e-cig and tobacco research, we developed a lower temperature HILIC/ESI-HR-QTOFMS method that separates polar molecules. Results reveal that, in addition to previously known volatile irritants, higher molecular weight organic compounds of lower volatility are produced in e-cig aerosols. We demonstrate that e-cig aerosol oligomers can be detected and characterized using HILIC/ESI-HR-QTOFMS, thus enabling more detailed research examining the physical properties, composition, biomarkers of exposure, and potential toxicological effects of e-cig aerosols.

11HA.3

Assessing E-cigarette Aerosol Physical and Chemical Changes Post-emission Using an Idealized Physical Throat Model.

KAITLYN SUSKI, Zarina Munshi, Raj Rao, Brad Ingebrethsen, Bryan Toth, Won Choi, Hosna Mogaddedi, *JUUL Labs*

E-cigarette aerosol is composed of only a few chemical compounds. Nevertheless, it is a complex system that undergoes rapid and constant chemical and physical change once emitted from devices due to its hygroscopic nature and range of component volatilities. During inhalation, volatile aerosol components deposit by a combination of vapor and particle deposition and the extent to which these deposition modes occur depends on particle size and number concentration as well as the vapor pressures of the volatile components in the aerosol. The vapor pressure of nicotine from e-liquids and how it changes based on e-liquid composition is not well characterized. This work aims to link changes in aerosol chemistry as e-cigarette particles travel through the respiratory tract to the vapor pressures of those components by measuring deposition rates in an idealized model airway.

The experiments presented here estimate deposition of e-liquid constituents using a humidified tube (RH ≈ 100%, 40 °C) with the same internal volume as the oropharyngeal region of the respiratory tract in an average adult male. E-cigarette aerosols were drawn through this model airway using a simulated human puff and inhalation flow sequence. Aerosol was collected and characterized ex-device and ex-airway via light scattering, gravimetric weighing, and gas and liquid chromatography. The light scattering and gravimetric results indicate rapid e-cigarette aerosol growth in the airway model due to water uptake. Additionally, there was greater removal of the more volatile components compared to lower volatility components based on the chromatography data. These results show that idealized model airways provide a relatively simple and low-cost approach to assess e-cigarette aerosol transport in human airways. While these experiments are limited to a physical model of the oropharyngeal region, similar water uptake kinetics and volatile component deposition processes would be expected to take place in more complex ways throughout the respiratory system, which will be explored by combining these results with modeling.

11IA.1

Long-Term Measurements of Particulate Matter in Residential Households: Case Studies with Cooking Methods, Cleaning, and Other Everyday Activities.

SIERRA LALTRELLO, Azita Amiri, Shanhu Lee, *The University of Alabama in Huntsville*

Humans spend approximately 80%-90% of their lives indoors, and past studies have shown that indoor particulate matter (PM) negatively affect human health. Previous indoor PM measurements were performed mostly in laboratories or “test-houses” without residents living inside under controlled conditions, thus not being fully-representative of real living environments. Continuous long-term measurements in real houses are essential for assessing diurnal and seasonal changes as well as PM response to everyday human activities. In this study, we show 1-year long continuous measurements using a prototype monitor (Portable Aerosol Spectrometer Dust Decoder, Model 11-D, Grimm Inc.) with a size range from 0.25 to 35 µm. This instrument does not require any chemicals, pumps, or radiation sources to operate, allowing long-term measurements of PM in residential households under safe and unperturbed conditions. We looked at three authentic households in the Southeastern U.S. from May 2019 to May 2020. Our study shows that oil-rich cooking releases more PM than methods like boiling and steaming, whereas time of day does not necessarily play a distinctive role. Cooking intensity plays a role in the amount of PM despite the type of appliance used. In particular, big cooking holidays, like Thanksgiving and Christmas, produce large amounts of $PM_{2.5}$ (averaging around 20 $\mu g/m^{-3}$ throughout the experiment) even with kitchen exhaust and house ventilation. Cooking produces more fine mode particles, whereas cleaning with a vacuum cleaner produces more coarse mode particles. Spraying air freshener and using the dishwasher also produce elevated coarse PM levels. Measurements during the pandemic period provide unique insights on how human occupancy affects indoor air quality. Our study reinforces the findings of previous research from simulated environments and further provides a big picture on how authentic household diversity plays a role in indoor PM levels.

11IA.2

Assessment of PM2.5 Concentration and Transport in Indoor Environments Using Low-cost Sensors. SUMIT SANKHYAN, Julia Witteman, Sameer Patel, Marina Vance, *University of Colorado Boulder*

Fine particulate matter (PM2.5) is an important constituent of air pollution and has been linked to a variety of health effects. Consumer-grade, low-cost PM sensors are gaining popularity as a convenient tool for consumers to monitor indoor air quality inside their homes. We investigated five commercially available air quality monitors (IQAir AirVisual Pro, Foobot Home, PurpleAir PA-II-SD, and PurpleAir PA-I-Indoor) and compared them to a research-grade optical particle monitor (TSI Optical Particle Sizer, OPS 3330) by deploying them in three homes of different sizes over a period of 9-12 weeks each. Two identical units of each monitor were deployed in the kitchen and bedroom of each home to evaluate PM2.5 transport between those spaces. Indoor monitors were collocated for 3 days at the beginning and end of each deployment period to assess their accuracy over time. A second component of the project included an investigation on the effects of deploying a consumer-grade portable air cleaner in the kitchen and in the bedroom on PM2.5 levels. A range of sensors (Samsung SmartThings) were also deployed to detect the opening of doors and windows and the operation of the air purifier. Preliminary results show a range of correlation levels between low-cost monitors and the OPS, with R2 values ranging from 0.75 to 0.94, and among pairs of the same low-cost monitor models, with R2 values between 0.60 and 0.99.

11IA.3

Does Residential HVAC Filtration Work? TIANYUAN LI, Masih Alavy, Zhang Yizhi, Jeffrey Siegel, *University of Toronto*

Residential filtration performance is understudied when compared to filtration in commercial buildings. There are substantial reasons to expect varied performance including predominantly recirculating systems that do not introduce ventilation air, low runtimes, the application of standardized laboratory tests to non-standardized residential systems, and the importance of dynamic source processes, among others. We measured particle concentrations, filter efficiency, and HVAC system-related parameters in 20 homes in Toronto, Canada in this year-long investigation. Over the course of the year, each home received four types of filters (MERV 8 uncharged media; MERV 8, 11, and MERV 14 electret media) for three months each and installed in a random order in each home. Major findings from the investigation include in-situ filtration efficiency varied widely between homes such that the difference between homes for the same filter was generally larger than the difference between filters with different nominal efficiencies. In most homes, the in-situ efficiency was smaller than the lab-tested efficiency largely due to bypass and face velocity differences. On average, the in-situ efficiency of the electret filters was smaller at the end of a three-month deployment than when new and the MERV 8 uncharged media was unchanged. Filter effectiveness showed similar large variations as in-situ efficiency. Filter pressure drop was very similar (and not significantly different) for all four types of filters, likely owing to differences in filter design as well as face velocity and air bypass interactions with filter flow resistance. Continuous hourly 0.5 – 2.5 µm particle number concentrations as measured with a low-cost optical monitor showed no discernable impact of different filters in these homes, likely due to low median runtimes (9.6%) across the investigation. This suggests that filters have to be selected and used well to have a meaningful impact on residential particle concentrations.

11ID.1

Environmental Effects on Betacoronavirus Resuspension and Transport at High Risk Facilities.

Sunil Kumar, Tatiana Baig, MARIA KING, *Texas A&M University*

To objective of this study is to understand the effect of the environment on the transmission, deposition and spread of virus aerosols in the ventilation airflow and enable early detection of virus particles in room size spaces. In an air-conditioned model hospital chamber bovine betacoronavirus (BCoV) aerosols as SARS-CoV-2 simulants were disseminated to test the effect of different environmental conditions including temperature, relative humidity and air velocity on the stability and movement of the virus. Particle tracking velocimetry was used to monitor the size distribution, deposition and resuspension of the BCoV virus particles aerosolized at different temperature, humidity and air velocity values. At regular time intervals after aerosolization, the viruses were collected from the surfaces and quantified using quantitative reverse transcription polymerase chain reaction (RT-qPCR).

Two portable VBAC collectors at 100 L/min flow rate were used to sample the simulant virus particles from the air at two locations (patient's bed and exhaust) in the chamber. The collected BCoV viruses were enumerated for viable and total counts. The aerosol collection results were used to gain information about the temporal and spatial concentration of the airborne viruses and whether they maintain their viability during aerosolization and transport. Based on the chamber mechanical blueprint, ANSYS Fluent computational flow model was created to simulate the entrainment of virus aerosols from a patient's breath in the ventilation airflow and validated by the virus aerosol collections at the different locations. The experimental data, in good agreement with the simulation showed the entrainment of the virus in powerful vortices before impacting on surfaces or exiting through the air outlet. Mitigation efforts to change the airflow pattern significantly reduced the virus concentration in the patient's breathing zone.

11ID.2

Influence of Wind and Relative Humidity on the Social Distancing Effectiveness to Prevent COVID-19 Airborne Transmission: A CFD Study.

YU FENG, Thierry Marchal, Ted Sperry, Hang Yi, *Oklahoma State University*

The ongoing pandemic caused by the novel severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has illustrated the global public health threat. It has been confirmed that the coronavirus disease 2019 can be transmitted through droplets created when an infected human coughs or sneezes. Accordingly, 6-feet social distancing has been advised to reduce the spread of the disease among humans. However, it is unknown whether 6 feet are sufficiently far or not. To provide evidence and insight into the "social distancing" guidelines, a validated computational fluid-particle dynamics (CFPD) model was employed to simulate the transient transport, condensation/evaporation, and deposition of SARS-CoV-2 laden droplets emitted by a cough or sneeze between two virtual humans with different environmental wind velocities. Initial droplet diameters range from 2 to 2000 microns, and the wind velocities range from 0 to 16 km/h, representing different wind forces from calm to gentle. Ambient relative humidities are 40% and 99.5%. Trajectories of SARC-CoV-2-laden droplets are visualized. Numerical results show that most of the large droplets fall to the ground in 6 feet. However, micro-droplets can suspend in the air much longer, causing a potential health risk to nearby people. HighER relative humidity will reduce the transmission distances of the virus-laden droplets due to less droplet evaporation effects. The 6-feet social distancing policy is not sufficient to protect the inter-person aerosol transmission, since the suspending micro-droplets were influenced by the convection effect and transport from the human who coughs/sneezes to the other human in less than 5 seconds. Thus, due to the complex real-world environmental ventilation conditions, a social distance longer than 6 feet needs to be considered. Wearing masks should be also recommended for both infected and healthy humans.

11ID.3

A Simple Effective Enclosure with Added Plastic Wrappings for Inexpensive Containment of Aerosolized COVID Viruses and Other Pathogens during Tracheal Operations.

LUKE MONROE, Jack Johnson, Howard Gutstein, John Lawrence, Keith Lejenue, Ryan Sullivan, Coty Jen, *Carnegie Mellon University*

SARS-CoV-2 (COVID-19) is a severe respiratory virus that quickly progressed into a global pandemic in early 2020 and can be transmitted through aerosol droplets that are produced by coughing, talking, and breathing. Medical procedures used to treat severe cases such as tracheal intubation, extubation, and tracheal suctioning produce large amounts of infectious aerosol droplets due to uncontrolled coughing in a sedated patient. This presents significant risk for viral exposure of health care workers. Given the serious morbidity and mortality associated with SARS-CoV-2 infection, preventing the spread of the virus from patient to healthcare providers during these procedures is essential. We tested a plastic enclosure to be used during intubation and extubation procedure in order to reduce aerosol spread and potential viral transmission. Four aerosol particle measurement instruments were used to verify the efficacy of aerosol containment using various techniques to seal side openings. The enclosure combined with two layers of plastic wrap sealing the holes reduced escaped particle concentrations (between 0.1 µm to 5 µm in diameter) by over 95% at 6 inches away from all sides. Furthermore, concentration decay experiments indicate that the enclosure should be left on the patient for 15 minutes following a tracheal procedure and cessation of any coughing to allow sufficient time for aerosol particles to settle upon interior surfaces. This enclosure is a cost effective, easily implemented additional layer of protection that can be used to reduce the risk of COVID-19 transmission and other aerosolized pathogens between patients and healthcare workers during and following life-saving tracheal medical procedures.

11IM.1

Isomer-resolved Quantification of Particle-phase Organic Compounds Using a Coupled GC-CIMS/FID.

CHENYANG BI, Jordan Krechmer, Graham Frazier, Wen Xu, Andrew Lambe, Megan Claflin, Brian Lerner, John Jayne, Douglas Worsnop, Manjula Canagaratna, Gabriel Isaacman-VanWertz, *Virginia Tech*

Atmospheric oxidation of volatile organic compounds generates thousands of unique chemicals that have distinctly different physical and chemical properties depending on their structure and chemical functionality. Measurement techniques that can achieve characterization with detail down to molecular structure (i.e. isomer-resolved resolution) are consequently necessary to understanding differences in fate and transport between isomers produced in the oxidation process. In this study, a field-deployable thermal desorption aerosol gas chromatograph (TAG) was simultaneously coupled to a time-of-flight chemical ionization mass spectrometer (“TAG-CIMS”) using iodide as a reagent, and a flame ionization detector (FID), providing near-universal response to all analytes. This instrument measures molecular formulas of unknowns alongside identification of known compounds and precise quantification of all analytes. We present here the 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). We found that chemical formulas identified in CIMS have an average of about five isomers and the sensitivities of those isomers can vary by up to two orders of magnitudes. Furthermore, we compare the directly measured sensitivity to currently adopted approaches to calibration (e.g. “voltage scanning”), yielding new insight into the capabilities and limitations of this reagent ion chemistry. Finally, a multi-reagent ionization mode is investigated in which both zero air and iodide are introduced as reagent ions, to examine the feasibility of extending the use of an individual CIMS to a broader range of analytes. While this approach reduces iodide-adduct ions by a factor of two, other product ions such as [M-H]- and [M+O2]- increase by a factor of five to ten, potentially providing additional structural information and measurements of compounds too non-polar to form an iodide adduct.

11IM.2

Molecular Analysis of Freshly Nucleated α-pinene SOA Using Droplet Assisted Ionization.

DEVAN E. KERECMAN, Murray Johnston, *University of Delaware*

Droplet Assisted Ionization (DAI) is an inlet ionization technique that allows for online detection of intact molecular ions from airborne droplets. In our laboratory, DAI is used to perform online analysis of aerosol particles by passing the aerosol through a condensation growth chamber (CGC) to create micrometer-size aqueous droplets. DAI is performed by subsequently sending the droplets through a temperature-controlled capillary tube that serves as the inlet to a Waters SYNAPT G2-S mass spectrometer. Because the sensitivity of DAI analysis increases as the original aerosol particle diameter decreases, this method is particularly well suited to the study of nanoparticle formation and growth. In this presentation, experiments are reported where the molecular composition of freshly nucleated SOA is studied by DAI. In an initial experiment, SOA having a median diameter of 20 nm, a number concentration of 2 x10^4 cm^{-3}, and a mass concentration of 0.25 μg m^{-3} produced signal with high ion intensity. Molecular characterization of the SOA was consistent with condensation of highly oxidized molecules (HOMs) that subsequently reacted within the particle phase. Further characterization of particle-phase chemistry is underway. The results have implications for understanding the relative roles of gas- vs. particle- phase processes that cause growth of newly formed particles.

11IM.3

Airborne Extractive Electrospray Mass Spectrometry (EESI) Measurements of the Chemical Composition of Biomass Burning Organic Aerosol.

DEMETRIOS PAGONIS, Pedro Campuzano-Jost, Hongyu Guo, Douglas Day, Melinda Schueneman, Wyatt Brown, Benjamin A. Nault, Kyla Siemens, Alexander Laskin, Felix Piel, Laura Tomsche, Tomas Mikoviny, Armin Wisthaler, Jose-Luis Jimenez, *University of Colorado-Boulder*

Fast quantification of organic aerosols (OA) at near-molecular level is necessary to quantify its sources, evolution, and fate. To that end, we carried out airborne extractive electrospray time-of-flight mass spectrometry (EESI) measurements of OA composition during the 2019 FIREX-AQ mission on the NASA DC-8. We demonstrate fast EESI response to spatial gradients within wildfire smoke plumes, allowing for 1-Hz quantification of individual components of OA. The EESI was operated with positive and negative ion polarity during different flights, and we report aerosol levoglucosan concentrations for EESI(+) operation, and nitrocatechol for EESI(-). Attribution of EESI signal to these compounds is supported by offline analysis of FIREX-AQ aerosol filter extracts using liquid chromatography coupled to ultra-high-resolution electrospray ionization mass spectrometry. We present the first in-field intercomparison of co-located EESI, Aerodyne high-resolution Aerosol Mass Spectrometer (AMS), and CHemical Analysis of aeRosol ONline Proton-Transfer Reaction Mass Spectrometer (CHARON PTR-MS) during a single FIREX-AQ flight. We developed methodology to allow for stable EESI quantification up to altitudes of 7 km, including optimization of the electrospray working solution for low-pressure operation, control of electrospray region pressure, and pre- and post-flight calibrations in parallel with an AMS. The effect of electrospray region pressure, particle diameter, and particle composition on EESI sensitivity were systematically investigated and are described here. EESI quantification was stable flight-to-flight within 60% (1 σ), and calibrations using the same electrospray hours apart were stable within 20% (1 σ), showing the importance of calibrating EESI response for each electrospray established. Using the EESI measurements of levoglucosan and nitrocatechol and AMS measurements of total OA, we show evidence for balanced rates of primary OA evaporation and secondary OA formation during aging of wildland fire smoke aerosol.

12AP.2

Multi-Spectral Digital Holography for Microparticles.

RAMESH GIRI, Gorden Videen, Matthew Berg, *Kansas State University*

Digital holography is now established as a useful technique to characterize the size and morphology of particles relevant to the coarse mode aerosols for size range (> 1um) [1]. Yet, knowledge of the material composition of particles observed with holography is limited. The understanding of the material compositions is important for many local and global climate modeling, for example, to characterize the radiative effects of mineral dust in the atmosphere. Here, we test a multiple wavelength method in digital holography to produce the color images of micro-particles. Color analysis is then used to investigate if the particles of differing material composition can be differentiated.

Reference

[1] Berg, M. J., and G. Videen, 2011: Digital holographic imaging of aerosol particles in flight. J. Quant. Spectrosc. Radiat. Transfer 112, 1776–1783.

12AP.3

Comparison of Characteristics of New Particle Formation (NPF) in the Arctic (Ny-Alesund, Norway) and Urban (Gwangju, Korea) Environments.

HAEBUM LEE, Kihong Park, *Gwangju Institute of Science and Technology*

New particle formation (NPF), which significantly increases the number of sub-micrometer particles in the ambient atmosphere, has been observed in various environments. The newly formed nanoparticles have the potential to form CCN affecting cloud formation. It has been reported that the NPF was affected by preexisting aerosols, RH, precursor gases. The sulfuric acid (H_2SO_4) which is one of the precursor gases plays a key role of nucleation and subsequent growth of particles with being formed as binary nucleation (H_2SO_4-H_2O), ternary nucleation (H_2O-H_2SO_4-NH_3). The NPF occurred regardless of pollution level (e.g. a clean or a highly/moderately polluted environment). This study compares the characteristics of NPF in the Arctic (Ny-Alesund, Norway) (very clean environment) and urban (Gwangju, Korea) (moderately polluted environment) by examining the NPF occurrence frequency, occurrence criteria (LΓ), intensity (formation rate and growth rate), meteorological parameters (RH, temperature, pressure, and solar radiation), and sulfuric acid concentration. The annual NPF occurrence frequencies at Ny-Alesund and Gwangju sites were 24%/year and 42%/year, respectively. The highest percentage of NPF events in Gwangju was observed in May and April, while in May to July in Ny-Alesund. The duration of NPF was not significantly different between two regions. The average growth rate in Gwangju was about 2-3 times higher than Ny-Alesund, and the formation rate was several tens of times higher. In particular, the sulfuric acid concentration for NPF events in Gwangju was ~10 times greater than in Ny-Alesund. Both regions met the LΓ criteria for the NPF events well, however, Fuchs surface area influence in LΓ was more dominant in Gwangju than in Ny-Alesund.

12AP.4

Effect of Brownian Rotation on the Drift Velocity of a Nanorod. GEORGE MULHOLLAND, Charles Hagwood, *National Institute of Standards and Technology, Gaithersburg*

A model set of equations including Brownian rotation dynamics is proposed to investigate the role of rotation on the drift velocity of nanorods in the direction of the external field (electrical, gravitational). The rotation dynamics is based on the Ornstein - Uhlenbeck type analysis for the calculation of the mean and variance of the rotation velocity and angle for a freely rotating nanorod which includes inertial effects (high frequency). The average drift velocity is computed from the spatial trajectory for each path and the ensemble average and confidence interval is computed from the average of 300 trajectories. The two time scales in the problem, rotation and translation, require a large number of time steps to resolve both motions. Calculations are carried out for a ratio of the time scales, α, ranging from 0.01 to 100. It is shown that in the limit of slow and fast rotation, the velocity approaches the values predicted based on previous studies. The simulations were validated by comparison with the analytic expressions for the rotational model and for the approach to the slow and fast rotation limit within 0.5 %. The value of α is found to be near unity based on kinetic theory calculation of the friction and rotation resistances. This value is closer to the fast rotation limit than the widely used slow rotation limit. Results are also presented for nanodisks and slender rods in the continuum limit.

12AP.5

The Prediction of Size and Charge of Particles Generated in an Electrospray System. HAO ZHOU, Pratim Biswas, *Washington University in St Louis*

Electrospray system attracts significant attention for the generation of uniform charged particles from nanometer to micrometer. The accurate prediction of final particle size and charge is critical in efficient utilization of electrospray method to synthesize nanomaterials. However, the evaporation of highly charge droplet often involves in various highly coupled processes such as Coulombic fission and solute/nanoparticle diffusion, which pose a challenge to predict the final size and resultant charge of the particles for different types of precursors. In this work, a holistic model accounting for solvent evaporation, solute/nanoparticle diffusion, collision and aggregation of nanoparticle inclusions, Coulombic fission and ion evaporation processes was developed. First, the model equations are cast into nondimensional form for generalization. Nondimensional governing parameters are derived and their influence on the final particle size was investigated by numerically solving the governing equations for two cases: dissolved solute and nanoparticle inclusions. The simulation shows that the non-dimensional characteristic diffusion time, non-dimensional characteristic coagulation time and Coulombic fission related loss have a major influence on the final particle size. Based on the relative magnitude of these parameters, there exists different scenarios for particle size. Then, an analytical expression to predict the final particle size was derived for both dissolved solute and the nanoparticle inclusion condition, in the case of slow drying. Finally, the relationship between the particle charge and size is investigated. An equation to predict final particle charge is proposed.

12AP.6

Comparison of Particle Concentration and Distribution during Different Dust Storm Types as Measured by AEROS in West Texas.

KARIN ARDON-DRYER, Mary Kelley, Moira Plantier, Xueting Xia, *Texas Tech University*

Dust particles are among the most common atmospheric aerosols; they can stay suspended in the atmosphere for a long period of time, ranging from several hours up to days. During a dust storm, the dust particle concentrations often exceed the World Health Organization (WHO) health-recommended daily threshold values for PM10 and PM2.5 (particles with aerodynamic diameter <10µm and <2.5µm respectively). Exposure to dust particles can lead to respiratory problems, particularly for people with asthma. Lubbock Texas is one of the most persistently windy inland areas of North America and is considered to be among the dustiest; dust storms in this region can form due to frontal passage or thunderstorm outflows. In this project, we are comparing multiple dust storm events that occurred in Lubbock TX. Measurements of particle concentration (PM10 & PM2.5), size distribution, meteorological conditions as well as elemental composition of samples were all captured by our Aerosol Research Observation Station (AEROS) which is located in Texas Tech University in Lubbock Texas. In our presentation, we will present the spatial and temporal behavior of each of these dust storm events as well as the similarities and differences between them.

12AP.7

Comparison of Bystander Asbestos Exposure Data to Fiber Migration Assumptions.

STEVEN COMPTON, *MVA Scientific Consultants*

When work involving asbestos or asbestos-containing materials results in the release of airborne asbestos fibers, both the asbestos worker and any bystanders in that area are at an increased risk of exposure to asbestos. Quantifying the exposure to bystanders is accomplished by collecting an air sample during the activity in question in the personal breathing zone (PBZ) of the bystander. Alternatively, a stationary (area) air sample can be collected some set distance from the activity as a proxy for a breathing zone sample.

If no bystander air sample data is available, then one may attempt to estimate what the exposure would have been from applying air flow models to exposure data for the asbestos worker. Individual airborne asbestos fiber sizes can be nanometers in diameter, whereas bundles can reach the millimeter range. This means the mechanics of particle migration after release can range from advective to practically newtonian. However, the widths of fibers collected in an air sample typically do not exceed the micrometer range, so a complex fluid dynamics model is best suited to approximate fiber migration. One such model was proposed by Donovan et al. in 2011.

Simulations of asbestos release from a variety of work practices performed in controlled conditions were conducted over a time span of several decades. The intent of each simulation was to investigate fiber release from a specific product type (gaskets, packing, brakes, pipes, joint compounds, etc.) and specific worker activities (sanding, mixing, drilling, grinding, cutting, etc.). Unlike historic studies, which are often limited in data regarding site conditions, these simulations are performed in reproducible conditions. Many of these studies also involved the collection of proximal air samples: bystander PBZ, area, or both.

This presentation will share a summary of that data as a metric for evaluating models of asbestos fiber migration.

12AP.8

Numerical Investigation of Ion-condensation. Jacob Svensmark, MARTIN BøDKER ENGHOFF, Nir Joseph Shaviv, Henrik Svensmark, *Technical University of Denmark*

The presence of small ions influences the growth dynamics of a size distribution of aerosols. Specifically, the often-neglected mass of small ions influences the growth velocity, which may be important for terrestrial cloud formation. To this end, we have developed a numerical model to calculate the growth of a population of aerosols in the presence of charges, which explicitly includes terms for ion-condensation (Svensmark et al 2019). It is shown that a positive contribution to aerosol growth velocity is obtained by increasing the ion-pair concentration, consistent with recent experimental findings (Svensmark et al, 2017).

The model is a zero-dimensional box model solving the general dynamics equation numerically using a 4th order Runge-Kutta algorithm. Six species are tracked individually: Neutral condensable gas, air ions of positive and negative charge, and stable aerosols of neutral, positive, and negative (single) charge. The aerosols are distributed in a number of logarithmically spaced nodes based on volume typically corresponding to aerosol diameters of 1-100 nm. Nucleation is not treated explicitly but input at a fixed rate which can be distributed between aerosols of all charges.

Unique to this model is that the addition of mass from the interactions between air ions and aerosols are taken into account.

Model runs for the sulphuric acid-water system are compared with an analytical expression for mass-dependent ion condensation, which is the classical condensation equation modified with a growth term relating to the ions.

The model can also be applied to other chemical systems if the interaction coefficients are recalculated.

The model can be downloaded at https://github.com/jacobsvensmark/ioncage

References

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12AP.9

Comparison of the Predictions of Langevin Dynamics-based Diffusion Charging Collision Kernel Models with Canonical Experiments. Li Li, Harjindar Singh Chahl, RANGANATHAN GOPALAKRISHNAN, *The University of Memphis*

Based on the prior work of Chahl and Gopalakrishnan (Aerosol Sci. Tech. 53(8): 933-957) to infer particle-ion collision time distributions using a Langevin Dynamics (LD) approach, we develop a model for the non-dimensional diffusion charging collision kernel β_i or H that is applicable for $0 \le \Psi_E \le 60, 0 \le \Psi_I/\Psi_E \le 1, Kn_D \le 2000$ (described in J. Aerosol Sci. 140: 105481). The developed model for β_i for attractive Coulomb and image potential interactions, along with the model for β_i for repulsive Coulomb and image potential interactions from Gopalakrishnan et al. (J. Aerosol Sci. 64: 60-80), is tested against published diffusion charging experimental data. Current state of the art charging models, Fuchs (1963) and Wiedensohler (1988) regression for bipolar charging, are also evaluated and discussed. Comparisons reveal that the LD-based model accurately describes unipolar fractions for 10 – 100 nm particles measured in air (Adachi et al., 1985), nitrogen and argon but not in helium (Adachi et al., 1987). Fuchs model and the LD-based model yield similar predictions in the experimental conditions considered, except in helium. In the case of bipolar charging, the LD-based model captures the experimental trends quantitatively (within ±20%) across the entire size range of 4 – 40 nm producing superior agreement than Wiedensohler’s regression. The latter systematically underpredicts charge fraction below ~20 nm in air (by up to 40%) for the data presented in Adachi et al. (1985). Comparison with the data of Gopalakrishnan et al. (2015), obtained in UHP air along with measurements of the entire ion mass-mobility distribution, shows excellent agreement with the predictions of the LD-based model. This demonstrates the capability to accommodate arbitrary ion populations in any background gas, when such data is available. Wiedensohler’s regression, derived for bipolar charging in air using average ion mass-mobility, also describes the data reasonably well in the conditions examined. However, both models failed to capture the fraction of singly and doubly charged particles in carbon dioxide warranting further investigation.

We thank The University of Memphis High Performance Computing Cluster for providing computational resources to carry out this research. Partial support for this work was provided by US National Science Foundation (NSF) PHY Grant Award Number 1903432 under the Directorate of Mathematical & Physical Sciences. Published as J. Aerosol Sci. 140: 105481.

12AP.10

The Effect of Potential Interaction and Atomic Mass on the Nature of the Scattering and Accommodation of Gas Molecules from the Surface of Charged Particles. Transitioning from Specular to Diffuse Reemission.

VIRAJ GANDHI, Jayden Pothoof, Carlos Larriba-Andaluz, *IUPUI*

Stokes-Millikan's (SM) slip correction equation has been shown to provide an accurate description of a charged particle's electrical mobility throughout a vast range of Knudsen numbers. The equation asymptotically agrees with the Stokes' flow in the continuum regime and with kinetic theory derivations in the free molecular regime, but only when a 91% diffuse/ 9% specular reemission law is chosen for colliding gas molecules. While this choice of reemission law has been shown to be valid for different gases, its universal validity remains in question. From a kinetic theory perspective, it is known that SM cannot hold for all molecules. Given that monoatomic collisions must be specular, the percentage of diffuse reemissions must become smaller as the number of atoms in the charged particle is reduced. This sets the 91%/9% reemission law as an asymptotic behaviour from two very different perspectives: 1) when reducing the size from the transition regime and 2) when increasing the size from the free molecular. This work focuses on the latter behaviour, i.e. trying to understand how the gas molecule reemission evolves into a predominantly diffuse scattering. Previously, our work has shown that this evolution occurs at various rates for different gases. Here, the effects of potential interaction and distinct atomic masses are observed through the study of alkali metal salts. Iodine salts of increasing cation masses are compared under Nitrogen environments. It is shown as the mass of the cation increases, the collisions seem to become more specular. This is tested by using IMoS, a mobility calculator that is able to predict electrical mobilities of all-atom entities to about 4% error. IMoS is also used to predict the Lennard-Jones gas-cation parameters that would be required to agree with the experimental results. Results suggest a correlation between increasing masses and decreasing potential well-depths, leading to the observation that smaller long-range interactions lead to more specular reemissions. Finally, MD simulations within IMoS are used to check whether the increasing specular reemissions may be regarded as due to the loss of scattering from increasing masses, due to smaller potential interactions, or perhaps due to a mixed of both.

12AP.11

A Universal Parameter to Describe the Reduction of Refraction Effects in the Scattering of Absorbing Spheres.

JUSTIN MAUGHAN, Christopher Sorensen, *Kansas State University*

The scattered intensity from large spheres are investigated as the radius R and imaginary part of the refractive index κ are varied. It is shown that the product of κ and the size parameter kR, κkR , is a universal parameter describing the quenching of the refraction phenomenon of the scattered light: the refraction hump, the rainbows, and the glory. The physical reason for this is that κkR is the inverse of the relative skin depth of light penetration into the sphere which is demonstrated by calculations of the internal fields that darken universally as κkR increases.

12AP.12

Radial Basis Neural Network Method for Solving Population Balance Equations for Particle Coagulation.

KAIYUAN WANG, Pei Wang, Suyuan Yu, Wei Peng, *Institute of Applied Physics and Computational Mathematics*

Many engineering applications and environmental processes involve population balances of particles, such as flame synthesis of nanoparticles, crystallization, polymerization, soot formation, atmospheric aging, and radioactive aerosols. The governing equation to describe the evolution of the number density function is called the population balance equation (PBE). The highly nonlinear nature and partial integral-differential characteristics of the PBE bring great challenges to the solution of this equation. Thus, it is of great theoretical and practical significance to study the numerical solution of the PBE. This study presents a radial basis neural network (RBNN) method for solving the PBE for particle coagulation. The new method approximates the number density function using an RBNN. The solution process of the PBE is comparable to the training process of a neural network. The final solution has an RBNN structure, which is also a bivariant analytical function of particle volume and time. Then the method is validated by comparing with analytical solutions and the sectional method for four numerical test problems. The comparison results show that the present method can almost accurately predict the time evolution of the number density function. The convergence analysis shows that the quality of the solution increases significantly with the increased number of center points.

12AP.13

Experimental Verification of the Kinetic Theory of Gelation.

Christopher Sorensen, RAIYA EBINI, *Kansas State University*

The sol-to-gel transition has been intensively studied and as all good aerosol scientists know, aerosols can gel. There are three main descriptions to understand this process: Kinetic, percolation, and phase separation, yet no consensus has emerged. Here we report studies of colloidal gelation of 40nm nanospheres. We chose a dilute monomer volume fraction to allow for a full investigation of the gelation from dilute sol to percolated gel. Growth of fractal aggregates was monitored by combining small angle static light scattering (SASLS), dynamic light scattering (DLS) techniques, and transmitivity measurements. The data verify the predictions of a kinetic theory, the ideal gel point (IGP) theory, where three regimes of kinetics are expected. First, the well-known cluster-dilute regime, with a kinetic exponent of $z = 1$ was observed, followed by a cluster-dense regime with an enhanced kinetics and $z \simeq 2$, and finally, a gelation regime was observed where the aggregate growth slows and ceases to grow at the IGP predicted size, Rg,G. We conclude that kinetics provides a complete theory of the gelation process from dilute sol to percolated gel. It will be interesting to expand this work into aerogels.

12AP.14

Investigating Homogeneous Nucleation of Propane and n-Butane in Supersonic Nozzle Expansions. JIAQI LUO, Barbara Wyslouzil, *The Ohio State University*

Supersonic separators have been proposed as a more environmentally friendly separation method than membrane, absorption, and adsorption in the separation processes of natural gas. From a technical perspective, understanding the non-equilibrium vapor-liquid phase transitions of n-alkanes is essential to the development of these devices. Homogeneous nucleation rates have been measured in supersonic nozzles for n-alkanes down to n-pentane. Thus, n-butane and propane are the next logical candidates to improve our understanding of vapor-liquid phase transitions of short-chain alkanes from both the experimental and theoretical points of view. Since a second goal of our research is to determine the critical cluster sizes from isothermal nucleation rate measurements, two supersonic nozzles with different cooling rates are used. All experiments use argon as the carrier gas. Pressure Trace Measurements (PTMs) are used to estimate the temperature, pressure, mass fraction of condensate, flow velocity, and area ratio of flow. The conditions corresponding to the onset of condensation and the characteristic times required by the phase transition are presented and discussed for n-butane and propane. Small Angle X-ray Scattering (SAXS) will be used to determine the nucleation rates by combining the measured number densities with the results of PTMs. SAXS experiments will be conducted once the Advanced Photon Source is again available for outside researchers.

12AP.15

Optical and Microphysical Properties of Aerosols Emitted from a Marine Engine. NILOFAR RAEOFY, Justin Dingle, Roya Bahreini, Andrew Metcalf, Gavin McMeeking, Tony Hansen, Yu Jiang, Jiacheng Yang, Kevin Thomson, Stephanie Gagne, Tak Chan, Jacob Swanson, Heejung Jung, Georgios Karavalakis, David R. Cocker III, Thomas D. Durbin, Wayne Miller, Kent Johnson, *University of California, Riverside*

Black Carbon (BC) emissions from ships have important implications on air quality, climate, and health. A study of aerosol emissions was carried out on a 2-stroke marine engine operated at 25%, 50%, and 75% load with three different fuels including distillate marine (DMA), low-sulfur residual marine (RMB-30) and high-sulfur residual marine (RMG-380). Aerosol emissions in the exhaust were sampled unconditioned or through a catalytic stripper/sulfur adsorber and analyzed by several instruments. In this analysis, we focus on the measurements related to optical and microphysical properties of the aerosols to gain insight on the emissions of climate-relevant components, namely BC and brown carbon (BrC). BrC are light-absorbing organic aerosols that exhibit a strong absorption wavelength dependence, increasing towards the shorter visible and ultraviolet (UV) wavelengths. A photoacoustic extinctiometer and an aethalometer were used to calculate single scattering albedo (SSA, λ=375 nm) and wavelength dependence of absorption (Absorption Ångström Exponent, AAE, λ=370 and λ=880 nm). The SSA values of unconditioned aerosols at 25% load were similar for all fuel types at ~0.23-0.33 while they all decreased to ~0.13 at 75% load, suggesting a higher contribution of strongly absorbing aerosols at the higher engine load. AAE values of the unconditioned aerosols for RMG-380, RMB-30, and DMA at 25% loads were 1.5-1.9, 0.7-0.9, and ~1, respectively. Different values of AAE suggest different types of aerosols were generated depending on the fuel, with the highest proportion of BC suspected to have been generated using the DMA fuel. The AAE values for all fuels also decreased in going from 25% to 75% load. A single-particle soot photometer (SP2) was used for measuring BC size distributions and microphysical properties. Data based on its color ratio and mixing state will be used to differentiate the nature of BC aerosols during the different runs and sampling conditions.

12AP.16

Effect of Volume Fraction and Hydrodynamic Interactions on Aerosol Particle Coagulation Using Langevin Dynamics Simulations. ZHIBO LIU, Vikram Suresh, Ranganathan Gopalakrishnan, *The University of Memphis*

Coagulation of aerosol particles at high concentration is modeled by tracking identical spheres in a periodic domain using Langevin Dynamics (LD) simulations. As the particle solid volume fraction is varied between 10^{-6}-10^{-1}, departing from the dilute coagulation regimes ($\eta_v \rightarrow 0$), it is seen that the coagulation rate constant or collision kernel increases by a factor of ~6 in the continuum regime (defined by the diffusive Knudsen number $Kn_D \rightarrow 0$) and is practically unaffected by particle crowding (or high volume fraction) in the free molecular regime ($Kn_D \rightarrow \infty$) of diffusional mass transport. We provide a parameterization for β across the entire Kn_D regime as a function of η_v, building on prior work on coagulation kernel development for dilute aerosols using Langevin Dynamics (Aerosol Sci. Technology 45(12): 1499-1509). The effect of hydrodynamic interactions on particle coagulation, calculated using the extended Kirkwood-Riseman approach developed by Corson et al. (J. Fluid Mechanics 855: 535-553), is parameterized as a function of the momentum Knudsen number Kn_D, providing a holistic description of the influence of free volume and particle-particle interactions on coagulation of dense aerosols. It is seen that hydrodynamic interactions are the strongest in the continuum regime of momentum transfer ($Kn \rightarrow 0$) and vanish in the limit of $Kn \rightarrow \infty$ (free molecular momentum transfer regime). The LD simulations allow the quantification of each parameter for a system of identical spheres. Preliminary results indicate the need to design particle coagulation measurements to understand the deviation of coagulation rate constants from the predictions of dilute models at high volume fractions and the precise role of hydrodynamic interactions in altering the coagulation kinetics. Further research on the inclusion of particle polydispersity, non-spherical shape and the associated rotational motion using LD simulations is underway.

12CM.1

Estimating Criteria Pollutant Emissions from Six Future Greenhouse Gas Mitigation Energy Scenarios in California. YIN LI, Christopher Yang, Michael Kleeman, *University of California, Davis*

California plans to reduce greenhouse gas (GHG) emissions in 2050 to a level 80% below emissions in the year 1990. This aspirational goal requires large scale adoption of low carbon fuel and new technologies in multiple economic sectors. The California Times model (CA-TIMES) was developed to explore economically optimized pathways to achieve the GHG mitigation, taking into consideration future activity, fuel, technology and any externally specified constraints.

Here we develop six different future energy scenarios using CA-TIMES to study the range of possible future energy systems in California. 1) “BAU”: A ‘business-as-usual’ scenario; 2) “GHG”: A climate friendly strict GHG reduction; 3) “2030CAP”: A loose GHG reduction scenario that only achieve 40% GHG reduction by year 2030; 4) “CCS”: A scenario focused on carbon capture & sequestration; 5) “NGB”: A scenario that allows more residential and commercial natural gas appliances; 6) “NGT”: A scenario that allows more natural gas combustion for electricity generation. Each scenario was then translated into criteria pollutant emission inventories using the California Regional Multisector Air Quality Emissions (CA-REMARQUE) model v2.0 which projected 2010 emission inventory to 2050 by accounting future changes in activity, fuel, technology and regulations.

Overall, the estimated emissions of criteria pollutants (PM2.5, CO, NOX, SOX) increased in the CCS scenario relative to the BAU. The 2030CAP scenario revealed a small emission decrease while the GHG scenario saw a large emission decrease due to the deep electrification and adoption of renewable fuels. The NGB and NGT scenarios were close to the GHG scenario with some variations observed in the residential and commercial building sector as well as the electricity generation sector. Notably, the emission did not consistently decrease across all economic sectors, demonstrating the complexity relationship between criteria pollutant emissions and future energy scenarios.

12CO.2

Physical and Chemical Characteristics and Oxidative Potential of Rice Straw and Pine Stem Burning Particles.

ILHWA SEO, Kwangyul Lee, Min-Suk Bae, Minhan Park, Shila Maskey, Arom Seo, Lucille Joanna Borlaza, Enrique Cosep, Kihong Park, *Gwangju Institute of Science and Technology*

Agricultural burning and forest fires have been often observed in Northeast Asia. Fine particles emitted from biomass burning affect radiative balance, cloud formation, human health, and regional and local air quality. In this study, the laboratory-scale chamber was used for determining the emission factor, size distribution, hygroscopicity, chemical composition, morphology, and oxidative potential (OP) of rice straw and pine stem burning particles. Emission factor (number and mass) was higher for pine stem burning particles than rice straw burning particles possibly due to lower combustion rate and combustion efficiency. Bimodal number size distributions (ultrafine and accumulation modes) for rice straw and pine stem burning particles were observed at the initial burning. The longer duration of ultrafine mode (~40 min) was detected during the rice straw burning, which would be caused by the longer periods of initial flaming combustion conditions of the rice straw burning than pine stem burning. OC, OC/EC, K^+/EC, Zn, and alkanoic acid in fine particles were higher for rice straw burning particles while EC, K^+/OC, K^+/Cl^-, Fe, Cr, Al, Cu, PAHs, and resin acids were higher for pine stem burning particles. Levoglucosan in OC was similar for rice straw (6.1%) and pine stem (6.3%) burning particles. The resin acids were significantly detected in pine stem burning particles as a useful organic tracer for wood-burning particles. The higher hygroscopic growth factor (HGF) and cloud formation potential (κ), and the less number of agglomerated soot particles for rice straw burning particles were observed. OP activity (mass-normalized) was 7 times higher for rice straw burning particles than pine stem burning particles. It could be related to the higher fractions of OC and Zn, Ba, As, and higher solubility (HGF) for rice straw burning particles than pine stem particles.

12CO.3

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. The tube with inset filter is subsequently analyzed using thermal desorption gas chromatography-mass spectrometry (TD-GC-MS) for targeted and non-targeted analysis of compounds with a wide range of volatilities (saturation concentration, C* ranging 10^{-3}-10^{7} µg/m3). We project VOC and S/IVOC measurements onto the VBS framework to gain insight into the gas-particle partitioning from woodstoves used for domestic heating, in-situ and simulated open burning and biomass cookstoves used in developing country households. Comparisons across sources indicate similar distributions for open and prescribed burns and are consistent with distributions from literature. We noted deviations in distributions for woodstove emissions with 20% in the particle phase at lower OA concentrations (<25µg/m3) compared to ∼40% for other fire types. These distributions were derived assuming compounds eluting at the same time as reference alkane standards have similar response factors as well. Current work involves validation testing with different classes of compounds (PAHs, methoxy-phenols etc.) to constrain distributions.

12CO.4

Cookstove Emissions and Performance Evaluation Using a Novel ISO Protocol and Comparison of Results With Previous Test Protocols. WYATT CHAMPION, Craig Williams, Larry Virtaranta, Mark Barnes, William Preston, Michael Hays, James Jetter, *ORISE, U.S. EPA*

In 2018, the International Organization for Standardization (ISO) 19867-1 “Harmonized laboratory test protocols” were released with the intent of establishing improved international comparability for data on air pollutant emissions, efficiency, safety, and durability of cookstoves. This study compares emissions and efficiency data between the ISO protocol and the formerly employed Water Boiling Test (WBT) on the same fuel/stove types [liquefied petroleum gas (LPG), wood pellet, wood fan, wood rocket, three stone fire, and charcoal] and tested in the same laboratory (US EPA). Additionally, comparisons in emissions data are made between the ISO and Firepower Sweep Test (FST) protocols for five of the six stove/fuel combinations, and for additional pollutants including polycyclic aromatic hydrocarbons. Using the ISO 19867-3 “Voluntary Performance Targets” tier system for carbon monoxide (CO) and fine particulate matter ($PM_{2.5}$) emissions (indicator pollutants specified by ISO), stove types remain similarly ranked using the ISO and WBT protocols (e.g., tier 5 for LPG, tier 4 for wood pellet, tier 0 for three stone fire and charcoal). Compared to the WBT, the ISO protocol results in higher CO and $PM_{2.5}$ emissions metrics for advanced biomass stove types, and lower emissions for traditional stoves. The FST results in generally higher emissions metrics compared to the ISO. This evaluation of the ISO protocol suggests that it provides data that are both a closer approximation to real-world emissions, yet also relatively consistent with former WBT data in terms of tier ratings for emissions and efficiency.

12CO.5

Towards a Standardized Measurement System for Black Carbon Emissions from Ships. Stephanie Gagne, JALAL NOROOZ OLIAEE, Fengshan Liu, Joel Corbin, Prem Lobo, Gregory Smallwood, *National Research Council Canada*

The International Maritime Organization (IMO) is considering reducing black carbon emissions from international shipping and, as of May 2019, IMO’s Pollution Prevention and Response sub-committee has been tasked to "develop a standardized sampling, conditioning and measurement protocol, including a traceable reference method and an uncertainty analysis" for the measurement of black carbon from ships. The subcommittee has already identified three methods for the measurement of black carbon from ships: namely Filter Smoke Number (FSN), Photoacoustic Spectroscopy (PAS), and Laser-Induced Incandescence (LII). None of these methods alone constitute a standardized and traceable sampling, conditioning and measurement system that can be applied in different contexts.

While standardized measurement systems for black carbon emissions exist for the aviation and automotive sectors, there are currently no standardized measurement systems capable of handling the wide variety and range of co-emitted species found in marine engine exhaust. The wide variation in marine fuels, engines and after-treatment system used by ships around the world leads to a wide range in exhaust emission conditions and co-emitted constituents. Measuring marine engine black carbon emissions in a standard and repeatable way under such a wide range of conditions brings many challenges.

In this study, we combine the lessons learned developing standardized systems for black carbon emissions from other sectors with systems used in the marine industry, and recommend a prototype sampling, conditioning and measurement system that takes the special features of marine engine emissions into consideration.

12CO.6

Aerosol Formation and Ejection via Pyrocumulonimbus Clouds in the British Columbia Fires of Late Summer 2017.

ALEXANDER JOSEPHSON, Eunmo Koo, Daniel K Thompson, Jon Reisner, *Los Alamos National Laboratory*

On August 12-13, 2017 the fires raging across central British Columbia and northern Washington created five pyrocumulonimbus (pyroCb) clouds which injected high volumes of pyro-aerosols into the upper stratosphere. In this presentation we investigate some of the causes of these pyroCb clouds through a series of high-fidelity simulations. These simulations include ground-fire simulations using FIRETEC which captures the fire spread and generation of pyro-aerosols at the ground level with conditions unique to the environment of British Columbia in the late 2017 summer. Results from these simulations are used to inform a larger HIGRAD simulation which captures the formation of multiple plumes and transport of aerosols from the fire to the stratosphere through these plumes. With these simulations, we are able to identify some of key characteristics of these fires which led to this injection of aerosols into the stratosphere and thus increased drastically the global impact of these fires.

12CO.7

Effect of Deionized-water and Steam Addition on Soot and NOx Emissions in a Lab-scale Flare.

OLANREWAJU WASIU BELLO, Milad Zamani, Larry W. Kostiuk, Jason S. Olfert, *University of Alberta*

Steam-assisted flares are often used in the upstream oil and gas industries as a strategy to produce “smokeless” combustion. Unheated liquid water addition to flames is also known to suppress soot formation but is rarely used in industrial flares. Since utilizing unheated liquid water saves the energy cost used to convert water to steam, it is useful to investigate the extent to which unheated water and steam individually affect soot formation and NOx emissions during flaring.

Measurements of the combustion products of a lab-scale flare were carried out using a photoacoustic extinctiometer, a chemiluminescence analyzer, and a non-dispersive infrared gas analyzer to measure black-carbon mass concentration, NOX concentration, and CO2 concentration, respectively. In addition, a Scanning Mobility Particle Sizer (SMPS) was used to characterize the concentration and the mobility diameter of the emitted particles. The three fuels used in this study were pure propane, pure methane, and a mixture of 90% methane and 10% propane; the latter one approximates a typical higher heating value of Alberta flare gas. The fuel flow rates were fixed at 20 SLPM in all cases, and deionized-water and steam were entrained into the combustion zone, while their flow rates varied from 0 to 30 grams per minute.

The result shows that both deionized-water and steam reduce NOx and soot emission indices; however, deionized-water reduces NOX and soot emissions more than steam. Likewise, the total particle number concentration decreases with an increase in deionized-water and steam, and deionized-water reduces the total particle number concentration more than steam at the same flow rate. These results suggest that water-assisted flares in the oil and gas industries would produce lower emissions with a lower operating cost compared to steam-assisted flares.

12CO.8

nvPM Across Decadal Length Scales: Dependence on Biofuel Content. John Kinsey, Bob Giannelli, Jeffrey Stevens, Robert Howard, Mary Forde, Cullen Leggett, Alla Zelenyuk, Kaitlyn J. Suski, Greg Payne, Julien Manin, Richard W. Frazee, Timothy Onasch, Andrew Freedman, Richard Miake-Lye, David Kittelson, Jacob Swanson, RANDY VANDER WAL, Jiawei Liu, Raju Kumal, *Penn State University*

Fuel composition has traditionally been assigned tight specifications given the numerous physico-chemical constraints imposed by engine type and operation. A prime example is Jet A, a fuel produced for commercial aviation and used all over the World. With a view towards renewable feedstock as a way to decrease the CO2 footprint associated with air travel, biofuels are receiving an increasing interest. Presently, biofuels are being tested as blends with conventional Jet A fuel, to avoid potential engine damage resulting from injection system's deposits, lack of lubrication or degradation of elastomer parts (seals and hoses). Biofuels, even blended, offer additional benefits such as reduced black carbon emissions. There is little data on the soot reduction mechanisms in jet engine combustion for such biofuel blends, in part because of the limited access to full-scale engine testing coupled with comprehensive emissions characterization. In this presentation, we provide an overview of black carbon emissions as evaluated by transmission electron microscopy (TEM) analyses of samples collected at the exhaust of a J-85 turbofan engine fueled with Jet A as well as blends of Jet A and Camelina biofuel. Aggregate morphology, primary particle size and their internal nanostructure are analyzed to provide insights into the combustion characteristics. It is hypothesized that aggregate size (and primary particle size) dependence upon power increases with fuel aromatic content, mediated by turbulent fuel air mixing. These tests were conducted by the U.S. Environmental Protection Agency, in cooperation with Arnold Engineering and Development Complex (AEDC, U.S. Air Force), as part of a series of studies entitled VAriable Response In Aircraft nvPM Testing (VARIAnT) field campaigns.

12CO.9

Laboratory-Generated Aerosols as Transfer Standards to Characterize Smoke Detector Performance. XIAOLIANG WANG, Judith Chow, John Watson, Marit Meyer, Gary Ruff, David Urban, John Easton, Gordon Berger, Paul Mudgett, *Desert Research Institute*

A smoke detector is critical for the early detection of a fire to save lives and avoid fire damage. Due to limited options to extinguish fires, rapid and accurate smoke detection is especially important for space activities. Performance testing of consumer smoke detectors requires specific facilities and experiments with smoldering and flaming emissions from different fuels (e.g., cotton lamp wick, paper, wood, gasoline, and polystyrene). Smoke detectors for use in spacecraft are tested using similar setups with representative fuel materials. To reduce the level of effort required to test smoke detectors and predict performance of future smoke detector designs, this study explored the use of laboratory-generated reference aerosols as transfer standards to evaluate smoke detector performance. Compared to smoke aerosols, reference aerosols can be generated with more precisely controlled chemical composition, size distribution, concentration, and optical properties. Among the three tested reference aerosols, mineral oil particles were reproducibly generated with a Gemini smoke detector tester, dioctyl sebacate (DOS) particles were generated with a wide concentration range and flexible size distributions using an atomizer, while polystyrene latex (PSL) particles were difficult to produce with the high concentrations needed for smoke detector testing. Reference aerosols generated from 1.5%–100% DOS solutions and mineral oil covered the response range of six types of smoke aerosols generated by oxidative pyrolysis of spacecraft-relevant materials. No single reference aerosol can simulate all the relevant spacecraft smoke aerosols and their corresponding detector responses within ±10% error; however, useful relationships between these reference and smoke aerosols were derived from this study.

12CO.10

Remotely-Sensed Aerosol Optical Properties Retrieved from a High Spectral Resolution Lidar (HSRL) Instrument during the FIREX-AQ Field Campaign. TAYLOR SHINGLER, Marta Fenn, Johnathan Hair, Amin Nehrir, Anthony Notari, *NASA*

The NASA Langley Research Center's High Spectral Resolution Lidar with Differential Absorption Lidar (HSRL-DIAL) instrument was flown on the NASA DC-8 aircraft during the Fire Influence on Region to Global Environments and Air Quality (FIREX-AQ; https://www.esrl.noaa.gov/csl/projects/firex-aq/) field campaign. The airborne HSRL-DIAL system retrieves aerosol backscatter and aerosol depolarization at 3 wavelengths (355, 532, and 1064 nm), aerosol extinction at 532 nm, and ozone concentration (differential at 290 and 300 nm). Additionally, the HSRL-DIAL system incorporates both a zenith and nadir telescope allowing for retrievals from in-smoke sampling to be integrated through the plume. During the first portion of the FIREX-AQ campaign, the DC8 aircraft sampled more than ten large-scale fires with varying fuels, combustion stages, and metrological conditions, with some fires being sampled multiple times across separate days. This presentation focuses on the retrievals of aerosol backscatter (at 532 and 1064 nm), aerosol depolarization (at 532 nm and 1064 nm), aerosol optical thickness (at 532 nm), lidar ratio, and color ratio to examine the changes in these properties in the smoke plume as they are advected downwind.

12CO.11

Biomass Burning Particle Emission Factors and Size Distributions Measured during FIREX-AQ. ELIZABETH WIGGINS, Richard Moore, Claire Robinson, Edward Winstead, Amber Soja, Emily Gargulinski, *NASA*

Biomass burning is a significant source of atmospheric aerosols that degrade air quality and exert a substantial radiative forcing on the climate system. During the summer of 2019 we collected in-situ measurements of the physical and optical characteristics of biomass burning aerosols emitted from wildfires in the Western US and agricultural fires in the Southeastern US as part of the joint NASA-NOAA mission FIREX-AQ. We measured aerosol number concentrations and size distributions for bulk aerosols and non-volatile aerosols along with their absorbing and scattering properties. The fires we sampled represent a rich variety of fuel types and compositions, environmental conditions at the time of burning, and fire characteristics such as combustion completeness. In this study we calculated particle number and mass emission factors and size distributions for total and non-volatile fire emitted aerosols. We compared our aerosol emission factors and size distributions to ground-based fire characteristics to better understand the factors that influence the physical properties of aerosol emissions. The results of this study will reduce variability in size resolved particle emission factors by isolating the influence of select fire characteristics and ultimately improve the representation of biomass burning aerosols and their radiative influence in atmospheric models including smoke forecasting and climate models.

12DP.1

Grain Charging Rate in High Ion Concentrated Dusty Plasma Using Langevin-Dynamic Simulations.

RANGANATHAN GOPALAKRISHNAN, Vikram Suresh, Zhibo Liu, *The University of Memphis*

Grain charging is modeled in instances wherein the ions are dense and strongly coupled (i. e.) $\Gamma_i>1$: $\Gamma_i \equiv (e^2/(4\pi\varepsilon_o n_i^{-1/3} k_b T_i))$. Langevin Dynamics is used to simulate the motion of multiple ions around a negatively charged grain in a periodic domain for 10^1 - 10^5 Pa. The ion flux coefficient is calculated using the grain-ion collision time distribution and the grain-ion pair correlation function $g^{(2)}(r)$ is used to deduce the influence of the ion space charge on the collision of individual ions with the grain during charging. In addition to Γ_i, the ion flux coefficient is influenced by the diffusive Knudsen number Kn_D $[\surd(m_i k_b T_i)/(n_i^{-1/3} f_i)]$ (an ion-neutral gas interaction parameter) and $\chi_{p\,\equiv}$ $(a_p/n_i^{-1/3})$ that compares the size of the grain to the mean inter-ion spacing). We also demonstrate that an effective grain-ion potential computed using $g^{(2)}(r)$ according to the effective potential theory accurately describes the grain-ion dynamics in a binary framework for $\Gamma_i<\sim20$, without the need to simulate multiple ions. Ion concentration has a significant effect across different ion coupling regimes and the analysis of the pair-correlation functions reveals the perturbation of ion structure in the plasma by the presence of grains. We hope our model development will spark experimental validation efforts.

We thank The University of Memphis High Performance Computing Cluster for providing computational resources to carry out this research. Partial support for this work was provided by US National Science Foundation (NSF) PHY Grant Award Number 1903432 under the Directorate of Mathematical & Physical Sciences.

12DP.2

Cold Atmospheric Pressure Plasma for the Microbial Inactivation of Contaminated Bioaerosols to Control Indoor Transmission of COVID-19 and Other Infection Diseases.

Alina Bisag, Cristiana Bucci, Filippo Capelli, VITTORIO COLOMBO, Giorgio Dirani, Matteo Gherardi, Pasquale Isabelli, Giulia Laghi, Romolo Laurita, Nikta Oveisi, Vittorio Sambri, *Industrial Engineering Department; University of Bologna*

Bioaerosols consist of airborne particles (from 0.001 to 100 µm) originated biologically from plants and animals and can contain living organisms such as viruses, bacteria, and fungi. Moreover, higher bioaerosol concentrations may be observed in indoors generally associated with human activities that could spread diseases such as influenza, allergies and respiratory syndromes. Transmission via aerosols has shown to be of great importance in the COVID-19 pandemic caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). In this field, non-equilibrium atmospheric pressure plasmas, thanks to their blend of bioactive agents (electrons, ions, UV rays and electromagnetic fields), enable the production of reactive oxygen and nitrogen species having antimicrobial proprieties, related to oxidation of cell membrane, protein molecules and DNA. Several studies demonstrated the cold atmospheric plasma (CAP) assisted inactivation of bioaerosol. In particular, the possibility to use dielectric barrier discharges (DBD) to deactivate bioaerosol could improve air quality and limit the infections diffusion. In this work, experiments aimed at evaluating bioaerosol inactivation by a direct DBD plasma source are presented. The plasma source is driven by a high voltage generator (AlmaPULSE, AlmaPlasma s.r.l.) and it consists of two symmetrical electrodes both covered by a dielectric layer with an interelectrode gap of 2 mm, allowing the flow of bioaerosol through the plasma discharge. A suspension of Staphylococcus epidermidis (ATCC 12228) or purified RNA of SARS COV 2 were used to produce bioaerosol. The DBD source showed the ability to reduce the bioaerosol's bacterial load and destroy the purified RNA, evaluating the integrity of ENRDRP gene by means of real time rt-PCR. These preliminary results demonstrated the possibility to use a non-thermal plasma generated by a dielectric barrier discharge to inactivate bioaerosols containing S. epidermidis and viruses.

12IM.1

Impacts of Data Completeness on Hourly Averaged PurpleAir PM2.5 Concentrations and AQI Category Estimation during Smoke Events.

SAMUEL FREDERICK, Karoline Barkjohn, Amara Holder, Andrea Clements, *U.S. EPA Office of Research and Development*

Air sensors can provide continuous PM measurements advantageous for rapidly changing concentrations due to wildfires. However, there may be increased uncertainty in sensor data due to interruptions in sensor connectivity or power. This work simulates the impact of data gaps in a smoke impacted PurpleAir $PM_{2.5}$ dataset. Data were collected during August 2018 at the Natchez wildfire in Northern California where a PurpleAir was deployed alongside an E-BAM. The PurpleAir logged data to an SD card every 80 seconds while the E-BAM recorded 1-hr averages. To simulate lowered completeness versions of the PurpleAir dataset, subsets within each 1-hr interval (e.g. 50% completeness=22 80s points/hour) were selected either at random or through an iterative process. Each hourly subset was averaged and corrected with a USEPA correction equation developed to make PurpleAir data more comparable to regulatory grade data making it possible to use the data for health messaging. Corrected PurpleAir data was then compared to both the full PurpleAir and E-BAM hourly averages. The NowCast AQI, a rolling 12-hr weighted average for $PM_{2.5}$ developed by USEPA, was calculated for datasets simulating 'worst-case' completeness (1 point/hour) alongside NowCast AQI values for the full PurpleAir dataset and E-BAM hourly averages. Estimations of NowCast AQI category for the 'worst-case' scenario with one data point sampled each hour indicate that the PurpleAir reports within one category of the E-BAM ~90% of the time. These results are important as sensor users develop methods for sensor data cleaning and analysis since applying overly strict completeness criteria could exclude limited data available during smoke events, while applying insufficient completeness criteria could provide misleading results.

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.

12IM.2

Performance Characterization of Low-Cost Sensor Observations in a Near-Source Environment in Rural Malawi.

ASHLEY BITTNER, Eben Cross, David Hagan, Carl Malings, Eric Lipsky, Andrew Grieshop, *North Carolina State University*

Low-cost sensor packages are one approach to increase the spatial and temporal resolution of ambient air quality (AQ) monitoring in low-resource settings. The accuracy, precision, long-term (>1 year) stability of low-cost sensors, and the transferability of calibrations built outside of the deployment environment remain some of the key questions for global low-cost monitoring efforts. To investigate these topics, we characterize long-term performance of three 'ARIsense' low-cost integrated sensor packages (QUANTAQ, Inc.; Aerodyne Inc.) using 13 months of ambient data collected from three sites in rural Malawi. Observations indicate minimal decay in sensor response, but issues related to intermittent solar power and blocked inlets. To characterize the performance of the ARIsense's integrated optical particle counter (OPC), we compare 130 hours of collocated particle measurements to an optical nephelometer/integrated filter measurement device (MicroPEM, RTI International) under ambient conditions in rural Malawi. We find that the performance of the OPC compared to the MicroPEM (using the Pearson correlation coefficient, r) varied with time of day ($-0.06 < r < 0.93$), relative humidity ($0.35 < r < 0.7$), temperature ($0.06 < r < 0.8$), wind direction ($0.02 < r < 0.83$) and the background concentration at the site ($-0.1 < r < 0.7$). In general, OPC performance decreased with increasing RH and increased with background concentration. To characterize the ARIsense's suite of integrated electrochemical gas sensors (CO, Ox, NO_2, NO), we compare 15 days of observations collocated with EPA reference instruments in Raleigh, NC. We compare the performance of calibration models (HDMR, MLR, kNN and RF hybrid) built using the collocation data and assess their robustness to reliably measure gas concentrations in the deployment environment. Finally, we discuss the ability of integrated sensor packages to inform source attribution and local AQ characterization, despite performance limitations.

12IM.3

Thermal-induced Alternation in Size Distribution of Gold Nanoparticles Characterized by Differential Mobility Analyzer.

ALICE CHINGHSUAN CHANG, Fang-Hsin Lin, *Industrial Technology Research Institute*

Nanoparticles have been widely considered because of its advantages involving high surface area and catalycity. Accompanied by the great growth in the research and fabrication of nanoparticles with size of sub-20 nm, it is getting more important to correlate the size and performance of nanoparticle. Commonly-selected techniques for the size measurement are transmission electron microscopy (TEM) and differential mobility analyzer (DMA), and the later additionally provides the size distribution of sample so that the statistic information could be directly obtained. The gas-phase DMA calculates the diameter of nanoparticle based on its electrophoretic characteristic and its main drawback is the larger detected size compared with the TEM results, which contributes to the inclusion of the non-volatile components in aerosol measured by DMA. In this study, a tube furnace was equipped with DMA for the removal of the organic, burnable impurities in the aerosols so that the composition of the non-volatile materials could be reduced. The reference gold nanoparticle with diameter of 10 nm (NIST-8011) was chosen and different heating temperatures were used for the size monitoring. At the temperature of 800 ˚C, most of the organic surfactants were flamed and the noise signals disappeared from the size distribution collected by DMA. On the other hand, the mean value and number concentration of gold nanoparticles showed little change. The comparable size of gold nanoparticle independent of heating temperature were connected to the reshaping and charging of the nanoparticle induced by the thermal treatment. Conclusively, the influence of the sample preparation and parameter selection on size measurement was illustrated and the correlation of DMA and TEM results were made in this work.

12IM.5

Development and Evaluation of a Low-Cost Black and Brown Carbon Filter Analyzer.

EMILY FLOESS, Andrew Grieshop, *North Carolina State University*

Carbonaceous aerosols from combustion are major contributors to climate forcing. Black (BC) and elemental carbon (EC) are both pure carbon produced by incomplete combustion which are quantified in two different ways, by using light absorption across all wavelengths and thermo-optically, respectively. Organic carbon (OC) is measured thermo-optically. Light absorbing OC, brown carbon, (BrC), absorbs light mainly in ultraviolet (UV) and blue wavelengths. Current methods to measure these components are costly but more measurements are needed globally, especially in developing countries, to understand their sources and climate forcing role. To increase the accessibility of these measurements, we are developing an open-source, easy to build, low-cost instrument for measuring these particles. The system uses a Raspberry Pi, UV/Infrared (IR) Pi-camera, UV (370 nm wavelength), IR (850 nm) and red (620 nm) LEDs to quantify light absorption from quartz filter samples. A camera image shows light absorbed through a filter under varying illumination and is compared with a calibrated reference. The instrument is calibrated and evaluated using filter samples from field based biomass burning emissions tests from multiple sources. The BC, EC, BrC, and OC of these samples is measured using the Magee Scientific Soot Scan Optical Transmissometer, Sunset Lab OC-EC Aerosol Analyzer, Aethlabs microAeth, and BrC extraction and compared with the low-cost analyzer results to evaluate the accuracy, repeatability, sensitivity, and limits of detection of the low-cost analyzer. The analyzer can detect particle loading from the range of collected field samples (0 to 38 μg/cm^2 EC), has accurately estimated filter EC loading, and preliminary results show promise in quantifying UV and IR absorption, which can be used to estimate black and brown carbon. The ability for the sensor to estimate OC loadings on filters will also be explored.

12IM.6

Laboratory and Modeling Evaluation of Particle-Dependent Inaccuracies in Low-Cost Optical Sensors.

AMANDA GAO, David Hagan, Eben Cross, Jesse Kroll, *MIT*

Light-scattering-based particulate matter (PM) sensors are beginning to achieve widespread usage in measuring air quality due to their low cost and ease-of-use, but their limitations are still poorly understood. More specifically, there are sensor inaccuracies that have yet to be characterized or explained—and this lack of knowledge can lead to sensor misuse and uninterpretable data. Here, we investigate the response characteristics of the commonly-used Plantower PMS nephelometer and Alphasense OPC-N2 optical particle counter to a series of laboratory experiments involving exposure to various distributions of monodisperse polystyrene latex (PSL) and ammonium sulfate aerosol, with the goal of characterizing low-cost inaccuracies in detecting particles with different size distributions and optical properties. We determine the size-dependent response of these PM sensors using measurements collected by reference instruments, and examine this data alongside the results of a physics-based open-sourced model (opcsim) that simulates sensor responses to experimental conditions using Mie theory. Taken together, these complementary approaches shed new light on the processes that lead to inaccuracies in low-cost measurements.

12IM.7

Recommended Calibrations for Aerodyne Aerosol Mass Spectrometers to Reduce Uncertainty and to Improve Quantificaiton. BENJAMIN A. NAULT, Pedro Campuzano-Jost, Douglas Day, Hongyu Guo, Melinda Schueneman, Weiwei Hu, Brett Palm, Jason Schroder, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

The Aerodyne Aerosol Mass Spectrometers (AMS and ACSM) are widely used 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 reliable quantification, to reduce the uncertainty in the measurements, and to properly interpret comparisons with other instruments, 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 this topic. Here, we describe the calibrations typically performed for a high-performance aircraft AMS, and break down which calibrations are accessible for most AMS users versus those that can be more challenging. We discuss which calibrations are necessary versus optional, the recommended frequency for the calibrations, and the associated uncertainties when neglecting to perform one type of calibration. 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 the context of comparisons with other measurements during recent studies.

12IM.8

Increased Temporal Resolution of Environmentally Persistent Free Radicals (EPFR) in Atmospheric Particulate Matter and Combustion Particles via Electron Paramagnetic Resonance (EPR) Spectroscopy.

HEATHER RUNBERG, Deborah Mitchell, Sandra Eaton, Gareth Eaton, Brian Majestic, *University of Denver*

Environmentally persistent free radicals (EPFRs) are an emerging area of atmospheric interest due to their implications in adverse health effects. Previous EPFR studies have looked at 24-hour averages of EPFR concentration within ambient $PM_{2.5}$, however, because $PM_{2.5}$ levels vary diurnally there is a need for higher resolution monitoring. This study demonstrates instrumental sensitivity that is adequate to assess EPFR concentrations at a much higher temporal resolution than previously reported. Ambient $PM_{2.5}$ samples were collected for 90 minutes at 96 L min^{-1} and analyzed quantitatively via electron paramagnetic resonance (EPR) spectroscopy. Environmental samples had no measurable $PM_{2.5}$ mass, to a sensitivity of ±10μg, however EPFR concentrations were found in the range of 10^{12} spins m^{-3} of air sampled, which is similar to values that have been reported previously in other urban locations, using longer sample collection periods. Additionally, because combustion products are likely to contribute to the EPFR portion of $PM_{2.5}$, and understanding how they are impacted by environmental conditions is necessary for interpreting the results of environmental samples, hexane generated soot was assessed for radical stability when exposed to water and ambient atmospheric conditions. Radical concentrations decreased by about 5% over the course of 88 days, but there was no difference in degradation rates between wetted and non-wetted soot. This study highlights the potential for sub-hourly EPFR monitoring which would allow for better insight into human exposure.

12IM.9

Aerosol pH Indicator and Organosulfate Detectability from Aerosol Mass Spectrometry Measurements.

MELINDA SCHUENEMAN, Benjamin A. Nault, Pedro Campuzano-Jost, Douglas Day, Duseong Jo, Jason Schroder, Brett Palm, Alma Hodzic, Jack Dibb, Paul Wennberg, Karl D. Froyd, Glenn Diskin, Jose-Luis Jimenez, *University of Colorado Boulder*

Aerosol sulfate is a major component of submicron particulate matter (PM1). Sulfate can be present as inorganic (mainly ammonium sulfate or AS) or organic sulfate (OS). Although OS are thought to be a smaller fraction of total sulfate in most cases, recent literature argues that this may not be the case in some environments. Aerodyne Aerosol Mass Spectrometers (AMS) measure total submicron sulfate, but it has been difficult to apportion AS vs. OS as the detected ion fragments are similar. Recently, two new methods have been proposed to quantify OS separately from AS with AMS data. We use observations collected during several major airborne field campaigns covering a wide range of sources and airmass ages (spanning the continental US, marine remote troposphere, and Korea) and targeted laboratory experiments to investigate the performance of the proposed OS methods. Four chemical regimes are defined to categorize the factors impacting sulfate fragmentation. In polluted areas with high ammonium nitrate concentrations and in remote areas with high aerosol acidity, the decomposition and fragmentation of sulfate in the AMS is variable, and the proposed literature methods cannot retrieve OS concentrations. In regions with lower acidity (pH>0) and ammonium nitrate (fraction in aerosol phase<0.3), the proposed OS methods may be more reliable. However, the fragmentation of ambient neutralized sulfate varies somewhat within studies, adding uncertainty, possibly due to variations in the effect of organics. Under highly acidic conditions, sulfate fragment ratios show a clear relationship with acidity (pH and ammonium balance). The HySOx+/SOx+ AMS ratio and measured ammonium balance are promising for rapid estimation of aerosol pH < 0, which is expected in ⅔ of the troposphere. These results allow an improved understanding of important intensive properties of ambient aerosols.

12IM.10

Aerosolization of Fine Lunar Simulant Particles for Size and Charge Characterization and Low-Cost Sensor Calibration.

ABHAY VIDWANS, Shruti Choudhary, Brad Jolliff, Pratim Biswas, *Washington University in St Louis*

In the Apollo manned lunar missions, lunar dust posed a great challenge. Electrostatic forces dominate transport of these dust grains, overcoming gravitational forces and leading to migration and adhesion to nearby surfaces. As upcoming manned lunar missions for extended human residence on the moon are being planned (ARTEMIS III), it becomes increasingly important to understand the characteristics of the fine content of dust that upon inhalation could adversely affect health. Studies on Apollo samples show that fine particles account for less than 20% by weight (1), but nearly 100% by number. While the fine particulate content of lunar regolith has been studied (2), little attention has been given to the fines of lunar simulant, a widely used Earth-sourced resource on which most of the lunar dust research has been performed.

In this study, we aerosolize JSC-1A simulant and use aerosol instrumentation to comprehensively examine the size, shape, and charging characteristics of fine particles in real time. Size distributions show unimodal shape with a mode in the realm of 0.2 to 0.3 µm. SEM imagery of these fine particles show highly irregular shape, consistent with lunar regolith. Tandem-DMA charge characterization indicates that nearly 100% of particles become charged when aerosolized, and the charge distribution is very widely spread across multiple charges. Next, calibration experiments were performed with the aerosolized simulant to evaluate the performance of two miniature low-cost sensors (Sharp GP2Y1010AU0F and Applied Particle Technology MINIMA). The two sensors, with different theories of operation, were calibrated against a Federal Reference Method PM monitor. Preliminary results show positive correlations for particle concentration. Further development of these sensors may enable in-situ concentration and size distribution measurements on the lunar surface.

[1] Carrier, W. D. (1973). Lunar soil grain size distribution. The moon, 6(3-4), 250-263.
[2] Greenberg, P. S., Chen, D. R., & Smith, S. A. (2007). Aerosol measurements of the fine and ultrafine particle content of lunar regolith.

12IM.11

Design and Characterization of a New OFR: The Particle Formation Accelerator (PFA).

NINGJIN XU, Don Collins, *University of California, Riverside*

Oxidation flow reactors (OFRs) are valuable tools for studying the formation and evolution of secondary aerosol (SA) in the atmosphere. Here we present a new all-Teflon reactor, the Particle Formation Accelerator (PFA), that was designed, constructed, and characterized through both experimental measurements and CFD modeling. We describe some of the design elements that were used to reduce flow recirculation and gas and particle losses and wall interactions. We report laboratory characterization of the reactor, including hydroxyl radical production, UV intensity distribution, residence time distributions (RTDs) for gases and particles determined using both computational simulation and experimental verification, gas and particle losses, and a comparison of aerosol yields of α-pinene and m-xylene with those reported in the literature. By wrapping the reactor with highly UV-reflective material, an overall UV intensity comparable to that in other OFRs is achieved using a relatively low power output lamp. Near laminar flow velocity profiles of gases and particles are suggested by CFD simulations and confirmed by the RTD experimental results. The transmission efficiencies of non-reactive gases and of particles are greater than 90%. Particle loss was reduced by minimizing static charge on the Teflon surfaces, resulting in higher inferred aerosol yields of α-pinene and m-xylene. Preliminary measurements of SA production when sampling ambient air in Riverside, CA, U.S. showed that the mass concentration of SA formed in the reactor was up to 1.8 times the mass concentration of the ambient aerosol at the same time. In the future, we will focus our efforts on measurement of the composition of the particulate and gaseous products during one or more field studies to evaluate how well the PFA reactor simulates atmospheric chemistry that typically requires hours or days.

12IM.13

Accurate Aerosol Absorption Measurements at Reduced Sample Pressures. MICHAEL COTTERELL, Kate Szpek, David Tiddeman, Jim Haywood, Justin Langridge, *University of Bristol*

Aerosol optical properties relate directly to their microphysical parameters and are used to interrogate differences in particle composition and mixing state. Recent years have seen optical spectroscopy on aerosols providing new insights into aerosol chemistry, reaction rates, water uptake in response to increasing humidity, and morphological evolution as aerosols age. Aerosol light absorption is poorly constrained in climate models, arising partly from a lack of accurate and direct observations of aerosol absorption. Photoacoustic spectroscopy (PAS) is the technique of choice for contact-free aerosol absorption measurements, and recent years have seen PAS instruments deployed in the field from aircraft measurement platforms for spatially resolved atmospheric aerosol measurements. The accuracy of these absorption measurements depends chiefly on the fidelity of instrument calibration and its dependence on sample pressure; measurements from aircraft platforms sample at varying pressures typically over the range 400 – 1000 hPa.

Strategies using O_3-laden gas samples at varying pressures are often employed to calibrate PAS instruments operating at visible wavelengths. We show that such calibration approaches enable high accuracy aerosol absorption measurements at ambient (~1000 hPa) pressures but provide for increasingly inaccurate calibrations as the pressure is progressively reduced below 1000 hPa. Instead, we show that the PAS instrument can be calibrated at ambient pressure and then a miniature speaker used to quantity the pressure response function for the microphone transducer. In this way, we show that we accurately measure aerosol absorption at reduced pressure for sub-micrometre diameter aerosols consisting of dyed polystyrene latex spheres or nigrosin dye. These results will be of utmost interest to those measuring aerosol absorption using PAS from airborne platforms or those calibrating PAS instruments for ground based or laboratory measurements.

12IM.14

Volatility Measurement of Organic Aerosol by Mass Fraction Remaining: Challenges and Advances. KAROLINA CYSNEIROS DE CARVALHO, Sohyeon Jeon, Christopher Oxford, Michael Walker, Brent Williams, *Washington University in St. Louis*

Organic matter contributes significantly to atmospheric aerosol, constituting a major fraction of submicron particulate matter. A crucial factor that controls the partitioning of the organic constituents of aerosols between the gaseous and condensed phases is their vapor pressure. This dynamic equilibrium influences the rate of reactions in the atmosphere and the fate of the corresponding compounds. Therefore, to be able to address their effects on Earth’s energy balance as well as on human health, accurate measurement of organic aerosol volatility is imperative.

Thermodenuders have been widely used in efforts to quantify the volatility of organic species. They consist of a heated tube in which the aerosol is evaporated and a denuder section to avoid re-condensation by removing the gas phase material. By exposing aerosols to different temperatures, it is possible to generate a mass fraction remaining curve (thermogram) using either a Volatility Tandem Differential Mobility Analyzer (V-TDMA) or an Aerosol Mass Spectrometer (AMS). However, determining volatility variables from AMS derived thermograms remains challenging. Volatility determination requires simultaneous computation of many parameters, including the mass accommodation coefficient, which is usually not known and often assumed to be unity for organic compounds.

Model predictions tend to yield steeper thermograms (i.e. higher volatility) in comparison to experimental data, and the uncertainty in the value of the mass accommodation coefficient has been suggested to play a role in the observed discrepancies. In this work, we studied the evaporation of azelaic acid by generating thermograms using both an AMS and a V-TDMA. Applying a new V-TDMA model, which takes into consideration the charging efficiency and the presence of multiple charges in the aerosol population, we compare the resulting curves from both instruments and discuss the role of the unity mass accommodation coefficient assumption in the calculations of organic aerosol volatility.

12IM.15

Effects of Inlet Temperature and Particle Transmission on Automated Mercury Analysis. Adriana Mustata, ELISABETH GALARNEAU, Geoff Stupple, Alexandra Steffen, *Environment and Climate Change Canada*

Atmospheric mercury is found predominantly in its gaseous elemental state, but small fractions are also present as oxidized gaseous and particulate forms. Previous research has suggested that inlet heating on automated analysers affects the phase distribution of measured mercury. Such effects could produce substantial errors when sampling at cold temperatures such as those found in the Arctic atmosphere or in winter at more temperate locations. In order to investigate these aspects of automated mercury analysis, laboratory experiments were conducted by dispersing a reference material and delivering it to an automated analyser whose temperature settings were varied over a range that bracketed their default values. Complementary experiments were also conducted in the high Arctic (83°N at Alert, Nunavut, Canada) using side-by-side instruments operated at different temperature settings. Results demonstrate that temperature affects measured mercury speciation and that particle transmission is an additional consideration when interpreting mercury measurements using automated analysers.

12IM.16

Performance Validation of Bio-Particle Counter by Using Inkjet Aerosol Generator. KENJIRO IIDA, Hiromu Sakurai, *AIST*

This study introduces a method to verify the counting capability of a bio-particle counter (BPC). A BPC counts and detects biological particles by analyzing the intensity of fluoresce signals from a sampled particle. The ratio of biological counts to total counts is called viable fraction (VF), and the VF and counting efficiencies (CE) should be two of the parameters to be tested in the verification experiment. Inkjet aerosol generator (IAG) is used to generate monodisperse test particles which are surrogate of biological particles. The test particles contain biological fluorophores in a trace amount, and the particle diameter is adjusted by the mass of lactose monohydrate in the test particles. In this study three biological fluorophores (tryptophan, NADH, and riboflavin) were added to lactose monohydrate (LM) particles, and these test particles are delivered to BioTrak (TSI Inc.). The mass of three fluorophores in the IAG-generated LM particles were optimized to maximize the VF measured by the BioTrak. After finding the optimum combination of the fluorophores the VF monotonically increased from 17% to 84% while the particle size was increased from 3.0 to 8.2 um. The experimental results validate that the IAG can generate test particles which a BioTrak can identify them as biological particles. Therefore, IAG can be used to periodically verify the counting capability of a BPC. Proposed method is practical since it does not involve the use of microorganisms and therefore does not raise any biosafety-concerns.

12IM.17

Determining the Cut-Off Diameter and Counting Efficiency of Optical Particle Counters With an Aerodynamic Aerosol Classifier and an Inkjet Aerosol Generator.

Steven Tran, KENJIRO IIDA, Yoshiko Murashima, Hiromu Sakurai, Jason S. Olfert, *University of Alberta*

A method to determine the cut-off diameter and counting efficiency of single-particle optical particle counters (OPC) is presented. An aerodynamic aerosol classifier (AAC) coupled with an atomizer was used to generate monodisperse dioctyl phthalate particles with a condensation particle counter (CPC) as the reference instrument. This method is accurate for capturing the counting efficiency of OPCs at lower size ranges and determining the cut-off diameter. The CPC was found to be a poor reference instrument for particles larger than 1 µm in which case an inkjet aerosol generator (IAG) was used as the monodisperse particle source and reference instrument. Two different particle materials were used with the IAG: lactose monohydrate and an ionic liquid (1-Ethyl-3-methylimidazolium trifluoromethanesulfonate). A combination of the AAC to size smaller particles (1 µm) was found to provide a comprehensive method capable of covering the counting efficiency over the entire operating range of OPCs.

12IM.18

Design and Characterization of an Ag Generator.

MARTIN IRWIN, Jacob Swanson, Adam M Boies, *Catalytic Instruments*

There currently exists few commercial options for the generation of aerosol particles in the 5-50 nm size range, limited mainly to spark generators, tube furnaces, electrospray generation, inverted burners, and diffusion flames. There is a requirement for a simple to use, solid particle generator capable of producing sufficiently high concentrations of small aerosol particles to calibrate particle counters, and general aerosol equipment. Many people have reported the production of metallic nanoparticles (including Ag) from inert-gas condensation using a tube furnace. The primary disadvantage of using an entire tube furnace is the size and cost of tube furnace that is required to produce the nanoparticles. A tube furnace also does not result in reproducible nanoparticle production as slight changes in the location of the Ag material placed within the furnace can result in large difference in both the concentration and size of particles produced. Silver particles are known to behave as a proxy for soot particles, but with a single elemental composition, offer reduced uncertainties to other generation techniques. Here we present the characterization of a new Ag-Generator, capable of producing sufficiently high concentrations of singly charged aerosol, ideal for e.g. the calibration of multiple CPCs in parallel, as well as a variety aerosol emissions equipment.

This novel Ag-Generator solves several key aspects associated with the production of metallic nanoparticle aerosols. By fixing the location and surface of metal exposed to the supplied gas stream, the stability of the nanoparticles produced is enhanced. Nanoparticle production on successive uses (heating up and cooling down between uses) is better controlled. The specific design allows for a more compact device design that allows for lower energy consumption and an ability to use with low voltage.

12IM.19

An Automated Approach to Identify and Quantify Compounds in Large GC-MS Datasets using Positive Matrix Factorization.

SOHYEON JEON, Michael Walker, Claire Fortenberry, Brent Williams, *Washington University in St. Louis*

Gas chromatography-mass spectrometry (GC-MS) has long been applied to identify and quantify individual chemical compounds in environmental samples. Typically, users identify each chemical compound by comparing mass spectral fragmentation patterns with known standards or MS libraries and quantify by integrating peaks to compare the variability between samples. Software that can automatically carry out these processes has been developed, but often requires manual quality control inspection of peaks. This can be particularly time-consuming for peaks with large retention time shifts or low abundance. In addition, this process may generate errors by the researcher's subjective correction. We evaluate here an automated approach of identifying and quantifying analytes of interest in the chromatogram for large dataset by using Positive Matrix Factorization (PMF) based on peak information obtained from Igor-based automated single-ion peak fitting method. To implement our automated analysis, a small sub-section of each chromatogram, corresponding to the retention time of an analyte of interest, is determined automatically based on a reference chromatogram before running PMF. Then, the PMF analysis generates solutions with increasing number of factors until a set of criteria related to the compound's mass spectrum and peak shape are met. With this approach, users can automatically implement PMF for all analytes of interest with minimal effort. Previously quantified peaks (compounds) from the Air Composition and Reactivity from Oudtoor aNd Indoor Mixing (ACRONIM) campaign are utilized to assess the strengths and limitations of this approach. This technique shows potential to improve data processing efficiency to identify and quantify analytes of interest in chromatograms from a range of environmental samples.

12IM.20

A New Moderate-cost Method for the Characterization of Organic Aerosol by Volatility and Elemental Ratios.

PURUSHOTTAM KUMAR, James Hurley, Nathan Kreisberg, Braden Stump, Susanne Hering, Patricia Keady, Gabriel Isaacman-VanWertz, *Virginia Tech*

Online measurements of the chemical composition of particulate matter have typically relied on expensive and complex research-grade instruments based on mass spectrometry and/or chromatography. Routine monitoring, which necessarily relies on economical alternatives that can be readily operated autonomously, generally provides only measurements of particle mass and, consequently provides limited chemical information. In particular, these instruments lack information on the degree of oxygenation of particles, a critical parameter in understanding the transformations and impacts of organic aerosols. We present here the development of a new aerosol chemical composition monitor ("Chemspot") to measure aerosol mass, volatility, and elemental ratios (O:C, S:C) in a way that maximizes reliability and autonomous operation at a moderate cost. Gas Chromatographic (GC) detectors, including a Flame Ionization Detector (FID) and Flame Photometric Detector (FPD), are combined with a CO_2 monitor to measure aerosol organic carbon, oxygen-to-carbon ratios, and total inorganic and organic sulfur. By relying on common and well-understood GC detectors, calibration can be easily automated using only a small number of gas-phase standards. Particles are sampled by impaction into a ~1 mm spot in a custom passivated quartz cell after passing through a condensational growth tube. The collected aerosol sample is thermally desorbed at different temperatures (for volatility binned composition) and the vaporized sample is passed through different detectors. Volatility resolution is achieved through controlled rapid temperature steps. We demonstrate here the efficient collection of particles between 10 nm and 1000 nm in diameter. Subsequent rapid thermal desorption at rates of 20 ^{o}C/s is shown to provide separation by volatility with a resolution of less than two orders of magnitude in vapor pressure. Volatility-resolved carbon, oxygen, and sulfur concentrations in ambient aerosol will be presented.

12IM.21

Influence of the Peaks Method Assumption on Variation in Volatility Tandem Differential Mobility Analyzer Measurements. CHRISTOPHER OXFORD, Brent Williams, *Washington University in St. Louis*

There is a significant amount of variation in Volatility Tandem Differential Mobility Analyzer (V-TDMA) aerosol measurements. As an example of such discrepancies, four authors have published V-TDMA volatility measurements for adipic acid (Tao 1989; Bilde 2003; Selah 2003; Salo 2010). The percent difference between the largest and smallest volatility measurement is: 129 % (surface energy), 142% (vapor pressure at 298 K), and 45% (enthalpy). Bilde et al. (2015) observed that the differences between the studies were often larger than the errors within each study. Thus, exploring the differences between the experiments could yield the cause of the variation.

The oven used in each V-TDMA was different, and each experiment used different experimental settings (aerosol-to-sheath ratio, etc.) to obtain the raw data and used different computational methods to solve for the volatility variables. In contrast, every study used the peaks method assumption to reduce the distributions to single values. In this assumption, the initial diameter is assumed to be the diameter at the peak of the size distribution entering the oven; the final diameter is assumed to be the diameter at the peak of the size distribution exiting the oven; and the residence time is assumed to be the residence time at the peak of the residence time distribution. Theoretically, differences in the experimental settings and oven designs should interact with the peaks method assumptions, which provide inputs to the different calculation methods.

In this work, we use a model to evaluate two different calculation methods (solving for vapor pressure, while assuming a surface energy value, versus simultaneously solving for both variables) used by V-TDMAs. We show that different V-TDMA settings and oven designs generate errors through the peaks method assumptions, and these errors can be amplified by the choice of calculation method.

12IM.22

Application and In-Field Assessment of a High Flow Rate Electrostatic Precipitator (ESP) in Collecting Fine Particulate Matter (PM2.5) for Toxicological Studies. MILAD PIRHADI, Amirhosein Mousavi, Constantinos Sioutas, *University of Southern California*

We evaluated the performance of a high flow rate electrostatic precipitator (ESP) as a fine particulate matter (PM2.5) collector to be used in toxicological studies. Optimum operational configuration of the ESP was determined based on the particle collection efficiency and associated ozone production of the instrument. Particle collection efficiency of the ESP was evaluated using various laboratory-generated aerosols such as NaCl and monodisperse polystyrene latex particles under different flow rates (i.e., 50, 75, and 100 lpm) and applied voltages (i.e., 8, 10, and 12 kV). The operating flow rate of 75 lpm and applied voltage of 12 kV were selected as the optimum configuration. On average, around 85% particle collection efficiency and 17 ppb ozone concentration were observed downstream of the instrument. Furthermore, field tests under the optimum configuration of the ESP were conducted at Los Angeles to assess the performance of our ESP under the ambient conditions. Chemical composition and oxidative potential of the PM2.5 samples collected on the ESP substrates were compared with those collected by versatile aerosol concentration enrichment system (VACES) operating in parallel including filters from VACES-diffusion dryer and PM slurries from VACES-BioSampler. Results showed that the ESP can preserve the labile species (i.e., total organic carbon and inorganic ions) more efficiently than the filters. The intrinsic oxidative potential of the PM samples collected on the ESP substrates was also higher than that of filters, most probably due to better preservation of the semi-volatile organic components. Nevertheless, concentration of the labile species and PM intrinsic oxidative potential of the samples collected by the ESP were rather lower than those in slurries collected by the VACES-BioSampler. In conclusion, considering the high flow rate of our ESP and its ability to collect PM samples accurately, it can efficiently be utilized in toxicological studies.

12IM.24

Integrated Aerosol Mass and Number Measurements with the Mass and Mobility Aerosol Spectrometer (M2AS). KINGSLEY REAVELL, David Walker, *Cambustion Ltd*

The Mass and Mobility Aerosol Spectrometer (M2AS) is an instrument which combines a unipolar diffusion charger, CPMA (Centrifugal Particle Mass Analyzer) mass classifier, Condensation Particle Counter, Electrometer and a novel mobility classifier. The M2AS allows the mass and mobility distributions of an aerosol to be simultaneously measured in a single scan. Currently we have demonstrated the measurement of aerosols between approximately 50 nm and 3 microns, depending on the particle density. The aerosol is first charged and then selected by mass : charge ratio in the CPMA. The aerosol charge level is determined by the ratio of particle count and electrometer measurements which avoids the need to make assumptions about the charge level. Direct measurement of the electrical mobility of the selected aerosol allows compensation for the width of the CPMA transfer function and provides a measurement of mobility diameter up to a larger particle size than traditional techniques. The particle effective density is thus directly measured.

In order for the integrated distributions from the M2AS to accurately match conventional measurements of the aerosol number and mass, it is necessary to characterise the particle losses and transfer functions of the constituent instruments. We describe a new technique for the measurement of the CPMA transfer function based on passing the sample aerosol twice through the same classifier.

We present validation of the accuracy of the M2AS measurement of total aerosol parameters by measurement of the density of aerosols of known density, comparison with weighing of samples collected on filter paper, and comparison with a condensation particle counter. Typically, the integrated distributions agree with the total aerosol measurements within approximately 10%.

12IM.25

Machine Learning Approaches to Characterizing Soot in TEM Images. TIMOTHY SIPKENS, Hamed Nikookar, Steven Rogak, *University of British Columbia*

Soot is a group of carbonaceous nanoparticles that contribute to climate change and can impact human health. The role soot plays in these scenarios depends significantly on their optical and transport properties, which are, in turn, largely determined by their size and shape. Transmission electron microscopy (TEM) remains one of the best ways of acquiring detailed information about particle morphology. However, the process of obtaining quantitative size information from these images requires image processing, which is often challenging due to the limited contrast of the carbonaceous nanoparticles against the carbon film often used on the TEM grids. While manual processing of the images remains one of the most robust ways of processing the images, the process is very time-intensive and greatly limits one’s ability to analyze a statistically significant number of particles. Machine learning approaches, including unsupervised clustering approaches and convolutional neural networks, have the promise to provide accurate image processing at the faster speeds necessary to characterize a meaningful number of images. We present a comparison of several of these techniques, as well as manual sizing, to determine both the projected area-equivalent diameter and primary particle diameter of soot aggregates. We then consider the relationship between these two properties for soot produced from a range of studies and consider the impact that the image processing approach may have on the results.

12IM.27

Effect of Relative Humidity on the Performance of Five PM Sensors.

PENG WANG, Feng Xu, Huanqin Wang, Da-Ren Chen, *Virginia Commonwealth University*

With the increasing awareness of adverse PM effect on the public health, air quality, atmospheric visibility and climate change, PM sensors with the initial costs significantly less than scientific ones have been widely proposed in the air quality monitoring network to measure the PM mass concentration. The study on the performance of these cost-effective PM sensors has been reported in literature. Many of these studies investigated low-cost sensors under the lab setting with relative humidity well controlled. However, the humidity is always present in the ambient. The effect of relative humidity on the readouts of low-cost PM sensors has not been reported yet. In this work, the performance of five widely used PM sensors were investigated using lab-generated particles under various humidity. As the reference, a tapered element oscillating microbalance (TEOM) was included. The effect of particle hygroscopicity, size and components on the performance of selected PM sensors was systemically studied. It was found the relative humidity has negligible effect on the selected PM sensor readings for hydrophobic particles, while measurable effect was observed on the readings of selected PM sensors when the relative humidity to some extent. More, the reading of PM sensors shows a different linear relationship with the TEOM reading for hydrophilic particles of different sizes and compositions under different relative humidity. Our investigation suggests that Low-cost PM sensors required to be calibrate under different relative humidity conditions and the recording of relative humidity of the ambient is necessary when applied PM sensors in the fields (for getting accurate PM data).

Keywords: Low-cost sensors; Relative humidity; Hygroscopicity; Particulate components

12IM.28

Performance Evaluations of Multiple Commercial PM Sensors in Research Triangle Park, NC.

SAMUEL FREDERICK, Karoline Barkjohn, Cortina Johnson, Ian VonWald, Andrea Clements, *U.S. EPA Office of Research and Development*

Recent developments in particulate air sensor technology have led to increasing access to air quality measurements and have facilitated individual and community-led actions for mitigating exposure. Central to enabling these discussions is determining sensor data accuracy relative to reference instruments and precision among sensors of the same model. This work summarizes evaluations of several air sensors measuring particulate matter (PM) at an urban background site in Research Triangle Park, North Carolina. Sensor models assessed include the APT Maxima, Aeroqual AQY, PurpleAir PA-II, SENSIT RAMP, Clarity Node-S, and AirVisual Pro. At least three of each sensor model were deployed simultaneously for at least 30 days with evaluation periods spanning March 2019 - February 2020. One-hour and 24-hour averaged PM_{10}, $PM_{2.5}$, and PM_1 sensor data were compared to collocated Grimm EDM180 and Teledyne T640x Federal Equivalent Methods, as available. Preliminary results suggest wide variability in precision among sensor models. The impact of meteorological effects, including temperature and relative humidity (RH), have been explored. For some models, higher RH did not lead to overestimation, stressing the importance of understanding manufacturers correction algorithms, which commonly include RH corrections. These results provide valuable information regarding the reliability of particulate air sensor data when compared to regulatory methods and provide context for EPA's sensor performance targets under development. These results highlight the importance of evaluating sensors in order to understand their limitations, have confidence in their data, and acknowledge the effort required to manage sensors marketed to those outside traditional air monitoring agencies.

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.

12IM.29

Experimental Characterization of Light Backscattering.

BLAINE FRY, Christopher Sorensen, *Kansas State University*

Climate models and remote sensing schemes require an accurate understanding of backscattering. Thus, there have been a great number of theoretical studies of backscattering in recent years. Despite this and the opportunity to uncover interesting physics, backscattering is largely unexplored empirically. Backscattering is both relatively dim and exceptionally sensitive to variations in particle size, shape, and refractive index. These factors, while creating potential obstacles, underscore the importance of practical characterization. Here we present a facile apparatus for collecting backscattered light in the range 168 to 179 degrees for both co- and cross-polarized scattered light. The apparatus draws strength from simplicity and is capable of the sensitive measurements necessary to characterize backscattering. Results for scattering by spheres and fractal aggregates demonstrate the device's utility.

12IM.30

Detailed Comparisons of Organic Aerosol Composition Measurements Using Advanced Mass Spectrometric Techniques.

ERIK HELSTROM, Abigail Koss, Jordan Krechmer, Manjula Canagaratna, Frank Keutsch, Alexander Zaytsev, Jesse Kroll, *MIT*

While the mass yield of secondary organic aerosol (SOA) from a number of volatile organic carbon precursors under different oxidation conditions has been measured for some time, the chemical composition of these condensed-phase products remains a source of substantial uncertainty. An incomplete understanding of the composition of SOA precludes the formulation of general formation mechanisms or a causal understanding of its overall physical and chemical properties. Therefore, it is necessary to develop instrumentation capable of measuring the full chemical range of carbon-containing species present. In recent decades, great strides have been made in detecting and quantifying additional organic species, owing to advancements in inlet design and the proliferation of ionization schemes for mass spectrometry. However, to our knowledge there is still uncertainty as to the observational intersections of these techniques – which species are measured by multiple instruments, and which species may remain unmeasured. A number of chamber oxidation experiments were performed to test the coverage of chemical identities detected in real time by a suite of these new instruments. Here we present an intercomparison of the measurements -- Filter Inlet for Gases and Aerosols-Iodide-Chemical Ionization Mass Spectrometer (FIGAERO-I-CIMS), Thermal Denuder-Proton Transfer Reaction-Mass Spectrometer (TD-PTR-MS), Thermal Denuder-Ammonium-Chemical Ionization Mass Spectrometer (TD-NH4-CIMS), and Aerosol Mass Spectrometer (AMS) -- of condensed-phase organic species collected during these experiments, identifying the remaining gaps and measurement overlaps this observing system provides. We use reduced-parameter frameworks which provide a solid foundation for assessing overall coverage in chemical space. Beyond this, we examine the evolution of individual species/ion signals over time to demonstrate consistencies and outstanding deficiencies across measurements. Ultimately this work aims to assist the development of systematic metrics by which future instrument deployments can be assessed.

12IM.31

The Impact of Structure on the Estimation of Atmospherically Relevant Physicochemical Parameters.

GABRIEL ISAACMAN-VANWERTZ, Bernard Aumont, *Virginia Tech*

Recent advances in field-deployable mass spectrometry of gas- and particle-phase organic compounds have provided unprecedented characterization of atmospheric mixtures. However, while organic carbon across the entire range of atmospheric properties has become measurable by current state-of-the-art tools, many of these instruments identify analytes only by elemental formula with little or no structural information. This lack of structural information stymies the estimation of many physicochemical properties, which have strong structural dependencies. Consequently, a substantial body of work has generated and utilized empirical parameterizations of molecular properties (e.g. volatility and reactivity) based on elemental formulas, and little work has quantified the extent to which ignoring molecular structure degrades estimates of these parameters. In this presentation, we compare the estimated vapor pressures, Henry's Law Constants, and OH reactivity of isomers of the same molecular formulas. Differences between isomers are compared to uncertainties between different structure-based estimation methods, and to errors in formula-based estimation methods. This analysis is performed using a set of ~35,000 structures (of ~1,200 formulas) predicted by the GECKO-A explicit chemical mechanism generator as atmospheric oxidation products of α-pinene, decane, and toluene. We find that differences between isomers are greater than differences between structure-based methods, indicating structural information improves estimates. Furthermore, particle-phase components suffer higher ranges and uncertainties in their estimated properties. However, formula-based estimation is possible for all three parameters with little bias and an approximately normally distributed error. Consequently, formula-based estimation is reasonable when necessary, but creates uncertainty commensurate with the lack of structural information.

12IM.32

Validating Wildfire Smoke Transport within a High-density, Low-cost Sensor Network.

KERRY KELLY, Derek Mallia, Adam Kochanski, Wei Xing, Tofigh Sayahi, Tom Becnel, Pierre-Emmanuel Gaillardon, Ross Whitaker, *University of Utah*

Short-term exposure to fine particulate matter ($PM_{2.5}$) pollution is linked to numerous adverse health effects. Wildfires can lead to substantial increases in $PM_{2.5}$ levels, and these impacts are becoming a growing concern as both the number and size of wildfires continues to increase. Although many smoke modeling tools exist, accurately simulating smoke production and dispersion is difficult, especially in regions with complex terrain where smoke plumes tend to exhibit substantial spatiotemporal variability. One of the fundamental problems associated with smoke modeling is the lack of highly resolved validation data. In this study, we use a network of 503 sensors (AQ&U and PurpleAir) located along Utah's Wasatch front to evaluate the performance of a coupled fire-atmosphere model (WRF-SFIRE-CHEM) to simulate fire emissions and smoke dispersion during the Pole Creek Wildfire. This fire burned an area over 260 km^2 adjacent the Wasatch Front during the summer of 2018 and led to $PM_{2.5}$ levels that exceeded 90 $\mu g/m^3$. The sensor measurements and modeling results reveal dramatic spatiotemporal differences in $PM_{2.5}$ concentration during this episode and suggest that coupled fire-atmosphere models such as WRF-SFIRE-CHEM can resolve local drainage flow and the downwind dispersion of wildfire smoke plumes in regions of significant topographic relief.

Conflict of Interest: Drs. Gaillardon and Kelly have a financial interest in the company Tetrad: Sensor Network Solutions, LLC, which commercializes solutions for environmental monitoring.

12IM.33

Comprehensive Detection of All Analytes in Large Chromatographic Atmospheric Dataset.

SUNGWOO KIM, Gabriel Isaacman-VanWertz, *Virginia Tech*

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. To gain insight into sources and transformations, individual components are frequently identified and quantified using gas chromatography/mass spectrometry. However, due to the complexity of this data and the highly dynamic nature of aerosol composition, data reduction is a significant bottleneck in analysis. Consequently, typically only a few dozen analytes are reported for a dataset, and a large amount of potentially useful data are discarded. We present here an automated approach of cataloging and potentially identifying all analytes in a large chromatographic dataset of ambient aerosols. We use a coupled factor analysis/decision tree approach to de-convolute peaks and comprehensively identify analytes. 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. We validate this approach using samples of known compounds, successfully cataloging all known analytes and resolving unknown contaminants. We demonstrate the separation of co-eluted peaks, including components with highly similar mass spectra and little-to-no chromatographic resolution, and the resolution of peaks that appear in only a fraction of chromatograms. As a case study, this method is applied to a complex real-world dataset representing months of hourly particle-phase organic composition, from which upwards of 400 analytes are resolved.

12IM.34

Development of a Personal Sampler Combined with Adenosine Triphosphate Bioluminescence Assay for the Rapid Measurement of Bioaerosols.

LI LIAO, Jeong Hoon Byeon, Jae Hong Park, *Purdue University*

Bioaerosols are defined as aerosol particles of biological origins (e.g., bacteria, virus, etc.) and associated with adverse health effects including infectious diseases, acute toxic effects, and allergies. To protect people against these biological threats, the first step is measuring the concentration of bioaerosols. To assess the individual exposure to bioaerosols, they are generally collected in the culture media using a personal sampler and then incubated in favorable conditions at least for 24 hours. However, these conventional culture methods are time-consuming and complicated. To overcome these limitations, we suggested an adenosine triphosphate (ATP) bioluminescence assay to rapidly measure the bioaerosol concentration and developed a personal bioaerosol sampler for combining with ATP bioluminescence assay. The personal sampler consisted of a respirable cyclone (cut-off diameter of 4 µm), a 3-jet impactor (cut-off diameter of 0.5 µm) to collect bioaerosols onto the head of swab used for ATP assay, a swab holder, and a personal sampling pump. The collection efficiency of 3-jet impactor was tested using aerosolized salt particles. The experimental cut-off diameter was 0.44 µm and slightly smaller than the designed size. Since the size of single bacteria is about 1 µm, the PB sampler can theoretically collect most bioaerosols. The performance of the PB sampler was evaluated and compared with a conventional Andersen impactor in the lab and the field. In the lab, concentrations of aerosolized *Escherichia coli*(*E. coli*) were measured. The results from the personal sampler were highly correlated to those from the Anderson impactor (R^2= 0.85). In the field, bioaerosols in the horse barn were measured. The PB sampler showed better performance than Andersen impactor.

12IM.35

Low Cost Detection Method for in Situ Detection of Aerosol Acidity Using Colorimetry Integrated With Camera.

AZAD MADHU, Myoseon Jang, Zechen Yu, *University of Florida*

Despite numerous studies that report the association of aerosol acidity with health effects of particulates and aerosol chemistry, the online detection of aerosol acidity is expensive and inaccessible. The Colorimetry integrated with Reflective UV Spectrometer (C-RUV) method has recently been developed to detect the aerosol acidity collected on a filter. This method innovates the online detection of aerosol acidity by using a micro-UV spectrometer that can be easily deployable in the field. However, the micro-UV spectrometer is still costly. In this study, a low-cost detection method that utilizes a commercialized camera (i.e., cellphone camera) with an LED light is demonstrated to measure aerosol acidity. The Colorimetry integrated with Camera (CICAM) images are used for the detection of the color change by the acidic aerosol collected in a filter that is impregnated with acid indicator (metanil yellow). Then, the resulting CICAM images are decoupled to the typical RGB (Red-Green-Blue) scale using a python-based computer program. The color change in the indicator of this study is most dramatic in the G component. Therefore, the calibration of the acidity of aerosol samples is performed with regard to the G value. In order to develop the relationship between CICAM and C-RUV, the spectral data originating from a micro-UV spectrometer is translated into the RGB values under the LED light source that is used for CICAM. There is a strong linearity between CICAM calibration and C-RUV. Therefore the previously derived C-RUV calibration can be directly applied to CICAM with a simple coefficient. The CICAM method and device are also applied to field data. Because of a user-friendly, easily deployable technique, the CICAM method will allow for field monitoring of aerosol acidity as well as citizen science.

12IM.36

New Inlet for Increasing Concentrations of Reactive Organic Gases in SCCM-Level Sample Flows.

NAMRATA SHANMUKH PANJI, Gabriel Isaacman-VanWertz, *Virginia Tech*

Organic aerosol (OA) in the atmosphere is of serious consequence to air quality, radiative climate forcing, and human health. A dominant fraction of this OA is formed through oxidation of reactive organic compounds, primarily emitted in the gas phase. These compounds, especially terpenes, contribute significantly to OA, O_3 production, and oxidant removal, but are typically present in sub-ppt to sub-ppb concentrations. Additionally, some highly reactive volatile organic carbons (VOCs) with lower volatilities, such as sesquiterpenes, present analytical problems in the form of losses to instrument lines and surfaces. Consequently, measurements of many reactive gases suffer high levels of detection. This has been particularly limiting for low-cost instrumentation (e.g., photoionization detectors), which frequently have levels of detection too high to be useful under typical ambient conditions. We present here a novel “enriching inlet” capable of increasing the concentration of organic gases in small sample flows (up to 5 sccm), thereby providing improved sensitivity and limits of detection. Inert gases are removed from the sample stream by selective permeation through Teflon™ AF-2400 tubing driven by a pressure gradient, concentrating remaining organic gases into a smaller flow for subsequent sampling. Significant enrichment (a factor of several) is demonstrated for several major classes of OA precursors; isoprene (C_5H_8), monoterpenes ($C_{10}H_{16}$, specifically α-pinene), and sesquiterpenes ($C_{15}H_{24}$, specifically β-caryophyllene). We present the relationships between pressure differential, inlet length, and sampling flow rate, to establish a model to predict enrichment of a given gas at a given sample flow.

12IM.37

Positive and Negative Emissions from Cooling Towers.

CHRISTOPHER WALLIS, Mason Leandro, Patrick Chuang, Anthony S. Wexler, *University of California, Davis*

Cooling towers are widely used in industrial and commercial applications to dissipate heat into the environment by spraying water droplets into air. The evaporation of these droplets cools the water which is then recirculated. Some droplets escape the cooling tower as spray drift and dry down, ultimately resulting in aerosol emission composed of impurities in the recirculating water. EPA AP42 designates these aerosols as PM_{10} and regulates their emissions. Cooling tower emissions are based on decades-old measurements. Since then measurement technology and cooling tower technology have been improved. We deployed modern aerosol instrumentation on a rack suspended by a crane over cooling towers at three power plants. Nafion dryers on the rack dried the droplets down to their aerosol core. IMPROVE samplers were used to obtain PM_{10} and $PM_{2.5}$ mass while a TSI APS measured particle size distribution. In parallel, droplet size distributions were measure by a Phase Doppler Interferometer. Although there are PM_{10} emissions as described by prior measurements, there are also $PM_{2.5}$ emissions, not previously appreciated. In addition, cooling towers scrub ambient PM_{10} and $PM_{2.5}$ such that under some circumstances the net emissions are negative. Instrumentation, emissions factors and scrubbing efficiencies will be presented.

12IM.38

Online Measurement of Semi-volatile Tracer Molecules in Workplace Room Air using Thermal Desorption Aerosol Gas Chromatography-Mass Spectrometry.

WEN XU, Philip Croteau, Nathan Kreisberg, Allen Goldstein, John Jayne, Douglas Worsnop, *Aerodyne Research, Inc.*

Knowing the chemical composition of aerosols is key to understanding their sources and to making effective control policies to reduce air pollution. Scientists often use offline filter-based techniques to capture detailed chemical compositions of aerosols. However, these techniques are usually labor-intensive and are not applicable when high time-resolution is a priority for accurate source appointment, especially in regions where the meteorology could change in hours.

In the current work, we demonstrate the application of online thermal desorption aerosol gas chromatography (TAG) mass spectrometry for measuring semi-volatile tracer molecules in room air of a workplace environment with a time resolution of about 1 hour. Time series of two organic compounds, levoglucosan and triethanolamine, were measured. The temporal profile of levoglucosan agrees well with the biomass burning organic aerosol (BBOA) factor measured using a collocated aerosol chemical speciation monitor (ACSM). The diurnal profile of levoglucosan shows elevated concentration during nighttime in winter, considered to be due to increased domestic wood-burning activity in local area homes and provides insight into the air exchange rates of the building HVAC system. The temporal profile of triethanolamine shows a strong weekday and weekend pattern. Its concentration is elevated when activities are going on in the machine shop inside the building, suggesting a possible source from metal cutting fluid. Filter blanking measurements show that both levoglucosan and triethanolamine are mainly in the particle phase. In summary, the TAG-MS system shows great potential in providing hourly molecular- resolved data for source apportionment, complementing both offline filter-based techniques and high time-resolution, but low molecular resolution, instruments, such as aerosol mass spectrometers.

12NM.1

On-the-fly Directed Assembly of Metal Nanoparticles from Electromagnetically Levitated Metal Droplets.

PANKAJ GHILDIYAL, Prithwish Biswas, Steven Herrera, Reza Abbaschian, Michael Zachariah, *University of California, Riverside*

Aerosol-synthesis techniques offer a scalable approach to production of metal nanoparticles and their assembly into well-defined structures. Fast particle diffusion rates in gaseous media typically cause rapid and uncontrollable, random aggregation, thus limiting controlled, directed assembly of nanoparticles in the aerosol phase. One approach to achieve directionality and control of nanoparticle assembly in the gas phase would be to employ an external magnetic field during particle formation and aggregation such that the directional interactions of the nanoparticles with the field compete with random, Brownian coagulation.

In this work, we explore an electromagnetic levitation technique to generate metal nanoparticles and tune their aggregate structure and morphology. This technique employs an electromagnetic levitation coil that levitates and inductively heat bulk metal pieces (~1cm) beyond their melting points. High temperatures (up to 2500K) and large evaporative flux achieved at the droplet surface result in a large supersaturation of metal atoms around the droplet, leading to nucleation and growth of metal nanoparticles that are transported and collected downstream by an inert carrier gas. Levitation allows the reactor to be wall-less and crucible-free and prevents crucible contamination at elevated temperatures. In addition, the magnetic field arising from the induction coil may also have a directional effect on the assembly and aggregate structure, particularly for magnetic metal nanoparticles. Morphologically distinct aggregates are obtained depending on the magnetic properties of the metal used. Aggregates from ferromagnetic metals such as Fe and Ni appear to be ‘stringier’ and chain-like (lower fractal dimension, Df), while for paramagnetic Cu, a more compact structure with a higher Df value is obtained. Thus, this technique offers a scalable, aerosol-phase approach to generate structurally distinct aggregate assemblies of metal nanoparticles.

12NM.2

Structure and Dynamics of Fractal-like Particles Made by Agglomeration and Sintering.

EIRINI GOUDELI, Maximilian L. Eggersdorfer, *University of Melbourne*

Aerosol synthesis of nanoparticles is a versatile process for production of commodities like titania, carbon black and fumed silica at scale. A critical design criterion for aerosol reactors is the high temperature particle residence time, which determines the nanoparticle growth by gas and surface reaction, coagulation and sintering. Typically, the chemistry is so rapid that coagulation and sintering dominate the particle growth and, thus, their structure that can impact significantly the material performance (e.g., catalytic or optical properties). Therefore, knowing the collision frequency and sintering time is necessary to model particle growth mechanisms accurately, which are currently modeled by making a priori assumptions on the particle structure.

Here, the growth of silica nanoparticles by agglomeration and viscous flow sintering is studied from free molecular to transition regime at high temperatures by discrete element method simulations. The effect of temperature on the aggregate mobility and gyration radii, particle morphology and collision frequency function is elucidated as function of the number of primary particles. The ratio between the characteristic sintering time and characteristic collision time controls the particle size and structure, quantified by the mass fractal dimension. The effect of this ratio of characteristic times on aggregate morphology is illustrated at various temperatures. Finally, when sintering is negligible, the overall collision frequency is 90% larger than that predicted by the classic Fuchs collision kernel for monodisperse agglomerates in the near free molecular and transition regime. For comparable coagulation and sintering rates, where aggregates with sinter bonds are formed, the overall collision frequency increases an enhancement of <90% is observed.

12NM.3

Synthesis of Multicomponent Metal-containing Nanomaterials in a Flame-driven High Temperature Reducing Jet Reactor. MOHAMMAD MOEIN MOHAMMADI, Shuo Liu, Chintan Shah, Sandeep Kumar Dhandapani, Shema Rachel Abraham, William Sullivan, Raymond Buchner, Mark Swihart, *University at Buffalo - SUNY*

Metal nanomaterials have great potential in various applications such as catalysis, gas sensing, bio-imaging and printed electronics. Single-step, continuous, gas-phase processes may provide the best means of producing these nanomaterials at low-cost and large-scale. Flame technology is widely used to manufacture different types of nanomaterials such as fumed silica and titania at industrial scale. However, production of non-noble metal nanomaterials via this technique is not common. We have developed a flame-driven High Temperature Reducing Jet (HTRJ) process in our group that enables flame-based synthesis of metal nanomaterials from aqueous salt precursors. In this process, a fuel-rich hydrogen flame passes through a converging-diverging nozzle. An aqueous precursor solution injected at the throat section of the nozzle is atomized by the high velocity gas stream. The resulting droplets evaporate and the precursor decomposes, initiating nucleation of particles in a reducing environment containing excess H2. After the reaction zone, particles are cooled immediately to prevent further particle growth and coalescence. The key advantage of the HTRJ system over common flame-based aerosol synthesis methods is the separation of flame and product formation zones, which allows synthesis of nanomaterials that can be reduced by H2 in the presence of H2O. We have utilized the capabilities of this reactor to synthesize two groups of nanomaterials. First, we present novel three-dimensional multicomponent metal-decorated crumpled reduced graphene oxide ball (M-CGB) nanocomposites. As a representative application, Pd-CGB nanocomposites were used for H2 detection in air at room temperature. Second, we introduce active and stable supported nickel-based nanocatalysts for the dry reforming of methane (DRM). The HTRJ process is a potentially scalable method to produce non-noble catalyst structures at low-cost to achieve high DRM activity at low temperature.

12NM.4

Synthesis of Sodium Yttrium Fluoride-based Phosphors by Ultrasonic Spray Laser Pyrolysis. MOHAMMAD MALEKZADEH, Vishvajeet Mane, Khirabdhi Mohanty, Mark Swihart, *University at Buffalo - SUNY*

$NaYF_4$-based nanomaterials exhibit advantageous properties such as sharp emission, high photostability, high chemical stability, and low toxicity which make them appropriate for numerous medical- and energy-based applications. Doping these nanomaterials with rare-earth elements such as ytterbium, thulium, europium, and erbium endows them with useful optical properties, including conventional and upconverted photoluminescence. To date, these nanomaterials have been synthesized only by solution-phase synthesis methods. In comparison with solution-phase synthesis methods, vapor-phase (aerosol) synthesis methods benefit from fewer steps in the synthesis process, continuous operation, low chemical waste, synthesis of nanomaterials with high purity and crystallinity, synthesis of nanomaterials of different composition without developing new recipes, and production of bare particles without ligands. In this study, we employed laser pyrolysis to synthesize $NaYF_4$-based nanoparticles. In laser pyrolysis, SF_6 is usually used as a photosensitizing agent to absorb the energy of the laser and transfer it to precursors that do not absorb at the CO_2 laser wavelength of 10.6 µm. However, it can also be used as a source of fluorine. We have developed a low-cost ultrasonic atomizer and employed it to spray an aqueous precursor solution of sodium acetate and yttrium acetate into the reaction zone where it is heated by a focused CO_2 laser beam, with SF_6 as the photosensitizer and the source of fluorine. This allowed us to produce $NaYF_4$ nanoparticles in a single step from aqueous salt precursors. In addition, we doped the nanoparticles with rare-earth elements to produce phosphors with useful optical properties.

12NM.5

Fabrication of Hollow Carbon Nanofiber Containing Metal Oxide Catalyst via Electrospinning and Thermal Treatment for Atmospheric VOCs Removal and Water Treatment.

SANGMO KANG, Jungho Hwang, *Yonsei university*

We propose a novel material which has high VOCs removal performance as an adsorbent and also as a catalytic oxidation agent. In addition, we propose a methodology of fabricating this material. By ejecting a PMMA solution containing manganese oxide (Mn3O4) precursor through the inner part of a dual nozzle while a PAN solution is delivered through the outer part, nanofibers impregnated with Mn3O4 (denoted as Mn3O4/NFs) are fabricated after the co-axial electrospinning (outer layer: PAN, inner layer: MnAc/PMMA). The Mn3O4/NFs are carbonized, become a hollow structure, and are activated (Mn3O4/HACNFs).Mn3O4 fabricated in this study are the most widely studied metal oxides due to the high activity, stability, relative low toxicity and redox properties. The fabricated Mn3O4/HACNFs are then tested for VOCs removal. The VOCs removal performance of is evaluated at low temperature (below 100) and high temperature (150~280), respectively, as a toluene adsorbent and a toluene oxidizing agent. The fabrication of Mn3O4/HACNFs using the dual nozzle co-axial electrospinning process is introduced for the first time, to the best of our knowledge.

A series of CoxMn3−xO4/HCNFs were also synthesized, and their catalytic performance in oxidative degradation of organic dye compounds in water was investigated. The results showed that, as an oxide composite of Co and Mn elements, CoMn2O4/HCNFs showed much stronger catalytic activity in peroxymonosulfate (PMS) oxidation than Co3O4, Mn3O4, and their physical mixture. Typically, the uses of 0.2 g/L CoMn2O4/HCNFs and 0.3 g/L PMS yielded a nearly complete removal of Rhodamine B (50 M) in 80 min at 25 ◦C. The efficiency of Rhodamine B decomposition increased with increasing temperature (15–55). Furthermore, CoMn2O4/HCNFs could maintain its catalytic activity in the repeated batch experiments. Moreover, hydroxyl and sulfate radicals participating in the process were evidenced using quenching experiments, and a rational mechanism was proposed. PMS oxidation with CoMn2O4 is an efficient technique for remediation of organic contaminants in wastewater.

The surface morphology and structure of the all nanofibers were characterized by field emission scanning electron microscopy (FESEM), energy-dispersive X-ray spectroscopy (EDX), transmission electron microscopy (TEM), powder X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS).

This work was supported by Railroad Technology Research Program (18RTRP-B082486-05) funded by Ministry of Land, Infrastructure and Transport of Korean Government.

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12NM.6

Characterization of Nanoparticles Emitted from Metallic Heaters in Electronic Cigarettes. KAUSHAL PRASAD, Mark D. Wilson, Jae Hong Park, *Purdue University*

Electronic (e-) cigarettes, also known as electronic nicotine delivery systems, are battery-operated devices that are growing in popularity worldwide. The e-cigarette consists of a heater to vaporize nicotine solution, a reservoir that contains nicotine solution, and a wick to deliver the nicotine solution to the heater. When the heater is operating, metal vapor can be produced from its surface, cooled by air, and then form nanoparticles (<100 nm) through condensation and nucleation. Although e-cigarettes are known to be safer than traditional cigarettes, their potential health risks have not been extensively reviewed yet. In this study, nanoparticles generated from e-cigarette heaters were characterized based on the total number concentration (TNC) and the size of the particles. Four heater wires (Kanthal A1, Nichrome, stainless steel 316L, and titanium) were tested for 30 minutes with a frequency of 0.1 Hz and a 50% duty cycle (5s on, 5s off). The size distribution of particles emitted from each heater was measured using a scanning mobility particle sizer (SMPS). In all cases, the TNC of particles decreased over time because the oxidation layer on the coil surface prevented further nanoparticle emission. A used coil may reduce the risk of metal exposure from e-cigarettes. The initial number median diameter (NMD) and TNC of particles ranged from 40 nm to 80 nm and 1.0 – 3.5 × 107 particles/cm3, respectively. The resistance of the heater material affected the generation of nanoparticles. Particles from the titanium heater have the largest NMD and the highest TNC. Lower resistance materials may produce more particles since they have a longer length and larger surface area. These findings can be used for developing safer e-cigarettes.

12NM.7

Controlled Explosion of Fine Dusts. SHUSIL SIGDEL, Justin Wright, Stephen Corkill, Christopher Sorensen, *Kansas State University*

Agricultural and coal dusts are known as explosion hazards and have a negative economic value. If these carbon containing dust could be detonated to form graphene, we can transform waste materials into valuable materials. This work primarily focuses on the design of a dispersion system for a dust explosion and preliminary results of the explosion of carbon containing dust in a 17-L aluminum chamber. To characterize the dispersion process of dust clouds, visualization experiments were conducted by using a transparent 17-L plastic chamber. In addition, we will talk about our future experiments in which finely divided materials like pyrophoric metals and coal dust are blown into the chamber with oxygen and detonated.

12NM.8

Effects of UV Intensity and Gas Composition on Photocatalytic Nitrogen Fixation on Titanium Dioxide Nanoparticles.

SABRINA WESTGATE, Nga Lee Ng, *Georgia Institute of Technology*

Nitrogen fixation, the conversion of atmospheric nitrogen to other nitrogen species, is an integral part of the nitrogen cycle and atmospheric chemistry. Prior work has suggested that up to a few percent of all fixed nitrogen in soil could be due to photocatalytic nitrogen fixation on naturally occurring semiconducting nanoparticles, though these processes are not well constrained. While some studies looking at nitrogen photo-fixation have reported the production of nitrogen-containing species, most experiments have been performed in the bulk aqueous phase and with limited instrument capabilities. Moreover, the details and driving forces of this reaction are largely unknown. In this work, we conduct experiments to investigate NOx production in the presence of titanium dioxide nanoparticles. In our setup, we expose the titanium dioxide to UV lights while flowing a mixture of gasses through the experiment. The effects of UV light intensity and gas mixture composition are studied. Using state of the art instrumentation, we are able to replicate ambient environmental conditions and capture real-time, highly accurate data for the gaseous products of the photocatalytic nitrogen fixation reaction. Results from these experiments will provide data for determining the reaction rates and mechanism pathways that occur in nitrogen photocatalysis.

12NM.9

Precursor Effects on the Properties of Detonation Graphene Aerosol Gel.

JUSTIN WRIGHT, Shusil Sigdel, Stephen Corkill, Jose Covarrubias, Levon LeBan, Jun Li, Stefan Bossmann, Christopher Sorensen, *Kansas State University*

Detonation of hydrocarbon gaseous precursors with oxygen in a chamber is a cheap, green, and scalable technique for producing multilayer graphene aerosol gels. Here we describe mixing oxygen and acetylene in various ratios to explore the range of properties of the graphene aerosol gels produced. The properties and characteristics we studied include Raman spectra, XRD spectra, mass density, appearance, and specific surface area. The higher the oxygen content in the chamber, the higher the detonation pressure, mass density, and crystallinity, with lower yield, specific surface area, and defect in the sample. For all samples, Raman peak intensities 2D/G=0.5 matching bilayer graphene, as well as all peaks having Lorentzian shape and positioning consistent with that of single layer graphene.

13ACa.1

Highly Viscous Secondary Organic Aerosol from Healthy and Stressed Pine Trees. NATALIE R. SMITH, Giuseppe Crescenzo, Yuanzhou Huang, Anusha P.S. Hettiyadura, Kyla Siemens, Ying Li, Celia Faiola, Alexander Laskin, Allan Bertram, Manabu Shiraiwa, Sergey Nizkorodov, *University of California, Irvine*

When plants are stressed, their volatile organic compound (VOC) emission profile changes in both quantity and types of compounds being emitted. For example, pine trees stressed due to aphid herbivory emit more sesquiterpenes, which can lead to the formation of different secondary organic aerosols (SOA) when compared to SOA formed from healthy plant emissions. In this study, the molecular composition, viscosity, and liquid-liquid phase separation (LLPS) were investigated for SOA derived from the photooxidation of VOC mixtures representing the emission profile of either healthy or aphid-stressed Scots pine (*Pinus sylvestris*) trees. Aerosols were generated in a 5 m^3 environmental chamber at 50% relative humidity. Detailed information on particle molecular composition was gained through nanospray desorption electrospray ionization –high resolution mass spectrometry. The observed neutral molecular formulas were used to predict the viscosity as a function of relative humidity using the parameterization developed by DeRieux et al. (2018). The predictions from the viscosity model were compared to the experimental values measured via the poke-flow method. Under low relative humidity both stressed and healthy plant SOA were highly viscous and had viscosities similar to tar pitch. Over all humidities investigated, stressed SOA had the highest viscosity followed by healthy SOA and α-pinene SOA. Phase separation experiments revealed that LLPS occurs over a wider relative humidity range for stressed SOA compared to healthy SOA. These findings suggest that SOA generated from a complex mixture of VOCs can result in higher SOA viscosity compared to SOA generated from a single component precursor, such as α-pinene. In addition, plant stress can lead to changes in the physicochemical properties of SOA.

13ACa.2

Atmo-ecometabolomics of Healthy and Stressed Riparian Shrubs: From the Plant Metabolome to Aerosol Production. FARZANEH KHALAJ, Alber Rivas-Ubach, Christopher Anderton, Swarup China, Kailen Mooney, Celia Faiola, *University of California, Irvine*

Vegetation contributes to production of secondary organic aerosol (SOA) via atmospheric processing of plant volatile emissions. SOA alters atmospheric radiative properties and thereby influences ecosystem function. Thus, there are tight ecosystem-atmosphere interactions linked through the plant metabolome that influence atmospheric composition and ecological processes, what we refer to as the “atmo-ecometabolome”.A better understanding of climate change effects on ecosystem function and SOA production could be achieved with a holistic atmo-ecometabolomics study approach. Within that framework, this study investigated the influence of aphid herbivory on the plant metabolome, volatile emissions, and SOA production of a common riparian shrub in California,Baccharis salicifolia–the first study to concurrently characterize these three components. The leaf-level metabolome was characterized using GC-MS and LC-MS. SOA was generated from plant emissions using an oxidation flow reactor (OFR).Chemically-speciated plant volatiles were characterized via thermo-desorption GC-MS-FID. Particle composition and size distributions were measured continuously with an aerosol chemical speciation monitor (ACSM) and scanning mobility particle sizer (SMPS), respectively. Results demonstrated that aphid herbivory significantly altered the leaf-level metabolome, and although there were some clear links between the leaf-level metabolome and volatile emissions, there was high intra-group variability in the volatile profile and SOA formation that hindered identification of clear herbivore effects. Of particular interest, SOA mass yield curves displayed as much variation within treatment groups as between treatment groups. The contribution of acyclic monoterpenes in the emission profile, such as beta-ocimene and beta-myrcene, were correlated with reduced SOA mass yield, but the relative contribution of acyclic monoterpenes was unrelated to herbivore treatment in this case. This study sheds light on the plant volatile structures controlling SOA formation from complex mixtures of plant volatiles, and can be used to improve predictions of SOA production in a future climate.

13ACa.3
Atmospheric Significance of the Aqueous-Phase Reactions of Green Leaf Volatiles: 1-Penten-3-ol, (Z)-2-Hexen-1-ol, and (E)-2-Hexen-1-al With Atmospheric Radicals.

KUMAR SARANG, Tobias Otto, Krzysztof Rudzinski, Irena Grgić, Nestorowicz Klara, Hartmut Herrmann, Rafal Szmigielski, *ICHF PAS, Warsaw, Poland*

Atmospheric particulate matter mostly consists of organic aerosols (OA), of which up to 90% exists as secondary organic aerosol (SOA). The incomplete knowledge of SOA precursors has led to the discrepancies between field measurements and the computer-modeled SOA budget. One of such potentially important, but missing sources of SOA is a class of compounds known as green leaf volatiles (GLVs). GLVs are C6-C5 unsaturated alcohols, aldehydes, or esters, which are released when a plant undergoes stress or mechanical wounding, such as cutting, freezing, or drying. The estimated annual global emission of C6 GLVs can alone give rise to 1-5 Tg C/yr SOA, i.e., at least one-third of that isoprene.

We investigated the temperature-dependent aqueous-phase kinetics of three GLVs: 1-penten-3-ol, (Z)-2-hexen-1-ol, and (E)-2-hexen-1-al with $SO_4^{\bullet-}$, and $^{\bullet}OH$ radicals. The second-order rate constants determined, range from 10^8-10^9 L $mol^{-1}s^{-1}$ for GLV+$SO_4^{\bullet-}$, and from 10^9 to 10^{10} L $mol^{-1}s^{-1}$ for GLV+$^{\bullet}OH$ kinetics. Various thermodynamic parameters, such as activation energy (E_A), molar enthalpy of activation ($\Delta H^{\ddagger}$), molar entropy of activation ($\Delta S^{\ddagger}$), and Gibb's free energy of activation ($\Delta G^{\ddagger}$) were calculated. The activation energies of less than 20 kJ mol^{-1} indicated the weak temperature dependence of the reactions. The second-order rate constants, especially of the order 10^9 L $mol^{-1}s^{-1}$, are diffusion-controlled, and therefore, we investigated them for the diffusion limitation; and diffusion-corrected rate constants were obtained. To explain the atmospheric significance of these aqueous-phase reactions, we calculated the aqueous-phase lifetime and the relative removal rate of GLVs by the overall gas- and aqueous-phase to the aqueous-phase reactions. The calculations demonstrated the dominance of aqueous-phase reactions of GLVs in cloud and rain waters under certain specific conditions for available radical concentrations.

13ACb.1
Oxidized Amines Enhance Particle Formation More Than Amines.

NANNA MYLLYS, Tuomo Ponkkonen, Sabrina Chee, James Smith, *University of California, Irvine*

Sulfuric acid plays a key role in atmospheric aerosol particle formation. Bases such as amines are known to stabilize sulfuric acid to form particles through salt formation. However, the role of oxidized amines in particle formation and growth is unknown. Trimethylamine oxide (TMAO), an oxidization product of trimethylamine, is studied here. As a weak base in the aqueous phase and a strong base in the gas phase, TMAO offers an interesting perspective for an argument "*base strength is a key factor in particle formation*." Another intriguing property of TMAO is related to its molecular structure: while steric hinderance of three methyl groups limits the hydrogen bonding sites to one, the zwitterionic bond causes a high dipole moment which enables the formation of stabilizing ion-dipole interactions. It seems clear that more than one base property is related to its capability to enhance aerosol particle formation. Molecular-level cluster formation mechanisms are resolved, and theoretical results on particle formation are confirmed with laboratory measurements. The enhancing effect of TMAO is compared to the other atmospheric bases and the factors, which make oxidized amines stronger stabilizer in clustering than amines, are discussed.

13ACb.2

A Generalized Semi-Empirical Model for Sulfuric Acid Nucleation in the Atmosphere. JACK JOHNSON, Sandra Fomete, Coty Jen, *Carnegie Mellon University*

Aerosol particles form in the atmosphere when gaseous phase compounds chemically react to form stable clusters in a process known as nucleation. In recent years, sulfuric acid has been shown to drive nucleation in the lower troposphere by reacting with various stabilizing compounds, such as ammonia or dimethyl amine. However, there are potentially hundreds of compounds that assist in sulfuric acid nucleation. These compounds could range in concentration from pptv to ppbv and vary in space and time. Consequently, modeling all the potential nucleation reactions in the atmosphere is challenging and requires a model that can broadly capture all pathways for sulfuric acid nucleation. For this study, we propose the use of a semi-empirical acid-base reaction scheme to determine an effective concentration of stabilizing compounds for sulfuric acid nucleation. Using a parameterization technique, we can determine the effective concentration of stabilizing compounds using particle concentration measurements. Our results show that the parameterized concentration is correlated with the measured concentration of stabilizing compounds and reflects the how strongly each compound stabilizes sulfuric acid particles. In addition, mixtures of stabilizing compounds were reacted with sulfuric acid to demonstrate how synergistic stabilization is captured by our model. The capabilities of the model to estimate stabilizing compounds will help improve accuracy for predicting nucleation rates in diverse regions around the world.

13ACb.3

Stochastic Effects in H2SO4-H2O Cluster Growth. CHRISTOPH KöHN, Martin Bødker Enghoff, Henrik Svensmark, *Technical University of Denmark*

The nucleation of molecular clusters is estimated to contribute about half of all cloud condensation nuclei, globally. A central molecule in nucleation is sulfuric acid nucleating together with H_2O molecules.

Based on a recently developed particle Monte Carlo (MC) Code [C. Köhn, M. Enghoff and H. Svensmark, 2018. A 3D particle Monte Carlo approach to studying nucleation. J. Comp. Phys., vol. 363, pp. 30–38], we here analyse how the growth of sulfuric acid-water clusters is influenced by stochastic fluctuations. We present the temporal evolution of the nucleation rate and of the size distribution as well as the onset time of the nucleation above a given cluster size with and without constant production of new monomers. We consider samples of H_2SO_4-H_2O clusters at T=200 K, with particle concentrations between 10^5 cm^{-3} and 10^7 cm^{-3} in volumes between 10^{-6} cm^3 and 10^{-2} cm^3.

Simulations are performed with a MC particle code following individual clusters. After every time step, we update the position of each cluster as a function of size-dependent diffusion coefficients and check for cluster collisions enabling cluster growth. Inversely, we check after every time step whether a polymer evaporates based on evaporation coefficients from literature [Yu, 2005. J. Chem. Phys., vol. 122, 074501; Yu, 2006. Atmos. Chem. Phys., vol. 6, 5193–5211].

Conclusively, we find clear evidence of fluctuations which are not apparent in deterministic continuum models. Recent research [Olenius et al, Nature Scientific Reports 8:14160, 2018] has shown that such stochastic processes can influence the early stages of growth which are critical for the survival rate of aerosol particles. We here find that fluctuations in the MC code favour a fast growth and thus an early occurrence of large clusters compared to simulations with less significant fluctuations.

13CC.1

Quantifying the Effects of Mixing State on Aerosol Optical Properties. YU YAO, Jeffrey H. Curtis, Nicole Riemer, *University of Illinois at Urbana-Champaign*

Calculations of the aerosol direct effect on climate rely on simulated aerosol fields. The model representation of aerosol mixing state potentially introduces large uncertainties into these calculations, since the simulated aerosol optical properties are sensitive to mixing state. The aim of this study is to systematically quantify the impact of aerosol mixing state on aerosol optical properties.

To this end, we created a large number of model scenarios using the particle-resolved model PartMC-MOSAIC. PartMC is a Lagrangian aerosol parcel model that tracks the evolution of composition and sizes of individual aerosol particles due to emission, coagulation, condensation and dilution without any a priori assumptions about aerosol mixing state. The model is coupled with the chemistry module MOSAIC, which deals with gas and aerosol phase chemistry. Aerosol optical properties are calculated using Mie calculations assuming spherical particles.

To cover a wide range of possible mixing states, we varied 41 input parameters that govern aerosol aging, including aerosol initial size distribution parameters, gas and aerosol emission rates, relative humidity, and temperature. The combinations of these variables for the individual scenarios are created by Latin Hypercube sampling where we prescribed a parameter range that represents the range encountered in different regions of the globe. The simulated aerosol optical properties in this scenario group capture the full diversity of the aerosols and can be used as the reference case. In order to quantify the errors due to the internal mixture assumptions used by many current aerosol models, we created another sensitivity scenario group with the same number and mass size distributions as the base scenarios but with averaged aerosol composition in prescribed size bins. Finally, we quantified the errors introduced by this composition averaging by linking the differences of optical properties with the mixing state metric chi. Preliminary results show the single scattering albedo (SSA) in the internally-mixed size bin cases are all lower than the particle-resolved reference cases, especially for the aerosols of intermediate mixing state (chi between 60% to 80%). The overestimation of the ensemble absorption in these internally-mixed particles is responsible for the SSA errors.

13CC.2

General Circulation Model Estimates of Aerosol Radiative Effects and Its Implication to Hydrology over the Hindu Kush-Himalayan (HKH) Region. SAUVIK SANTRA, Amit Kumar, Shubha Verma, *Indian Institute of Technology Kharagpur*

We present an analysis of aerosol transport simulations carried out in the Laboratoire de Me´te´orologie Dynamique (LMD-ZT) General Circulation Model (GCM) over the Hindu Kush Himalayan (HKH) region. The seasonal mean of GCM estimated aerosol optical depth (AOD) and single scattering albedo (SSA) were found to be consistent with the measured values. The pre-monsoon mean AOD was estimated to be 20% higher than that of the winter mean. About 75% of the simulated AOD was found to be from anthropogenic emissions and was mostly constituted of sulfate (45-65%), followed by organic carbon (OC) (40-50%), and black carbon (BC) (4-8%). One of the prominent features was the discrete spatial gradient in the distribution of sulfate and BC aerosols, thereby indicating their origin from different source regions. A substantial variation was seen in the spatial distribution of SSA between the HKH region and the neighboring regions of IGP. Aerosol radiative forcing was found to be positive at the top-of-atmosphere (TOA), indicating a net warming effect. Notably, the value of aerosol radiative forcing at TOA during pre-monsoon was about 4-6 times the value during the winter season. A strong influence of transport from far-off regions, which contributed as high as 60% of the total positive radiative effects, was inferred. Furthermore, the relative percentage of snow albedo reduction (SAR) and the annual increase in surface runoff due to deposition of both anthropogenic and natural aerosols were found to be significantly high, with their values being 13-15% and 3-12 cm of water equivalent respectively. The radiative transfer calculations are further used as input to a hydrological model, and sensitivity studies of surface runoff to aerosol deposition is carried out and validated with available observational data.

13CC.3

Investigating the Clear Sky Bias: Cloud-Relevant Aerosol Chemistry. MADISON FLESCH, Amy Christiansen, Virendra Ghate, Annmarie Carlton, *University of California, Irvine*

Measurements of aerosol physical, chemical, and radiative properties at cloudy times are critical to accurately understand and predict aerosol-cloud interactions necessary to improve atmospheric models. The uncertainty surrounding aerosol-cloud interactions and their effects on the radiation budget still persists, despite decades of study and improvements in measurement and modeling tools. Low level shallow cumulus clouds interact with boundary layer aerosol, which can serve as cloud condensation nuclei. The fundamental controlling chemistry among inorganic and organic particulate matter constituents and how they affect uptake of aerosol liquid water (ALW) is the same at the surface and at cloud height. Remotely sensed and ground-based measurements of optically-relevant aerosol properties during cloudy periods are often removed from final, quality assured data products due to increased error during such times. This contributes to a clear sky bias in the quantitative understanding of atmospheric aerosol burden, and in particular chemical composition and hygroscopicity that affect water uptake, a controlling factor of particle size and light scattering. Holistic evaluation of optical and physicochemical properties of aerosols can establish a greater understanding of this relationship. We combine surface measurements of Angstrom exponents and particulate matter chemical composition from six co-located AErosol RObotic NETwork (AERONET) and Interagency Monitoring of PROtected Visual Environments (IMPROVE) sites across the U.S. and statistically analyze their relationships as a function of satellite-derived cloud flags in aerosol optical depth (AOD) files. We find aerosols are physically larger and ALW content is enhanced by 20% on cloudy days over clear sky days across the U.S. This suggests that the inability by current atmospheric models to accurately describe aerosol-cloud interactions is caused, in part, by a clear sky bias in the recording of aerosol optical properties.

13HA.1

Ascorbate Oxidation by Iron, Copper and Reactive Oxygen Species: Review, Model Development, and Derivation of Key Rate Constants. JIAQI SHEN, Paul T. Griffiths, Steven J. Campbell, Battist Uttinger, Markus Kalberer, Suzanne E. Paulson, *UCLA*

Ascorbic acid is among the most abundant antioxidants present in the lung, and the chemistry of ascorbic acid plays a key role in the mechanism by which air pollution particles elicit a biological response. Because ascorbic acid (AH_2) is a highly redox active species, it engages in a far more complex web of chemical reactions than a typical soluble organic molecule, reacting not only with oxidants such as the hydroxyl radical, but also with redox-active transition metals such as iron and copper. The literature provides a solid outline of this chemistry, but there are several gaps and disagreements about reaction mechanisms, stoichiometries and reaction rates, particularly for the iron and copper reactions. Here we synthesize available data in the literature to develop a chemical kinetics model. We then use seven sets of laboratory measurements to constrain the mechanisms for iron and copper-mediated oxidation of ascorbic acid and derive key rate constants. The model built from existing literature is in poor agreement with the data without adjustment, although it does show that both ascorbic acid and ascorbate (AH^-) are oxidized primarily by Fe(III) and Cu(II) rather than the reduced forms of these metals. Further, micromolar concentrations of the transition metal reactions are more important sinks for AH_2 and AH^- than the reactive oxygen species. We find that the evidence supports catalytic mechanism for the reactions, rather than a redox mechanism as suggested in some of the literature, with the stoichiometry for iron: $Fe(III) + AH_2$ (or AH^-) $+ O_2 \rightarrow Fe(III) + DHA + H_2O_2$ ($- 2H^+$ for AH^-) and copper: $Cu(II) + AH_2$ (or AH^-) $+ O_2 \rightarrow Cu(II) + DHA + H_2O_2$ ($- 2H^+$ for AH^-), and rate constants of 5.7×10^4 and 4.7×10^4 $M^{-2}s^{-1}$ for the $Fe(III) + AH_2/AH^-$ reactions and 1.0×10^5 and 2.5×10^6 $M^{-2}s^{-1}$ for the $Cu(II) + AH_2/AH^-$ reactions, respectively.

13HA.2

Characterization and Comparison of PM2.5 Oxidative Potential Assessed by Two Acellular Assays. DONG GAO, Krystal Godri Pollitt, James Mulholland, Armistead G. Russell, Rodney J. Weber, *Georgia Institute of Technology*

The capability of ambient particles to generate *in vivo* reactive oxygen species (ROS), known as oxidative potential (OP), is a potential metric for evaluating the health effects of particulate matter (PM) and is supported by several recent epidemiological investigations. A variety of acellular assays have been developed to assess PM OP. In this study, we systematically compared two health-relevant acellular OP assays that track the depletion of antioxidants or reductant surrogates: the synthetic respiratory tract lining fluid (RTLF) assay that tracks the depletion of ascorbic acid (AA) and glutathione (GSH), and the dithiothreitol (DTT) assay that tracks the depletion of DTT. Year-long daily samples were collected at an urban site in Atlanta, GA during 2017, and both DTT and RTLF assays were performed to measure the OP of water-soluble $PM_{2.5}$ components. $PM_{2.5}$ mass and major chemical components, including metals, ions, and organic and elemental carbon were also analyzed. The results showed that the OP assays differ in their sensitivities to PM chemical components. OP as measured by the DTT and AA depletion (OP^{DTT} and OP^{AA}, respectively) were correlated with both organics and some water-soluble metal species, whereas that from the GSH depletion (OP^{GSH}) was exclusively sensitive to water-soluble Cu. These OP assays were moderately correlated with each other due to the common contribution from metal ions. Multivariate linear regression models were developed to predict OP measures from the particle composition data. Variability in OP^{DTT} and OP^{AA} were attributed to not only the concentrations of metal ions (mainly Fe and Cu) and organic compounds, but also antagonistic metal–organic and metal–metal interactions. OP^{GSH} was sensitive to the change in water-soluble Cu and brown carbon (BrC), a proxy for ambient humic-like substances.

13HA.3

Oxidative Potential of Fine Particulate Matter - Implications of Emission Source Sectors, Particle Chemical Composition and Acidity, and Metal Dissolution. POURYA SHAHPOURY, Zheng Wei Zhang, Andrea Mario Arangio, Valbona Celo, Ewa Dabek-Zlotorzynska, Tom Harner, Athanasios Nenes, *Environment and Climate Change Canada*

Air pollution is a major global health risk. It has been associated with respiratory-cardiovascular diseases as well as increased mortality. Inhalation of particulate matter with aerodynamic diameter ≤2.5 µm ($PM_{2.5}$) is a major cause of air pollution adverse effects. Oxidative potential (OP) is defined as the ability of PM-bound chemicals to oxidize the lung antioxidants either directly or through catalytic generation of reactive oxygen species. This process may result in oxidative stress, inflammation of the epithelial tissue, and chronic diseases. OP depends on various factors such as PM chemical composition and mass-size distribution. Among PM components, water-soluble organic species, quinones, and transition metals are the major contributors to OP. In this work, we investigated the OP of $PM_{2.5}$ from the National Air Pollution Surveillance sites across Canada, covering urban traffic, industrial, residential, and biomass burning source sectors. We applied a novel in-vitro OP assay that we developed in-house, which considers the reaction of PM with major lung antioxidants in simulated lung lining fluid and determines the redox state of the samples. The results were evaluated through correlation analysis with $PM_{2.5}$ constituents including organic matter, black carbon, transition metals, biomass-burning markers, organic ligands, as well as the aerosol pH. Our findings indicate that $PM_{2.5}$ oxidative burden was influenced by the emission source sectors, with traffic emission having the highest activity followed by industry and biomass burning. Water-soluble metals and black carbon were the major contributors to OP, with the former being influenced by the levels of aerosol-bound oxalate as well as pH in the aerosol aqueous phase. This study provides an insight into how current trends in urbanization and anthropogenic activities, as well as various emission sources, contribute to PM composition, human exposure and health risks associated with fine inhalable PM.

13IA.1

Evaluating an Indoor Air Quality Model Using Simultaneous Measurements of Cookstove PM2.5 Emissions and Indoor Concentrations.

MOHAMMAD MAKSIMUL ISLAM, Roshan Wathore, Hisham Zerriffi, Julian Marshall, Rob Bailis, Andrew Grieshop, *North Carolina State University*

Combustion of biomass in residential cookstoves is a major source of household air pollution (HAP), an acknowledged threat to human health. Multiple studies explore the effect of cookstove use on HAP, but few had simultaneous measurements of both emission and indoor air quality in different seasons and locations. Measurements of air exchange rate (AER) in houses in developing countries are also limited. Thus, the quantitative linkage between cookstove emission and indoor air quality is still poorly constrained. Here, we aim to improve links between estimates of cookstove emissions and indoor $PM_{2.5}$ using data collected during a cookstove intervention trial in two rural areas in India (Kullu in Himachal Pradesh State; Koppal in Karnataka State). 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. We use these data to evaluate a Monte-Carlo single box model for HAP, developed by the World Health Organization (WHO), and used to establish emission rate targets (performance tiers) for clean stoves.

In general, Kullu households had ~50% lower $PM_{2.5}$ concentration than those in Koppal, consistent with the observed higher estimated AERs and shorter cooking times in Kullu compared to Koppal. We applied multilinear regression modeling, which showed that ventilation and cooking characteristics have a large influence on indoor PM. We used the WHO model with measured emissions rates and other household characteristics (volume, AER) and compared the results to observed indoor $PM_{2.5}$ concentrations. We find that model greatly overestimates (by a factor of ~10) average kitchen concentration. Further analysis explores various factors (e.g. stove types, presence of chimney, AER, monitoring height and kitchen volume) that may affect model estimations.

13IA.2

Modeling Indoor Aerosol Dynamics during HOMEChem.

SAMEER PATEL, Sumit Sankhyan, Donghyun Rim, Atila Novoselac, Delphine K. Farmer, Marina Vance, *University of Colorado Boulder*

In the US, people spend about 90% of their time indoors, and indoor $PM_{2.5}$ exposure has been estimated to account for more than a quarter of fine particulate matter (PM) mortality burden. We conducted a field study titled HOMEChem (House Observations of Microbial and Environmental Chemistry) to comprehensively characterize the indoor chemistry of a three-bedroom, two-bathroom 110 m^2 manufactured test house while everyday activities such as cooking, cleaning, human occupancy, and opening doors and windows were performed.[1] Our previous work provided an overview of indoor concentrations of PM (~1 nm – 20 µm) observed during HOMEChem.[2]

Modeling of indoor PM emissions provides insights into PM formation rate, transport, and fate which might facilitate the development of mitigation strategies to reduce personal exposure. The present work focuses on an aerosol dynamics model including coagulation, wall depositions, and other sources and sinks of particles (4-500 nm) to (1) calculate deposition characteristic of the test house, (2) calculate activity-wise emission rates or source strength, (3) attribute PM loss to different sinks (deposition and exfiltration). We also performed a sensitivity analysis to assess the effects of house parameters on indoor concentrations, and therefore, personal exposure. Model results show coagulation and deposition as the major factors contributing to the decay of PM number concentrations. Exfiltration accounted for less than 30% of the particle losses. Sensitivity analysis results indicate that while increasing the air exchange rate (AER) reduces indoor PM mass concentration, the PM number concentration increases at higher AERs.

[1] Farmer et al. (2019), Environmental Science: Processes & Impacts, 21(8), 1280-1300.
[2] Patel et al. (2020), Environmental Science & Technology, 54, 7107-7116.

13IA.3

Modeling Indoor Aerosol Inorganic Thermodynamics with ISORROPIA.

BRYAN BERMAN, Bryan Cummings, Anita Avery, Shannon Capps, Peter F. DeCarlo, Michael Waring, *Drexel University*

Many indoor aerosols originate from the outdoor environment. However, certain aerosol components may be physically or chemically processed upon transport from outdoors to indoors. For instance, temperature and relative humidity (RH) gradients between the indoors and outdoors may influence the repartitioning of certain aerosol components. Cummings and Waring (2019) developed a model that simulates indoor organic aerosol (OA) concentration, composition, partitioning behavior, and secondary formation. We expand this model to predict inorganic aerosol (IA) repartitioning by integrating the thermodynamic model, ISORROPIA, which predicts concentrations of various inorganic species in the aerosol and gas phases at chemical equilibrium. To our knowledge, this is the first instance of applying ISORROPIA in an indoor model to simulate indoor IA thermodynamics. Specifically, we modeled inorganic concentrations and compared them to indoor aerosol concentration measurements from aerosol mass spectrometer (AMS) data obtained by Avery et al. (2019). To evaluate the model, sulfate normalized indoor-to-outdoor concentration ratios, which may be used to distinguish repartitioning losses from physical loss mechanisms, were computed for inorganic NO3 ($[I/O]_{NO3/SO4}$) across the simulation set. Our simulated $[I/O]_{NO3/SO4}$ were then compared to observed data from Avery et al. (2019). Both exhibited qualitatively similar exponentially decaying curves with respect to the indoor-outdoor temperature difference, ΔT. The simulated $[I/O]_{NO3/SO4}$ were heavily influenced by ammonia concentrations. However, the exponential trends of both were in agreement when sufficient indoor ammonia sources were modelled, from both human occupants and surface reservoirs. This model evaluation serves as a proof of concept towards modeling chemical processes of inorganic aerosols and gases at key points in a heating, ventilating, and air-conditioning (HVAC) system, in the summer and winter, with ISORROPIA. Therefore, future work will involve exploring how HVAC systems influence indoor aerosol composition and chemical processing, with a focus on indoor aerosols of outdoor origin.

13VC.1

Secondary Organic Aerosol Yields from the Oxidation of Benzyl Alcohol.

SOPHIA CHARAN, Reina Buenconsejo, John Seinfeld, *California Institute of Technology*

Benzyl alcohol is a widely used compound in consumer products that can be found in soaps, inks, paints, and, consequently, indoor and outdoor air. Experimental and computationally simulated environmental data from chamber experiments of benzyl alcohol and OH provide an understanding of aerosol yield and chemistry under relevant urban conditions (5–200 ppb NO and 291–312 K) and give insight into the effect of volatile chemical products on the production of secondary organic aerosol (SOA). This research especially considers the physicochemical processes occurring in environmental chambers; in particular, the loss of particles and vapors to the chamber walls is accounted for. Analysis of the measured yield as a function of initial seed surface area concentration shows a clear seed surface area effect. Benzyl alcohol is found to have a large SOA formation potential; at NO concentrations of ~80 ppb and 291 K, SOA mass yields for benzyl alcohol can reach 1. This is much larger than previously predicted. Time-resolved SOA yields are presented as a function of temperature and NO_x concentration. The SOA yield decreases with rising temperatures, and the aerosol formed at lower temperatures is more oxygenated and may contain fewer organonitrates. As the NO mixing ratio increases, the SOA yield decreases due to differing aerosol formation pathways. This study of benzyl alcohol indicates that SOA yields for similar volatile chemical products could be even larger than previously predicted.

13VC.2

Formation of Highly Oxygenated Molecules and Nitro Aromatic Compounds from the Oxidation of Benzyl Alcohol. MOHAMMED JAOUI, Havala Pye, Karl Seltzer, Kenneth S. Docherty, Michael Lewandowski, David R. Cocker III, Sophia Charan, Reina Buenconsejo, John Seinfeld, Tadeusz Kleindienst, *U.S. Environmental Protection Agency*

Detailed chemical analysis of Secondary Organic Aerosol (SOA) produced in a 14.5 m3 chamber from the photooxidation of benzyl alcohol (BnOH) in the presence of NOx, and H2O2 was carried-out in this study. BnOH is a constituent of volatile chemical products (VCPs) and commonly used as a solvent for inks, paints and coatings and in a wide variety of personal care products, foods, beverages, and pharmaceutical industries. VCPs have become a dominant source of organic emissions in urban settings due to a significant decrease of NMVOC emissions from the mobile sector. Gas phase species and SOA collected on denuders and glass-fiber filters respectively were solvent extracted, derivatized using BSTFA, and GC-MS analyzed. GC-MS analysis showed the occurrence of more than 60 and 20 oxygenated compounds in SOA and gas phase, respectively. Highly oxygenated molecules (HOMs) and nitro aromatic compounds (NACs) were among the main reaction products identified in SOA and/or the gas phase. SOA associated with the BnOH/NOx system was yellow to light brown compared to those generated from BnOH/H2O2 system consistent with the presence of NACs in the BnOH/NOx system. Six NACs were identified including 3-nitrobenzyl alcohol, 4-nitrocatechol, and 2-hydroxy-5-nitrobenzyl alcohol. Three isomeric HOM products were identified in SOA including tartaric acid, 2,3,5-trihydroxy-4-oxo pentanoic acid, and pentaric acid belonging to three groups with the general chemical formula C4H6O6 (3 isomers); C5H8O6 (8 isomers); and C5H8O6 (4 isomers), respectively. SOA yields, OM/OC ratio are presented in this study. Proposed reaction schemes are provided for selected HOMs and NACs products. H-abstraction from the CH2 group leads to the formation of benzyl aldehyde and OH radical addition to the ipso and ortho positions of the aromatic ring leads mainly to the formation of 5-hydroxy-4-oxo-2-pentenal, proposed in this study as the main precursor to BnOH HOMs. Small carbonyls (aldehydes and ketones) in the gas-phase have been examined as their 2,4-dinitrophenylhydrazones derivatives using a HPLC method.

13VC.3

Low Secondary Organic Aerosol Production from Oxygenated Volatile Chemical Products. MACKENZIE HUMES, Mingyi Wang, Sunhye Kim, Jo Machesky, Drew Gentner, Neil Donahue, Albert Presto, *Carnegie Mellon University*

Traditional anthropogenic Secondary Organic Aerosol (SOA) research has focused on various combustion sources, including emissions from factories, vehicles, and biomass burning. Emissions of Volatile Chemical Products (VCP) and Intermediate Volatility Chemical Products (IVCP) such as cleaning solvents, pesticides, coatings, and personal care products are now larger than emissions from more traditional sources, in part because of control measures on those sources and in part due to their near unity emission factors. Current models under-predict SOA formation and the oxidation products of I/VCPs are likely an overlooked source. These include various I/VCPs containing oxygen groups such as glycol ethers, esters, and oxygenated aromatics, whose SOA formation potential are poorly understood. I/VCPs containing oxygen groups may have a greater probability of undergoing fragmentation and inhibiting intramolecular hydrogen shifts when oxidized, resulting in less polar, lower molecular weight products. As the volatility is inversely dependent on molecular weight and polarity, the addition of these groups may prevent SOA formation. In this study, we observed the oxidation of common I/VCPs containing oxygen groups under high and low NOx conditions to determine their potential as SOA precursors.

We oxidized four glycol ether I/VCPs, two oxygenated aromatic VCPs, and two ester VCPs using an Oxidation Flow Reactor (OFR) at 50% RH with and without the presence of NOx. We measured SOA concentration and composition using an AMS and SMPS and gas phase I/VCPs and products using PTR-MS and iodide CIMS. All non-aromatic species had SOA yields of zero. The two aromatic ring-containing compounds: 2-phenoxyethanol and 1-phenoxy-2-propanol had SOA yields of approximately 15%. This supports the idea that oxygen groups can inhibit SOA formation and that some oxygenated VCPs may be used in consumer products without making SOA.

14AC.1

Secondary Organic Aerosol Formation from the Oxidation of Camphene.

QI LI, Jia Jiang, Isaac Afreh, Kelley Barsanti, David R. Cocker III, *University of California, Riverside*

Camphene is one of the dominant monoterpenes measured from biogenic and biomass burning (BB) emissions. However, camphene has not been well-studied in smog chambers and very little is known about its potential to form secondary organic aerosol (SOA). 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. In this study, a series of conventional environmental chamber experiments were performed in the UCR environmental chamber to explore camphene SOA yields and properties under atmospherically-relevant conditions. Camphene SOA yields of up to 27% were measured under no/extremely low NOx conditions. Experiments performed in the presence of NOx resulted in completely different SOA formation in terms of SOA yield and particle size distribution, possibly indicating different reaction pathways. At 300k, in the presence of 100ppb of NOx and 1 ppm of H_2O_2, an SOA mass yield of 70% was measured, in contrast to only 27% under low/no NOx conditions and 10%-40% of typical SOA yield of α-pinene. In addition, oxidation reactions in the presence of NOx formed much larger particles (dp>600nm) than formed without NOx (100-200nm) in the same amount of time. To further advance the understanding of camphene and improve representation in air quality models, chamber results were compared with simulations using two box models, GECKO-A and SAPRC. The chamber experimental results and box modeling simulations will be presented, along with parameterizations for use in air quality models.

14AC.2

Chemical Mechanism of Atmospheric Oxidation of Benzyl Alcohol.

REINA BUENCONSEJO, Sophia Charan, Paul Wennberg, John Seinfeld, *California Institute of Technology*

Recent work indicates the growing importance of volatile chemical products (VCPs), particularly as air pollution regulations drive down the contribution of vehicular-based emissions. This work presents the chemical mechanism of benzyl alcohol, a VCP used in consumer care products and as a solvent in manufacturing processes. Specifically, this work identifies the primary oxidation products from benzyl alcohol reaction with hydroxy radicals and elucidates the pathway to secondary organic aerosol (SOA) formation using both laboratory studies and Master Chemical Mechanism (MCM) data. Benzyl alcohol oxidizes to form hydroxybenzyl alcohol via addition of OH to the aromatic ring, and benzaldehyde via hydrogen abstraction from the -CH2OH group. Experiments are conducted over a range of NO mixing ratios in order to probe the role of NO in the oxidation mechanism. This work also quantifies the contribution of each pathway (hydroxybenzyl alcohol versus benzaldehyde) to SOA formation.

14AC.3

Bimodal Size Distribution in Secondary Organic Aerosol Formed via Sequential Ozone and Nitrate Oxidation of Catechol.

LAUREN A. GAROFALO, Matson A. Pothier, Carley D. Fredrickson, Brett Palm, Joel A. Thornton, John Orlando, Xuan Zhang, Delphine K. Farmer, *Colorado State University*

The condensation of secondary organic aerosol (SOA) onto existing aerosol has profound effects not only on the chemical composition, but also on the size distribution, of the aerosol. Changes in chemical and physical properties can, in turn, alter how the aerosol interacts with the atmosphere including radiative and air quality effects. Catechol, an oxygenated aromatic that is directly emitted from wildfires as well as produced in wildfire smoke undergoes oxidation reactions with O_3, OH and NO_3 radical to form SOA; oxidation via NO_3 or OH in the presence of NO_x yields nitrocatechol – a nitrogen-containing chromophore that can drastically change the optical properties of the aerosol. In the chamber study reported here, we investigate the SOA production of catechol with various oxidants in the presence of ammonium sulfate seed. In the experiment in which catechol was first exposed to ozone and subsequently to NO_3, we observe a bimodal size distribution where an organic aerosol (OA) mode appears independent of the size mode for the existing OA from ozone oxidation and that of the seed aerosol. This behavior was only observed for this sequential oxidation scheme and not for oxidation of catechol by OH/NO_x. We describe possible quasi-equilibrium and non-equilibrium effects that may cause a size distribution to diverge from the size distribution expected by equilibrium growth.

14CC.1

In-situ Physical and Chemical Characterization of Cloud Droplet Residuals, Interstitial, and Background Aerosol Particles During the HI-SCALE Field Campaign.

GEORGES SALIBA, Alla Zelenyuk, David Bell, Kaitlyn J. Suski, John Shilling, Fan Mei, Gourihar Kulkarni, Jian Wang, Jason Tomlinson, Jerome Fast, *Pacific Northwest National Laboratory*

Shallow cumulus clouds are an important part of the Earth’s radiative budget with radiative cooling forcing on the order of tens of W/m2. However, shallow cumulus clouds are an important source of uncertainty in most climate models because these clouds have length scale that are smaller than grids cell size and their representation in climate models often rely on parameterizations. Some geographic regions, like the southern Great Plains, are an ideal place to study land-atmosphere interactions that significantly affect the shallow cumulus clouds formation and lifetime because of strong gradients in soil type and moisture, biogenic and anthropogenic emissions, as well as frequent new particle formation events. Here, we present results from the Holistic Interactions of Shallow Clouds, Aerosols and Land Ecosystems (HI-SCALE) field campaign at the U.S. Department of Energy’s Atmospheric Radiation Measurements (ARM) Climate Research Facility’s Southern Great Plains (SGP) site in Oklahoma. Measurements were conducted during the spring and summer seasons of 2016, when strong surface heating induces intense turbulence and higher biogenic fluxes of organic vapor precursors. Airborne measurements onboard the ARM Aerial Facility’s Gulfstream 1 (G-1) included particle number size distributions of background, interstitial, and cloud droplet residuals aerosol particles between 0.01 and 10 µm dry diameter and chemical composition of submicron bulk (using an Aerosol Mass Spectrometer, AMS) and individual aerosol particles (using PNNL’s single particle mass spectrometer, miniSPLAT), cloud condensation nuclei (CCN) concentrations, and cloud droplet concentrations. We will present a detailed comparison between the size distributions, densities, and size-dependent mixing state of aerosol sampled below cloud, cloud droplet residuals, and interstitial particles to understand the effect of particle physicochemical properties on their CCN activity and examine the effect of cloud processing and aqueous chemistry on size and composition of cloud droplet residuals. In addition, we will explore the variability in droplet and particle number concentrations, aerosol size, and chemical composition, which can alter in-cloud maximum supersaturations, to understand the large observed variability in the fraction of activated cloud droplets during the HI-SCALE campaign.

14CC.2

Linking Upwind Marine Biological and Meteorological Processes to Local Marine Particle Concentrations With Flexpart. KEVIN SANCHEZ, Bo Zhang, Hongyu Liu, Michael Shook, Ewan Crosbie, Luke Ziemba, Matthew Brown, Claire Robinson, Taylor Shingler, Kenneth Thornhill, Edward Winstead, Bruce Anderson, Chris Hostetler, Georges Saliba, Chia-Li Chen, Savannah Lewis, Lynn Russell, Michael Behrenfeld, Richard Moore, *NASA*

Marine biogenic particles contribute to cloud condensation nuclei (CCN) concentrations and hence cloud optical properties. Correlations between local marine biological processes and marine particle concentrations are often observed to be weak in published studies. In this study, several satellite measured and model simulated ocean biological quantities were analyzed along air parcel backtrajectories derived from FLEXPART, a Lagrangian particle dispersion model, to identify links between upstream marine biological variables, representative of the marine biomass, to shipboard measurements of particle concentrations and composition. Similarly, meteorological variables associated with particle sources and sinks were analyzed along these FLEXPART trajectories to identify the contribution of physical meteorological processes to particle measurements and further deconvolute the parcel hysteresis effect on measured marine particle concentrations. This analysis uses data from the North Atlantic Aerosols and Marine Ecosystems Study (NAAMES), which was conducted to better understand the effect of marine biological processes on marine particle concentrations. NAAMES consisted of four combined ship and aircraft field campaigns, between November 2015 and April 2018 that aligned with changes to the annual phytoplankton bloom cycle. This study is ideal for examining differences in seasonal marine biogenic contributions to particle concentration and composition. Results indicate phytoplankton net primary production correlated with organic aerosol mass, and down welling shortwave forcing correlated with both organic and sulfate aerosol mass when averaging over two day FLEXPART trajectories. In addition, wind speed negatively correlates with aerosol mass and number over five day trajectories. Observed wind speed enhance primary marine emissions and enhance total particle surface area. This suggest upstream wind speed may influence measured particle mass and concentration by enhancing total particle surface area, leading to increased scavenging of volatile compounds, decreasing the potential of smaller particle growth and new particle formation.

14CC.3

Analysis of CCN Number, Hygroscopicity, and Droplet Activation in the Western Pacific Measured during CAMP2Ex. MICHAEL BATTAGLIA JR., Athanasios Nenes, Rodney J. Weber, *Georgia Institute of Technology*

As part of the NASA CAMP2Ex field campaign, we observed cloud condensation nuclei (CCN) spectra between 0.1 and 0.6% supersaturation onboard the NASA P-3B research aircraft during seven research flights over the Pacific Ocean originating from Clark Freeport in the Philippines. The CCN spectra were measured with a Droplet Measurement Technologies CCN-100 continuous-flow streamwise thermal gradient chamber (CFSTGC) operating at Scanning Flow CCN Analysis mode (SFCA) at 500 mbar pressure. Combination of the CCN spectra and submicron aerosol size distributions from the fast integrated mobility spectrometer (FIMS) are used to obtain size-resolved CCN hygroscopicity - which are also compared against bulk hygroscopicity calculated with aerosol mass spectrometer (AMS) data. During periods of high sulfate fraction, the data is used as an in-flight calibration.

The hygroscopicity and aerosol observations, together with the observed distributions of updraft velocity are used as inputs to a cloud droplet parameterization to investigate the levels of cloud supersaturation values that would develop in clouds. From these simulations we also determine the degree to which clouds respond to aerosol perturbations, and quantitatively determine the contribution of aerosol and vertical velocity variability to the droplet number variability. Finally, we related our results to a growing body of studies focused on the drivers of droplet variability in the eastern Mediterranean, South Atlantic Ocean and southeastern United States.

14HA.1

Comparing the Toxicity and Composition of Particulate in Multiple Canadian Air Zones. DANA UMBRIO, Alison Traub, Cheol H. Jeong, Scott Weichenthal, Hongyu You, Ryan Kulka, Greg J. Evans, *SOCAAR, University of Toronto*

Exposure to ambient fine particulate matter ($PM_{2.5}$) has been linked to adverse respiratory and cardiovascular health outcomes. In Canada, $PM_{2.5}$ is regulated by its mass concentration, but this does not adequately capture how differences in its composition or origins may influence associated health risks. $PM_{2.5}$ is postulated to initiate some adverse health-effects by generating reactive oxygen species when inhaled, which leads to oxidative stress and inflammatory responses. Oxidative potential (OP) and oxidative burden (OB) are thus being explored as more health-relevant metrics for assessing the risk of particulate matter. These metrics have already been shown to be associated with a range of health outcomes. Moreover, correlations with different metals have also been reported, although the findings are often conflicting, and thus not readily generalizable across locations or airshed.

Approximately 1000 samples, collected from June 2016 until December 2018 in forty cities across Canada, were analyzed using three standardized acellular assays: ascorbate (AA), glutathione (GSH) and dithiothreitol (DTT). These assays measured the rate of depletion of AA, GSH and DTT when exposed to $PM_{2.5}$ samples. Linear and multilinear correlation analyses were used to evaluate how $PM_{2.5}$ metal composition influenced OP and OB and how these relationships differed in six air zones across Canada. Moreover, cluster analysis was applied to classify the metals into source-related groups and identify marker metals. These findings will be discussed in terms of how the associations of OP and OB with composition and sources can be generalised across a large geographic area.

14HA.2

Effect of Biomass Burning, Firework Emissions, and Haze Events on the Oxidative Potential of Ambient Particulate Matter in Delhi, India. JOSEPH V PUTHUSSERY, Ashutosh Shukla, Jay Dave, Sreenivas Gaddamidi, Atinder Singh, Dilip Ganguly, Neeraj Rastogi, Sachchida N. Tripathi, Vishal Verma, *University of Illinois Urbana-Champaign*

Delhi, the capital of India, has the worst air quality among all major megacities in the world. Delhi experiences annual daily peaks of fine particulate matter ($PM_{2.5}$) concentrations in the months of October - January, because of the various episodic events [biomass burning (BB), Diwali fireworks and the frequent haze events] which occur during this period. This increase in the $PM_{2.5}$ mass concertation is expected to have an extremely adverse impact on the local and regional public health. Recent studies have shown that the oxidative potential (OP) of $PM_{2.5}$ is a promising health metric over mass concentrations to estimate the $PM_{2.5}$ toxicity.

In this study, we investigated the effect of BB emissions, fireworks emissions, and haze events on the OP [based on a dithiothreitol (DTT) assay] of ambient $PM_{2.5}$. We sampled ambient $PM_{2.5}$ at Delhi intermittently from October 11, 2019, to January 8, 2020 (~50 days). We used an automated OP measuring instrument, which was recently developed in our lab, to measure the hourly averaged real-time OP of ambient $PM_{2.5}$. The chemical composition of $PM_{2.5}$ was also measured using various collocated online instruments such as high-resolution time-of-flight aerosol mass spectrometer, aethalometer, and Xact® (total metals). Preliminary results showed extremely elevated ambient $PM_{2.5}$ OP on the night of Diwali and during haze events, reaching up to 13 nmol/min/m^3, which is among the highest reported DTT activity at any site in the world. We are currently combining the OP data with the chemical composition to perform source apportionment modeling, which is aimed to quantify the relative contribution of each of these episodic events on the $PM_{2.5}$ OP. The results from this study would assist epidemiologists in quantifying the health risks associated with short term exposure to $PM_{2.5}$ derived from these episodic events.

14HA.3

Spatiotemporal Variability and Source Apportionment of Oxidative Potential Associated with Water-soluble PM2.5 in the Midwest United States.

HAORAN YU, Joseph V Puthussery, Yixiang Wang, Yicen Liu, Vishal Verma, *University of Illinois Urbana-Champaign*

Oxidative potential (OP) of ambient $PM_{2.5}$ has been linked with numerous adverse health outcomes in humans. Multiple chemical endpoints have been developed to evaluate the OP of $PM_{2.5}$, while different endpoints showing different mechanisms of aerosol catalyzed ROS generation. To investigate the comprehensive redox properties of ambient particles, we used five commonly used OP endpoints [ascorbic acid (AA) and glutathione (GSH) consumption in surrogate lung fluid (SLF), dithiothreitol (DTT) consumption and •OH generation in SLF and DTT]. We collected 72 h integrated $PM_{2.5}$ samples weekly from five sites in the Midwest US (including Illinois, Indiana and Missouri) during May 2018 – May 2019. A semi-automated multi-endpoint ROS activity analyzer (SAMERA), which was recently developed in our lab, was used to analyze all the samples. We also measured the chemical composition of these samples, including carbonaceous species [i.e. elemental carbon (EC), organic carbon (OC) and water-soluble organic carbon (WSOC)], inorganic ions (nitrate, sulfate and ammonium) and thirteen metals. Spatial profiles of the OP were analyzed by calculating coefficient of divergences (CoD) between different site pairs. We also investigated the correlations between various chemical components and OP for different sites and seasons. Preliminary results showed that OP was highest during the summer season at all the sites. Significant correlations were found between multiple OP endpoints and transition metals (i.e. Cu, Fe and Mn) during summer at most of the sites, while the correlation with WSOC was more significant during winter at all the sites. The source apportionment modeling by positive matrix factorization (PMF) is currently underway, which will lead us to identify the emission sources contributing to different OP endpoints. Our study provides the first large-scale development of spatiotemporal profiles of OP, involving almost all possible modes of chemical ROS generation, and investigating their sources in the Midwestern United States.

14SA.1

Investigations of the Spatial and Temporal Variations in Organic Aerosol Sources within Europe Using 24 Long-term ACSM Datasets.

GANG CHEN, MariCruz Minguillon, André S.H. Prévôt, Team COLOSSAL, *Paul Scherrer Institute*

Atmospheric aerosol is a suspension of liquid or solid particles in gas, which not only causes serious adverse health effects but can also reduce visibility and interact with ecosystems and climate. Organic aerosol (OA) has been identified as one of the major components of air pollution, representing 20 to 90% of the total submicron aerosol mass. However, the spatial/temporal variabilities of OA sources remain poorly characterized in Europe. Europe has a well-established air quality monitoring infrastructure with >50 Aerosol Chemical Speciation Monitors, ACSMs (Aerodyne Research Inc., MA, USA) in operation. Among these sites, 24 datasets have long-term (>1 year) measurements since 2016. In this study, we performed source apportionment (SA) applying Positive Matrix Factorization (PMF) analysis using some novel techniques within SoFi Pro (Datalystica Ltd., Villigen, Switzerland), including rolling mechanism, a-value approach, bootstrap re-sampling, criteria-based selection, and uncertainty assessments. Ultimately, by following a standardized SA protocol, this work will compile and assess an updated, robust, stable, and accurate overview of OA sources/types with extensive spatial and temporal variability across Europe.

This study aims at being beneficial for policymakers to optimize air quality mitigation strategies, and to assess the effectiveness of already implemented policies. In addition, it will provide sound constraints to regional and global climate or air quality models to improve their precision and accuracy.

This work has been mainly supported by the COST Action CA16109 Chemical On-Line cOmpoSition and Source Apportionment of fine aerosoL (COLOSSAL), the related SNSF International Co-operation project SAMSAM (IZCOZ0_177063), and the Aerosol, Clouds and Trace gases Research Infrastructure (ACTRIS).

14SA.3

Dispersion Normalized PMF Provides Insights into the Significant Changes in Source Contributions to Atmospheric Particulate Matter after the COVID-19 Outbreak. Qili Dai, Yinchang Feng, PHILIP K. HOPKE, *Nankai University*

An effective source apportionment tool, factor analysis, utilizes the covariance of compositional variables to separate sources of ambient pollutants like particulate matter (PM). In addition to the variations in source emission rates, meteorology provides another important source of variation through transport and dilution. Conventional positive matrix factorization (PMF) loses information in the observation data due to variations in dilution. To reduce the influence of dilution, dispersion normalized PMF (DN-PMF) is proposed to incorporate the ventilation coefficient into the PMF analysis. This approach has been applied to hourly speciated particulate data measured at a suburban location in a field campaign that included the COVID-19 outbreak. Compared to standard PMF, the results from DN-PMF increased the morning peaks of coal combustion, and traffic rush hour peak of traffic emissions, lowered the daytime peak of soil and aged sea salt and a point source of waste incinerator. It is provided more subtlety defined source directionality. DN-PMF enhanced the local influence of coal combustion, traffic emissions and incinerator, and highlighted the regional transport nature of soil and aged sea salt. The enhanced emission patterns indicated that the DN-PMF is a useful addition to current source apportionment methods. This work also highlights the significant changes in source contributions after the outbreak of COVID-19. During this unprecedented pandemic, secondary inorganic aerosol (SIA) was the predominant source of PM2.5, with averaged mass contribution of 50.5% that formed via gaseous precursors mostly emission from coal combustion, followed by firework emissions (32.0%), primary emission of coal combustion (13.3%), primary traffic emissions (2.1%), soil and aged sea salt (1.2%) and incinerator (0.9%). The traffic contribution has decreased dramatically (70%) compared to other sources. Soil and aged sea salt contributions decreased by 68%, also likely related to decreased traffic volume.

14UA.1

Reduced Traffic Volumes and Air Quality during the COVID-19 Shutdown. CHEOL H. JEONG, Nathan Hilker, Taylor Edwards, Jon M. Wang, Jerzy Debosz, Yushan Su, Anthony Munoz, Dennis Herod, Greg J. Evans, *SOCAAR, University of Toronto*

The COVID-19 shutdown is providing an unprecedented natural experiment to explore the impact of markedly reduced sources of pollution on air quality. Analysis of traffic volumes during the shutdown allows a greater understanding of improved air quality due to reduced vehicular emissions. In addition to the change in total traffic volume, the fleet composition can also be analyzed to elucidate the influence of the fleet composition of gasoline and diesel vehicles on traffic-relate air pollutants (TRAPs). However, understanding the influences of local and regional sources is challenging due to the temporal and spatial variabilities of TRAP and potential confounding factors in determining the change of air quality. Thus, a comprehensive analysis is necessary to properly assess the impact of the shutdown on urban air quality.

In this study, continuous air pollution data from February to June in 2017-2020 at two near-road sites (NR) located near Highway 401 and downtown in Toronto, Ontario, Canada were used to compare the levels of TRAP pre-, during, and post-shutdown. Urban background (BG) concentrations were obtained from two other sites in Toronto. The TRAPs measured include: nitrogen oxides, carbon monoxide, black carbon, ultrafine particles, and PM2.5. Hourly concentrations of organic and inorganic aerosol and trace elements were also determined using an Aerosol Chemical Speciation Monitor (ACSM, Aerodyne) and Xact metals monitor (Cooper Environ), respectively, at the downtown site. The number, length, and speed of motor vehicles measured at the NR sites were measured to identify the changes to the proportion of gasoline passenger cars and diesel trucks within the fleet.

Urban background concentrations were estimated through baseline subtraction using a spline of minima approach. Regional contributions thereby estimated were compared to data from the BG sites which are representative of regional air quality superimposed with city-wide emissions. Receptor modeling was performed to assess the change of local and regional scale PM2.5 sources using continuous organics, inorganic ions, and trace elements at the downtown NR site. Moreover, the changes observed in 2020 were compared with data from February to June 2017-2019, to estimate an excess change in 2020 due to the shutdown. Finally, the changes in TRAP concentrations were compared to the changes in total traffic volume and fleet composition to resolve how changes to the mix of gasoline and diesel vehicles influence TRAP. This study can help support the development of more specific policies and regulations to reduce local air pollution effectively.

14UA.2

Influence of the COVID-19 Lockdown on Delhi's Air Quality. KANAN PATEL, Mark Campmier, Sahil Bhandari, Nisar Ali Baig, Gazala Habib, Joshua Apte, Lea Hildebrandt Ruiz, *University of Texas at Austin*

To reduce the spread of COVID-19, a nationwide lockdown was implemented in India from Mar 24-May 31, 2020. Here, we assess the impacts of this lockdown on ambient air quality in Delhi, building on nearly four years of ongoing measurements of non-refractory submicron aerosol (NR-PM_1) composition using an aerosol chemical speciation monitor and black carbon (BC) via an aethalometer from the Delhi Aerosol Supersite (DAS). We obtained additional pollutant data ($PM_{2.5}$, CO, NO_x, O_3, SO_2) from the regulatory monitoring sites across the city.

Average NR-PM_1 dropped sharply (~40%) at the outset of the lockdown, assessed based on comparing multi-week periods before and after Mar-24. While the lockdown likely had a role to play, meteorology was also an important factor considering the influence of unseasonable precipitation around the initial period of the lockdown, as well as the usual seasonal increase in ventilation and temperature in the spring/summer period. Considering the full lockdown period, the bulk NR-PM_1 concentration was strikingly similar to the previous three years, with only modest changes in the lockdown period compared to prior years. The largest difference relative to prior years was a ~two-fold reduction in particulate sulfate. Relative to prior years, we also observed large reductions in BC, CO, and NO_x, and increases in O_3, likely because of sharp reductions in traffic emissions.

Positive matrix factorization (PMF) of the organic aerosol (OA) mass spectra resolved three factors–HOA (hydrocarbon-like-OA), OBBOA (oxidized-biomass burning-OA) and OOA (oxidized-OA). Comparing the lockdown period against pre-lockdown conditions, average HOA and OOA concentrations decreased by ~33-35% while average OBBOA remained practically unchanged, likely due to influence of regional agricultural burning in May.

Overall, our results provide valuable evidence on atmospheric aerosol dynamics in Delhi, and by inference, how future large-scale modification of activity and/or emissions might contribute to improvements in Delhi’s air quality.

14UA.3

On the Impacts of COVID-19 Pandemic on Air Quality in Florida. MARWA EL-SAYED, Yasin Elshorbany, Kirsten Koehler, *Embry-Riddle Aeronautical University*

Earlier this year, the world has faced an unprecedented pandemic caused by the novel COVID-19 virus. Although directly infecting more than 10 million and killing almost half a million people around the globe to data, this pandemic has indirectly impacted the lives of many. The shutdown associated with the pandemic has profound negative economical and social impacts. Most cities worldwide have been locked down leading to significant reduction in daily commutes, changes in transportation patterns and traffic load, as well as increases in emissions from liquefied petroleum gas due to residential uses. Even though preliminary studies show improvements in air quality in several places during the lockdown, yet this impact is not fully understood. The goal of this study is to investigate the impact of this lockdown on air quality in six major cities across the state of Florida, namely: Orlando, Miami, Tallahassee, Gainesville, Jacksonville, and Tampa. Hourly measurements of $PM_{2.5}$, ozone, NO_2, SO_2, and CO in addition to meteorological data were provided by the US EPA through six sites operated by Florida Department of Environmental Protection during mid-March to mid-April in 2020, the period in which the state was mostly shut down. The significance of the lockdown on the atmosphere is tested in Florida by comparing levels of pollutants in 2020 to average concentrations in 2015-2019 at all sites. Satellite data of the pollutants are also used to investigate regional patterns. Using these remote sensing products, the spatial distribution of atmospheric pollutants is examined to better understand the effect of transport on the levels of pollutants in Florida. The impact of the pandemic on human exposure is also presented. Results herein provide insight into the soures of atmospheric pollutants and their significance in the state of Florida.

14VC.1

Asphalt-related Emissions are a Large Urban Source of Secondary Organic Aerosol Precursors. DREW GENTNER, Peeyush Khare, Jo Machesky, Megan He, Ricardo Soto, Albert Presto, Andrew Lambe, Jordan Krechmer, Manjula Canagaratna, *Yale University*

Recent studies show that non-traditional emissions (e.g. volatile chemical products; VCPs) are becoming dominant contributors of reactive organic gases in developed megacities. Asphalt is a heavily used, non-combustion-related source of gas-phase precursors to urban secondary organic aerosol (SOA). Yet, its emissions are largely absent from inventories due to their complex mixture of predominantly intermediate- and semi-volatile organic compounds (IVOCs, SVOCs), which emit over long timescales (e.g. days to weeks), are not present in the "product formulation", and also closely resemble motor vehicle emissions. We constrained their emissions via a combination of laboratory tests of commonly used PG 64-22 road asphalt and roofing materials under environmentally-relevant thermal, solar irradiation and ozone stresses, and supplement these observations with multi-city field measurements. To further investigate the SOA formation potential, we oxidized asphalt-related emissions in a potential aerosol mass (PAM) reactor under daytime and nighttime conditions and measured the SOA formation and chemical composition using an aerosol mass spectrometer (AMS), a scanning mobility particle sizer (SMPS), and a high-resolution proton transfer reaction time-of-flight mass spectrometer (PTR-TOF).

We report emission factors for total emissions and their distribution of aliphatic, aromatic, and sulfur/oxygen-functionalized compounds as a function of typical temperatures for asphalt while in-use, storage, and during paving. We also evaluate changes over time and provide the most detailed chemical speciation of asphalt-related emissions to date using both a high-resolution atmospheric pressure chemical ionization quadrupole time-of-flight mass spectrometer (APCI-QTOF) and a vacuum electron ionization mass spectrometer (EI-MS) coupled to a gas chromatograph. Together, this combination of laboratory emission experiments, oxidation experiments, and field measurements demonstrate that asphalt is a major non-combustion source of reactive intermediate- and semi-volatile SOA precursors with significant implications for urban air quality.

14VC.2

Improving the Representation of Secondary Organic Aerosol from VCP Sources in Air Quality Models. SREEJITH SASIDHARAN, Qi Li, David R. Cocker III, Mackenzie Humes, Albert Presto, Neil Donahue, Jo Machesky, Drew Gentner, Jeffrey R. Pierce, Shantanu Jathar, *Colorado State University*

Volatile chemical products (VCPs) that include consumer products, pesticides, paints, and surface coatings are emerging as dominant sources of volatile organic compounds (VOCs) to the urban atmosphere. These VCP VOCs can oxidize in the atmosphere to form secondary organic aerosol (SOA), yet there are large uncertainties surrounding the oxidation pathways that lead to SOA formation and the contribution of VCP sources to the urban SOA budget. In this work, we leverage two unique laboratory datasets and a state-of-the-science model (i.e., SOM-TOMAS) to develop parameters to represent the SOA formation from key VCP VOCs. The datasets currently represent the only chamber and flow reactor data available for SOA formation from VCP VOCs. The SOM-TOMAS (Statistical Oxidation Model-TwO Moment Aerosol Sectional) model simulates the chemistry, thermodynamic properties, and microphysics of SOA. SOA parameters were developed for several different classes (glycols, glycol ethers, esters and oxygenated aromatics) of VCP VOCs that accounted for the effects of multi-generational aging and losses of vapors to the reactor walls. A chemical scheme, based on the branching ratio of the peroxy radical, allowed for the development of a universal set of parameters that explained the SOA formation under both low and high NO_X conditions. Ongoing work is focused on box model applications that quantify the (i) SOA mass yields for VCP VOCs under atmospherically-relevant conditions and (ii) SOA formation from anthropogenic sources, including VCPs, in Los Angeles (CalNex-2010) and New York City (NYICE-2018). Future work will incorporate these parameterizations into a chemical transport model to study air quality and atmospheric chemistry in urban environments.

14VC.3

A Comprehensive Understanding of Predicted SOA Formation from Volatile Chemical Products. ELYSE PENNINGTON, Karl Seltzer, Havala Pye, Melissa Venecek, John Seinfeld, *California Institute of Technology*

Volatile chemical products (VCPs) have important implications for air quality but are not well characterized. Field studies have demonstrated the prevalence of gas-phase VCPs in urban environments, but few chamber studies have been performed to quantify their ability to form secondary organic aerosol (SOA). Structure-activity-relationships (SAR) are used to describe the properties and activities of compounds based on their chemical structure. Quantitative SAR models are useful to predict a compound's activity in the absence of empirical data. We use existing SAR models to estimate reactivity against OH and other oxidants, volatility, partitioning and heterogeneous uptake coefficients, and other parameters relevant to SOA formation. We compare the results from multiple reactivity models, partitioning mechanisms, and multigenerational aging schemes. SOA yields are estimated using published yields of structurally similar compounds. We compile the results of these simulations to present a broad level understanding of the ability of VCPs to form SOA. This model improves our understanding of the environmental fate of VCPs, specifically the impact on SOA mass and speciation. This model can be used to better represent anthropogenic SOA formation in box and regional models.

15AC.1

Automating the Search for New Pathways in Atmospheric Oxidation Chemistry. VICTORIA BARBER, Jesse Kroll, *MIT*

Understanding the routes by which secondary organic aerosol (SOA) is formed via oxidation of volatile organic compounds represents a key challenge in atmospheric chemistry. In recent years, a number of "exotic" transformations not typically found in standard atmospheric oxidation mechanisms (e.g. Peroxy radical isomerization, epoxide formation) have been shown to be important in the formation of low-volatility organic compounds and SOA. These discoveries suggest that there may be other non-traditional mechanisms that play a role in oxidative aging and aerosol formation, and point to the need for a systematic way to look for such pathways. The Reaction Mechanism Generator (RMG) is an open-source program developed for and typically applied to combustion systems. RMG uses a combination of an extensive database of known chemical information and a functional group based methodology for kinetic and thermodynamic parameter estimation to automatically develop reaction networks with very little *a priori* information. Here, we use RMG to systematize and automate the search for new mechanisms in atmospheric organic oxidation chemistry. RMG is used to generate reaction networks for the OH-intiated oxidation of a set of approximately 200 monofunctionally and bifunctionally substituted pentanes in the gas phase at atmospheric temperatures and pressures. In addition to the canonical reactions expected for organic radicals in the atmosphere, a number of "exotic" reactions are identified. These include the recently explored but historically underappreciated reaction mechanisms described above, as well as examples of novel chemistry which may impact SOA formation. The results demonstrate the utility of RMG as a tool for atmospheric reaction discovery, and provide several interesting targets for further study via quantum mechanical calculations and experiments.

15AC.2

Application of Machine Learning to Development of Atmospheric Chemical Mechanisms. YUANLONG HUANG, Weimeng Kong, John Seinfeld, *California Institute of Technology*

Atmospheric chemistry plays an important role in climate change and human health. The temporal evolution of species emitted to or formed in the atmosphere is evaluated by three-dimensional chemical transport models (CTMs) simulating simultaneous chemical reactions and transport. The number of all the species comprising atmospheric chemistry can be immense. Moreover, representing the detailed steps that proceed from initial oxidation of a volatile organic compound (VOC) with the principal oxidants, OH, O_3, or NO_3, to important products is a major challenge in atmospheric chemistry. Generally, chemical mechanisms employed in atmospheric models are limited to a few hundred species and reactions, which still can require up to 90% of the overall computational resources for solving the overall chemical transport model. This is a severe limitation on the ability to simulate atmospheric chemistry. Machine learning has been demonstrated to be successful in handling complex simulations by significantly reducing computational burdens but keeping precision. Here we explore the potential of employing machine learning in atmospheric chemical mechanisms to reproduce with fidelity the molecular routes leading from compounds emitted into the atmosphere to ultimate oxidation products, including aerosol species. Chemical reaction networks generated by machine learning offer the opportunity not only to replace existing mechanisms used in atmospheric models but also to be computationally efficient. Machine learning-derived reaction mechanisms based on the explicit atmospheric chemical mechanisms (e.g., isoprene oxidation) that have been developed in the laboratory and theoretical studies will be trained by state-of-the-art long short-term memory networks.

15AC.3

First-Generation Alkyl and Alkoxy Radical Fates Foreshadow SOA Yields from Cyclic Monoterpenes. DANIELLE C. DRAPER, Thomas Almeida, Michelia Dam, Nanna Myllys, Theo Kurten, James Smith, *University of California, Irvine*

It is widely accepted that oxidation of monoterpenes can be a significant source of secondary organic aerosol (SOA). However, numerous studies have shown that different combinations of monoterpenes and oxidants can lead to drastically different SOA yields, and this observation is still poorly understood from a mechanistic perspective. NO3 radical oxidation of cyclic monoterpenes (e.g. α-pinene , β-pinene, Δ-carene, sabinene, limonene) is one such example where reported experimental SOA yields range from 0% to >100% for different monoterpenes. Using quantum chemical calculations of unimolecular reaction kinetics, we have determined that the fate of the first-generation alkyl and/or alkoxy radical are quite different for each of these structurally similar molecules. Radical intermediates such as these can either continue propagating through additional oxidation steps or may terminate from uni- or bi-molecular chemistry. Our results show that the monoterpenes with higher observed SOA yields generate radical intermediates with readily available radical propagation pathways, whereas those with lower yields have dominant termination pathways early in the oxidation mechanism. These computational mechanisms are supported with chemical ionization mass spectrometry (CIMS) measurements during monoterpene+NO3 chamber experiments. While specifically applied to organonitrate radical intermediates in this study, this inter-monoterpene comparison provides valuable insight for mechanism development for other oxidant / monoterpene systems as well.

15CC.1

Characterization of Coarse-Mode, Iron-Containing Aerosols Transported to South America: Implications for Biogeochemical Cycles and Radiative Balance. ANNE BARKLEY, Nicole Olson, Joseph M. Prospero, Alexandre Gatineau, Kathy Panechou, Nancy Maynard, Patricia Blackwelder, Swarup China, Andrew Ault, Cassandra Gaston, *University of Miami*

The long-range transport and subsequent deposition of nutrients associated with African aerosol to South America fertilizes nutrient-depleted ecosystems, such as the Amazon and Tropical Atlantic Ocean (TAO). Quantifying the physio-chemical properties of long-range transported aerosols is important both for nutrient delivery and the radiative properties. In this work, we collected African aerosol at a coastal site on the northeast coast of the Amazon Rainforest in South America from February to March 2016. Using scanning electron microscopy (SEM) coupled to energy dispersive X-ray spectrometry (EDX), we detected a wide diversity of iron (Fe) containing, coarse-mode particles including mineral dust, freshwater diatoms (FDs), primary biological aerosol particles (PBAPs), and biomass burning aerosols. Number size distributions for FDs peaked between 7.6 and 10 µm and PBAPs peaked between 10.0 and 17.7 µm. Additionally, we show that with increasing particle size, FDs and PBAPs made up a larger percentage of particles. These findings highlight that long-range transported aerosols can be larger than predicted by gravitational settling. We also found that the FDs, likely from paleo-lakes within the Saharan, often contained inclusions of mineral dust within the holes in their frustules and were more aspherical than mineral dust particles. Using elemental mapping, we show that these FDs with mineral dust contain small “hotspots” of Fe. We propose that FDs facilitate increased nutrient transport because they are more easily kept aloft due to their large aspect ratios, light density, and high surface area-to-volume ratios. Thus, these FDs could be vectors for increased nutrient transport to the Amazon and western TAO. Our findings contribute to the growing literature that show coarse and super-coarse mode aerosol are globally important aerosols and need to be included in global biogeochemical and radiative balance models.

15CC.2

Size-dependent Impacts of Atmospheric Oxidation on Ice Nucleating Particles from Sea Spray Emissions.

PAUL DEMOTT, Thomas Hill, Kathryn Moore, Russell Perkins, Josephine Rudd, Liora Mael, Chathuri Kaluarachchi, Hansol Lee, Kathryn Mayer, Alexei Tivanski, Vicki Grassian, Kimberly Prather, *Colorado State University*

Certain particles emitted as sea spray from bubble bursting act as ice nucleating particles (INPs) via containing ice nucleation active entities as molecular components. The ocean thereby provides a source for glaciating marine supercooled clouds. Many factors impact the atmospheric lifetime of marine INPs. One factor not previously evaluated is the impact of photochemical aging. We have explored the potential for this via measurements made using wave flume production of sea spray aerosols, an oxidation flow reactor for exposing particles to atmospheric oxidation by hydroxyl radicals, two INP measurement methods, and morphological and compositional analyses of collected singe INPs. Immersion freezing ability was determined from -10 to -28ºC through droplet freezing assays of filter-collected aerosols (PM10), and at -30ºC for single INPs at PM1.5 sizes using a continuous flow diffusion chamber (CFDC). Single INPs from the CFDC were collected for analysis (and refreezing) in cold stage Atomic Force Microscopy and Raman spectroscopy systems, and for transmission electron microscopy analysis.

Any amount of aging (0.5 to 5 days equivalent) by hydroxyls led to decreases in INP concentrations by up to 50 times at a single temperature. This effect varied over the course of a laboratory phytoplankton bloom, and PM10 INPs, that dominated nascent INP emissions, suffered roughly an order of magnitude higher loss of ice nucleation activity than did PM1.5 INPs. Morphological and compositional data indicated that periods with the least oxidation impact at submicron sizes were periods dominated by organic/inorganic particles other than core-shell sea salt/organics. Alternately, core-shell particles were most associated with destruction of INPs by oxidation. Results imply a constant competition between production and destruction of marine INPs over oceans, and the size-dependent and chemical nature of this process requires elaborated study in order to be accounted for in atmospheric modeling.

15CC.3

Size-Dependent Aerosol Climate Forcing and Chemistry in the Lower Stratosphere.

DANIEL MURPHY, Karl D. Froyd, Gregory Schill, Charles Brock, Agnieszka Kupc, Christina Williamson, *NOAA ESRL*

We examine the climate forcing of aerosol particles in the lower stratosphere in the present-day stratosphere as well as the implications for volcanic or intentionally added material. Infrared absorption is more important for aerosol in the lower stratosphere than it is in the lower troposphere. Sulfuric acid particles in the background stratosphere are near the peak efficiency for cooling the Earth. Mixed tropospheric particles that make their way into the stratosphere are less efficient at climate forcing but have significant surface area for possible heterogeneous chemistry that can affect ozone. There is no optimum size for added material that simultaneously minimizes all potential side effects such as heterogeneous chemistry and reduction of direct sunlight. Sulfuric acid particles after the Mount Pinatubo eruption had relatively little surface area compared to their climate impact. Added material could easily have more impact on heterogeneous chemistry than an analogy to volcanic eruptions would suggest.

15HA.1

Chemical and Cellular Superoxide Generation by Secondary Organic Aerosols in Epithelial Lining Fluid.

TING FANG, Jinlai Wei, Jessica Monterrosa Mena, Michael Kleinman, Manabu Shiraiwa, *University of California, Irvine*

Inhaled particulate matter (PM) produces reactive oxygen species (ROS), such as superoxide radical (O_2^-), which have been implicated in the initiation and development of lung inflammation and cardiovascular diseases. PM can trigger release of superoxide in epithelial lining fluid through redox reactions or can induce macrophages to generate superoxide biologically after they phagocytize particles. However, the relative importance of the source of the PM on chemically and biologically generated ROS is poorly understood. Very little is known, especially, about the role of secondary organic aerosols (SOA) from specific sources in the generation of superoxide. In this study, SOA particles were generated from specific volatile organic compounds including isoprene, toluene, and naphthalene by hydroxyl radical oxidation using a Potential Aerosol Mass (PAM) chamber. Superoxide generation by SOA from aqueous redox chemistry was measured using an Electron Paramagnetic Resonance spectrometer coupled with a spin trapping technique. For cellular superoxide release, RAW 264.7 macrophage cells were incubated with SOA particles on 96-well cell culture plates at physiologically relevant conditions and the production of superoxide was monitored over 2 hours using a calibrated chemiluminescence assay. The total amount of O_2^- generated from macrophages was compared to that from SOA aqueous chemistry. Dose-response curves were used to compare the role of different SOA on superoxide production. Preliminary results suggest that isoprene SOA generates more superoxide compared to other types of SOA.

15HA.2

Strong Association between More-Oxidized Oxygenated Organic Aerosols (MO-OOA) with Cellular Reactive Oxygen Species Production upon Particulate Matter Exposure.

FOBANG LIU, Taekyu Joo, Gabriela Saavedra, Dong Gao, Jenna Ditto, Jean Rivera-Rios, Drew Gentner, Rodney J. Weber, Nga Lee Ng, *Georgia Institute of Technology*

Health risks associated with exposure to ambient particulate matter (PM) are a major concern around the world. Adverse PM health effects have been proposed to be linked to oxidative stress through the overproduction of reactive oxygen species (ROS). However, the associations between PM components and ROS production are not well understood, especially for organic aerosols (OA), which constitute a substantial fraction of fine PM and comprise hundreds to thousands of compounds. In this study, we collected ambient fine PM at an urban site (Jefferson Street, SEARCH network) in Atlanta, GA, during summer and winter. PM-induced cellular ROS production and oxidative potential (OP) of PM were measured. OA components were identified by high-resolution mass spectrometry (HR-ToF-MS and LC-ESI-Q-ToF). Water-soluble metals (e.g., Fe, Cu, and Mn) were also analyzed. We find a positive nonlinear correlation between cellular ROS with OP determined by two acellular assays. A strong association is observed between more-oxidized oxygenated OA (MO-OOA) and cellular ROS for both summer and winter PM. The contribution of different components to cellular ROS and OP is further evaluated by multivariate linear regression analysis. The results resolve a predominant contribution of MO-OOA to cellular ROS production, while OP could be attributed to metals (i.e., Cu and Mn), MO-OOA, less-oxidized oxygenated OA (LO-OOA), and biomass burning OA (BBOA). Our work highlights an important role of MO-OOA in cellular ROS production upon PM exposure.

15HA.3

Role of Organic Aerosol in Cardiovascular and Respiratory Disease Deaths. HAVALA PYE, Cavin Ward-Caviness, Karl Seltzer, Benjamin Murphy, K. Wyat Appel, *United States Environmental Protection Agency*

Fine particulate matter, $PM_{2.5}$, is associated with negative health outcomes including cardiovascular and respiratory disease deaths. As a result, total mass is regulated in the United States by the Clean Air Act and the National Ambient Air Quality Standards (NAAQS). Over the past few decades, the composition of $PM_{2.5}$ in the United States has undergone significant changes including a decrease in sulfate and increase in relative abundance of organic aerosol (OA). A significant fraction of this OA is formed in the atmosphere and is thus called secondary organic aerosol (SOA). SOA is produced throughout the year and is a major component of total OA even in urban locations. The shift in $PM_{2.5}$ composition towards OA, as well as advances in modeling of SOA formation pathways (e.g oxidation of monoterpenes, isoprene, and anthropogenic volatile organic compounds) allows for examination of SOA components not previously available due to the lack of robust prediction algorithms and dominance of other components. In this work, we use concentrations of $PM_{2.5}$ constituents from the Community Multiscale Air Quality (CMAQ) modeling system v5.3 (ww.epa.gov/cmaq) to examine the relationship between $PM_{2.5}$ OA components and total cardiovascular and respiratory disease deaths. Using county-level data from the Centers for Disease Control on the cardiovascular mortality rate, we model changes in mortality rates by county as a function of OA and SOA in $PM_{2.5}$ while adjusting for a broad array of relevant confounders. Results highlight the role of OA in cardiovascular and respiratory disease deaths in the 2016 United States atmosphere.

15IM.1

Ultrasonic Aerosolization of Powder Phase Materials to Generate High Concentration Aerosol. Rayhan Ahmed, Vikram Suresh, Li Li, RANGANATHAN GOPALAKRISHNAN, *The University of Memphis*

A continuous supply of high concentration aerosol is needed for many aerosol-based additive manufacturing technologies. Dispersion of powder phase materials as aerosol is attractive due to its relative simplicity to solvent based techniques and lower costs. However, generation of steady high concentration aerosol from powders is challenging due to particle-particle and particle-surface adhesion forces. Building on our prior work on using ultrasonic aerosolization to disperse dry powders (Pokharel et al. (2019). Aerosol Sci. Tech. 53(3): 321-331), we describe here improvements to increase the concentration output, stability and tunability of the device. The improved ultrasonic aerosol generator is capable of generating number concentrations $>10^7$ cm^{-3} from commercially available TiO_2 powder. Moreover, the aerosol generation method is scalable and could potentially be scaled by increasing the number of ultrasonic transducers which also increase the stability and concentration of the aerosol output. Using three ultrasonic transducers, we generate aerosol concentrations in the range of $\sim 10^7$ cm^{-3} from raw TiO_2 powder of mean primary particle size ~225 nm. Milling and heat treatment of the raw powder seem to improve the dispersibility considerably. The mass concentration of particles >0.3µm is of the order of ~ 500 mg/m^3. It is hypothesized that the superior dispersibility of the milled powder compared to raw powder is due to the coating of ultrafine particles on the surface of fine and coarse powder particles. The conclusions derived herein are supported with upper bound estimates of number concentration and size distribution of aerosols. Altogether, the described improvements may be used to the generation of high concentration aerosol ($10^7 – 10^8$ cm^{-3}) in the size range of ~0.3 – 2 µm using off the shelf parts that may cost <$3000 to assemble.

Published as Ahmed, R., V. Suresh, L. Li and R. Gopalakrishnan (2020). "Scalable generation of high concentration aerosol in the size range of 0.1–10 µm from commercial powders using ultrasonic dispersion." Powder Technology 376: 52-59.

15IM.2

Interferences on Aerosol Acidity Quantification due to Gas-phase Ammonia Uptake onto Acidic Sulfate Filter Samples.

BENJAMIN A. NAULT, Pedro Campuzano-Jost, Douglas Day, Hongyu Guo, Duseong Jo, Anne Handschy, Demetrios Pagonis, Jason Schroder, Melinda Schueneman, Bruce Anderson, Charles Brock, Michael Cubison, Jack Dibb, Glenn Diskin, Karl D. Froyd, Weiwei Hu, Agnieszka Kupc, J. Andrew Neuman, Brett Palm, Eric Scheuer, Gregory Schill, Christina Williamson, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

Measurements of the mass concentration and chemical speciation of aerosol are important to investigate their chemical and physical processing from near emission sources to the most remote regions of the atmosphere. A long-standing, common method to analyze aerosol is to collect it onto filters and to analyze the aerosol off-line; however, this method is prone to biases due to the handling and preparation of the sample. These artifacts affect the chemical composition of aerosol, which in turn affects our understanding of numerous physico-chemical processes and aerosol radiative properties. We show, using filters collected onboard the NASA DC-8 and NSF C-130 during six different aircraft campaigns, a consistent, substantial difference in ammonium mass concentration and ammonium-to-anion ratios, when comparing the aerosols collected on filters versus the Aerodyne Aerosol Mass Spectrometer (AMS). Another on-line measurement is generally in agreement with the AMS, showing the aerosol has lower ammonium-to-anion ratios than obtained by the filters. Using a simple gas uptake model with literature values for accommodation coefficients, we show that for ambient ammonia mixing ratios greater than 10 ppbv, the time scale for ammonia reacting with acidic aerosol on filter substrates is less than 30 s for typical aerosol volume distributions. Measurements of gas-phase ammonia inside the cabin of the DC-8 show ammonia mixing ratios greater than 10 ppbv (45±20 ppbv), consistent with mixing ratios observed in other indoor environments. In addition, using constraints from satellite observations of ammonia indicates that ammonium mass concentrations collected on filters are not thermodynamically possible in remote areas. This analysis provides insight into what the filters' ammonium limit-of-detection should be when the sample is prone to exposure to ammonia and that this interference is an issue for any filters (ground-based included) when the filter is exposed to ammonia for long periods.

15IM.3

Temperature Dependent Phase Separation and Ice Nucleation Studies of Model Aerosols Using Droplet Microfluidics.

PRIYATANU ROY, Cari Dutcher, *University of Minnesota*

Phase transitions in ambient aerosols are significant in prediction of their primary and secondary effects including optical properties and cloud formation in global climate models. In situ studies of the phase state is expensive and requires complex instrumentation. We present droplet microfluidic platforms for experiments on phase transitions at low temperatures liquid-liquid phase separation (LLPS) in statically trapped aerosol droplets and high-throughput temperature detection of model ice-nucleating particles. LLPS studies at temperature down to -20°C showed that for ternary aqueous droplets containing ammonium sulfate, 3-methylglutaric acid (3MGA) and water, the initial phase transition happens at a lower solute concentration at lower temperatures. Thermodynamic models for activity coefficients E-AIM and AIOMFAC were used to convert solute concentration to separation relative humidity (SRH) showing the SRH for this system was slightly higher for lower temperatures. Similar studies were performed for NaCl and 3MGA system which again showed a slight temperature dependence of the RH at which crystal growth initiated. Other organics studied did not show any significant temperature dependence of LLPS. Ice nucleation study was conducted on a platform with a controllable temperature gradient and a flow-through microfluidic channel. Snomax was used as a model ice nucleating particle (INP) freezing at <-10°C. Rapid detection of ice nucleation was attempted with polarized optics utilizing birefringence of droplets with ice crystals vs. liquid droplets, and a deep neural network using supervised learning to classify frozen vs. liquid droplets with an accuracy >99.8%. Future work would include incorporation of on-chip platinum thin film temperature sensors and investigating INPs from varied sources such as mineral dust, sea spray aerosol, agricultural emissions. These measurements will be used to predict the cloud and ice formation activity of land-based and sea spray aerosols.

15SA.1

Elucidating the Sources of Fine Particulate Matter (PM2.5) in the City of Calgary, Canada. MD. AYNUL BARI, Sharif Nawyaz, Warren Kinderzierski, *University at Albany, SUNY*

With ongoing interest and concern about the state of fine particulate air pollution in urban centers, a study was done to better elucidate fine particulate matter (PM2.5) sources in the City of Calgary, Canada. The study was carried out using available $PM_{2.5}$ speciation data for 4 years (June 2013–May 2017) at Calgary downtown. Twenty-four hour arithmetic and geometric mean concentrations of PM2.5 were low i.e., 6.7 $\mu g/m^3$ and 5.2 $\mu g/m^3$, respectively and ranged from 0.23 to 75 $\mu g/m^3$. Nine PM2.5 sources were identified using a multivariate receptor model positive matrix factorization (PMF). Secondary particulate matter including secondary organic aerosol (SOA), secondary nitrate and secondary sulfate was the largest contributor to PM2.5 (3.7 $\mu g/m^3$, 57%), consistent with results obtained in a previous source apportionment study recently completed (secondary aerosol 54%) using hourly concentrations of gaseous pollutants. Other notable sources include traffic (0.78 $\mu g/m^3$, 12%), road-salt (0.49 $\mu g/m^3$, 7.7%), biomass burning (0.43 $\mu g/m^3$, 6.7%) and soil (0.52 $\mu g/m^3$, 8.1%) with minor contributions from aluminum- and zinc-rich sources. Further work is needed to understand the origin of potential SOA and secondary sulfate precursor sources in Calgary and the surrounding region. These findings provide an improved understanding of ambient concentrations and contribution of different source emissions to $PM_{2.5}$ in Calgary and this information can aid in developing appropriate air quality management strategies for $PM_{2.5}$.

15SA.2

Long-Term Trends of Urban Activity Sources Contributing to Organic Carbon (OC) in Different Urban Areas: A Focus on the PM Emission Regulations. ABDULMALIK ALTUWAYJIRI, Milad Pirhadi, Amirhosein Mousavi, Constantinos Sioutas, *University of Southern California*

Organic carbon (OC) is extensively attributed to different adverse health outcomes. In this study, we investigated the long-term temporal variations in the sources contributing to OC in central Los Angeles (CELA) and Riverside as source and receptor sites over the 2005-2015 years, a time period during which the tailpipe emissions were stringently regulated. Concentration of different components such as OC, EC, inorganic ions, and ozone were obtained from Chemical Speciation Network database to be input to the positive matrix factorization (PMF) source apportionment model. Five factors including 1) tailpipe emissions, 2) non-tailpipe emissions, 3) biomass burning, 4) secondary organic aerosol (SOA), and 5) local industrial activities were identified for each of the years. Our results showed a decreasing trend in the absolute contribution of tailpipe emissions as well as local industrial activities to the total OC concentrations in the 2005-2015 period at both sites. The contribution of tailpipe emissions to total OC, peaking at cold season, decreased by nearly 60% at both sites, from 3.52 µg/m3 (50%) in 2005 to 1.81 µg/m3 (34%) in 2010 and 1.48 µg/m3 (32%) in 2015 in CELA , and from 3.29 µg/m3 (49%) in 2005, to 1.7 µg/m3 (32%) and 1.24 µg/m3 (34%), respectively, in 2010 and 2015 in Riverside. The SOA contributions to ambient OC showed oscillations over time at both the sampling sites. The biomass contributions were almost constant over the whole period. Furthermore, a general increasing trend in the relative contributions of non-tailpipe emissions to OC were observed in the CELA and Riverside sampling areas. This finding underpins the need for further investigation of and potential regulations on the non-tailpipe emissions in various urban areas, given the developed mitigation strategies for the tailpipe emissions over the recent years.

15SA.3

Laser Derivatized Black Carbon Nanostructure: Characterization and Tests for Identifying Emission Sources. Madhu Singh, RANDY VANDER WAL, *Penn State University*

Source identification is important to pollution receptor models that require knowledge of source contributions at receptor sites. In this study black carbon samples from known sources are imaged via transmission electron microscopy (TEM) before and after laser heat treatment. Image processing algorithms quantify nanostructure characteristics including fringe length, fringe tortuosity, fringe spacing, stacking and curvature for nascent and laser heated black carbon. These metrics collectively comprise the identification marker or "fingerprint" for black carbon particulate. Unknown samples can then be compared against information available from existing samples to identify its source or have a close estimate of what the source may be, both qualitatively and quantitatively. Quantitative comparison for identification uses statistical analyses. By this approach, laser derivatization uses the changed black carbon nanostructure post laser heat treatment to identify the particulate source.

Soot source identification by analysis of laser-annealed nanostructure is premised on black carbon particulate from different combustion sources differing in nascent nanostructure. Combustion conditions of temperature, pressure, fuel, fuel-air-ratio, fuel-air mixing are specific to each emission source and differ between sources. Thus, black carbon particulate originating from different sources will vary in chemical composition and physical nanostructure reflecting its formation conditions. With distinct nanostructure TEM imaging followed by application of image analysis algorithms can quantify nanostructure parameters. When sufficiently distinct, contrasting nanostructure can identify the black carbon origin. In black carbon where nanostructure is poorly contrasted, it can be magnified by laser annealing (derivatization) to enhance lamellae recognition and quantification. Additionally, subtle differences in chemical composition (e.g. bonding, elemental content) between black carbons also contribute to the annealing trajectory and differentiation. The term derivatization is applied stemming from analytical chemistry where derivatization is a process by which a compound is chemically changed to improve recognition or detectability. Laser derivatization is used here in a similar manner to enhance differences in black carbon nanostructure and chemistry upon laser heating. In this talk laser annealing results for differentiating black carbons from varied sources; turbo-combustor, diesel engine, wildfire along with reference carbon blacks will be shown – highlighting initial differences in chemistry and improving nanostructure recognition and differentiation.

15UA.1

Exploring Sources of Ultrafine and Nucleation Mode Particles. Alyssa Zimmerman, Markus Petters, NICHOLAS MESKHIDZE, *North Carolina State University*

Ultrafine particles with diameters less than 100 nm suspended in the air are a topic of interest in air quality and climate sciences. Sub-10 nm particles are of additional interest due to their health effects and contribution to particle growth processes. Ambient measurements were carried out at North Carolina State University in Raleigh, NC between April to June 2019 and November 2019 to May 2020 to investigate the temporal variability of size distribution and number concentration of ultrafine particles. A mobile lab was deployed between March and May 2020 to characterize the spatial distribution of sub-10 nm particle number concentration.

The three key findings, that may be important for the near ground-level particle number concentration and size distribution for a typical SE US city, will be discussed in this presentation:

1. New particle formation (NPF) and growth events, both Class A and Class B, were observed regularly (about 5 per month). Particles exhibited prolonged modal growth over 8 hr, which may indicate a regional scale nucleation event. The NPF events happen under relatively clean as well as polluted conditions (particularly Class B events).

2. The spatial patterns observed during both stationary and mobile deployments suggest that multiple temporally stable and spatially confined anthropogenic point sources are responsible for direct emissions of nucleation mode particles. These sub-10 nm sized particles dominated number concentration during periods of low planetary boundary layer height and low solar radiation. These particles were present during both the regular and the NPF days.

3. The slight reduction in ultrafine particle number concentration was observed during reduced economic activity caused by the COVID-19 pandemic. However, this reduction was within interseasonal variability and significantly smaller than a ~75% reduction in the average daily traffic.

15UA.2

Long-term Analysis to Elucidate the Origins of Ultrafine Particles in a Major City. HOSNA MOVAHHEDINIA, Nathan Hilker, Cheol H. Jeong, Greg J. Evans, *SOCAAR, University of Toronto*

Ultrafine particles are both directly emitted and produced through atmospheric processes. In this research, we explored the origins of ultrafine particles in an urban area by analyzing 15 years of particle size distribution data collected from 2006 to 2020 near a busy roadway in downtown Toronto, Canada, along with meteorological and other pollutant concentration data (NO, NO_x, SO_2, BC). These data for particle diameters in the range of 6 nm to 560 nm were measured by a Fast Mobility Particle Sizer (FMPS). We manually classified days into five categories: strong nucleation, weak nucleation, midday pollution, traffic pollution, and reference. Strong and weak nucleation days showed long (3hr ≤) or short (< 3hr) nucleation events with a daily-average particle number concentrations of $(19\pm7)\times10^3$ and $(17\pm5)\times10^3$ #/cm^3, respectively. Midday pollution days exhibited higher particle number concentrations around noon with a daily-average of $(22\pm7)\times10^3$ #/cm^3. The high number concentrations on these days appear to be associated with anthropogenic sources. The traffic pollution days ($(20\pm5)\times10^3$ #/cm^3) showed morning or afternoon traffic emissions, with no midday rise. Lastly, 46% of the days had lower particle number concentrations ($(12\pm2)\times10^3$ #/cm^3) throughout the day. Although the number concentrations were lower on these "reference days", the influence of traffic emissions was still observable in the diurnal pattern. Time series analysis of these categories shows that the occurrence frequency of midday pollution, and strong and weak nucleation days has decreased in recent years with the number of reference days correspondingly increasing. Moreover, meteorological analysis showed that midday pollution days happen more often in winter while strong nucleation days are more frequent in summer.

15UA.3

Rapid Growth of New Atmospheric Particles by Nitric Acid and Ammonia Condensation. MINGYI WANG, Weimeng Kong, Ruby Marten, Xucheng He, Dexian Chen, Joschka Pfeifer, Arto Heitto, Jenni Kontkanen, Lubna Dada, Andreas Kürten, Taina Yli-Juuti, Hanna Manninen, The CLOUD collaboration, Rainer Volkamer, Ilona Riipinen, Josef Dommen, Joachim Curtius, Urs Baltensperger, Markku Kulmala, Douglas Worsnop, Jasper Kirkby, John Seinfeld, Imad El Haddad, Richard Flagan, Neil Donahue, *Carnegie Mellon University; The CLOUD Collaboration*

New-particle formation is a major contributor to urban smog, but how it occurs in cities is often puzzling. If the growth rates of urban particles are similar to those found in cleaner environments (1–10 nm/h), then existing understanding suggests that new urban particles should be rapidly scavenged by the high concentration of pre-existing particles. Here we show, through experiments performed under atmospheric conditions in the CLOUD chamber at CERN, that below about +5 degrees Celsius, nitric acid and ammonia vapors can condense onto freshly nucleated particles as small as a few nanometres in diameter. Moreover, when it is cold enough (below −15 degrees Celsius), nitric acid and ammonia can nucleate directly to form ammonium-nitrate particles. Given that these vapors are often one thousand times more abundant than sulfuric acid, the resulting particle growth rates can be extremely high, reaching well above 100 nm/h. However, these high growth rates require the gas-particle ammonium-nitrate system to be out of equilibrium to sustain gas-phase supersaturations. In view of the strong temperature dependence that we measure for the gas-phase supersaturations, we expect such transient conditions to occur in inhomogeneous urban settings, especially in wintertime, driven by vertical mixing and by strong local sources such as traffic. Even though rapid growth from nitric acid and ammonia condensation may last for only a few minutes, it is nonetheless fast enough to shepherd new particles through the smallest size range where they are most vulnerable to scavenging loss, thus greatly increasing their survival probability. We also expect nitric acid and ammonia nucleation and rapid growth to be important in the relatively clean and cold upper free troposphere, where ammonia can be convected from the continental boundary layer and nitric acid is abundant from electrical storms.

16CA.1

Long-Term Trends of PM2.5 and Its Carbon Content in the South Coast Air Basin: A Focus on the impact of Wildfires.

FARAZ ENAYATI AHANGAR, Sina Hasheminassab, Payam Pakbin, Scott A. Epstein, Andrea Polidori, 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 resulted in a substantial reduction of ambient concentrations of and its carbonaceous content including elemental carbon (EC) and organic carbon (OC) in the South Coast Air Basin (SCAB). With these reductions in concentration levels, the contribution from wildfire, as a major source of and EC which cannot be controlled through regulations, is gaining more significance. Dry conditions in recent decades have also contributed to increased frequency and intensity of wildfire events throughout the SCAB.

Many studies have addressed the short-term effects of wildfires on concentration levels during fire episodes; however, few have analyzed and quantified the long-term influence of wildfires on air quality in the SCAB. These studies have suggested that the long-term levels of EC concentration might be impacted by the wildfire contributions. In this work, we have analyzed the long-term trends of , EC, and OC at four monitoring sites in the SCAB from 2004 to 2018. Using a back-trajectory model combined with a fire emission inventory we determined the days that were affected by wildfires and compared the air quality levels on these days to the rest of the study period. The results suggest that while wildfires caused elevations in concentration of , EC, and OC in SCAB in relatively short temporal scales around fire episodes, their impacts on long-term trends were not statistically significant as some of the previous studies have suggested.

16CA.2

An Algorithm for Soot Aggregate Restructuring.

Ogochukwu Enekwizu, DIVJYOT SINGH, Alexei Khalizov, *New Jersey Institute of Technology*

Soot aggregates, derived from the incomplete combustion of fossil fuels and biomass burning, are ubiquitous in the atmosphere and adversely impact air quality and global climate. The fractal-like structure of soot aggregates undergoes significant restructuring due to interaction with condensable trace-gas chemicals during atmospheric aging. This morphological change affects the properties of soot aggregates including their light scattering and absorption, surface chemistry, cloud nucleation efficiency and atmospheric lifetime. In this study, we develop an algorithm to simulate the condensation-induced restructuring of soot aggregates. The restructuring algorithm accounts for adhesion forces between soot monomers, forces exerted by liquid bridges between non-contacting monomers, capillary forces due to coating trapped in junctions between monomers, and viscous dissipation forces. We test our restructuring algorithm on an ensemble of initially fractal aggregates and track the morphological evolution of the aggregate backbone. We also compare our predictions of final aggregate morphology against compact aggregates generated directly via traditional Diffusion Limited Cluster Aggregation (DLCA) methods. The results of our findings will provide a framework that facilitates predictions of morphologically dependent soot properties.

16CA.3

Organic Tracers of Low and High Molecular Weight in Particulate Matter with Thermal Desorption -- Pyrolysis -- Gas Chromatography/Mass Spectrometry. ALENA KUBATOVA, Brett Nespor, Richard Cochran, Haewoo Jeong, Frank Bowman, David Delene, Evguenii I. Kozliak, Bin Yao, *University of North Dakota*

Particulate matter (PM) consisting of both organic carbon (OC) and elemental carbon (EC) causes a wide range of effects in the atmosphere, yet only a fraction of OC is fully characterized. Typically thermal optical analysis (TOA) is employed to determine the OC and EC distribution. Further chemical speciation for source apportionment of OC compounds is typically accomplished with either thermal desorption (TD) or solvent extraction followed by GC-MS. Nevertheless, these current methods tend to favor the detection of low molecular weight, semi-volatile compounds and may discriminate against higher molecular weight species.

In this study, we investigate TOA in comparison to TD-pyr-GC-MS to identify various organic compounds for samples obtained at rural North Dakota and during the CARES campaign. The combination of TOA quantitative data with the qualitative characterization of the semi-volatile fraction (TD) was complemented with structural information on larger molecular weight species using stepwise pyrolysis (pyr), which enabled improved insight on characterization of OC and its high molecular weight fraction. TD (300 °C) and pyr (> 500 °C) GC-MS data provided specific homology profiles for alkanes, alkenes, polycyclic aromatic hydrocarbons (PAHs) and a variety of other organic compounds, where TD was mostly associated with biogenic origin. In the pyr fractions of carbonaceous PM, highly abundant homologous series of n-alkenes, n-alkylbenzenes, PAHs, n-alkanes, and substituted phenols were observed. The occurrence of these compounds based on newly developed pyrolytic indicators reflects the breakdown of biogenic sources, e.g., plant lipids, although certain sampling periods showed a contribution of anthropogenic origin.

16CA.4

Assessing Polarimetric Measurement Sensitivities to Light-Absorbing Aerosol. CHENCHONG ZHANG, William Heinson, Benjamin Sumlin, Michael Garay, Olga Kalashnikova, Rajan K. Chakrabarty, *Washington University in St. Louis*

Aerosol absorbs and scatters solar radiation, thus affecting the earth's energy budget through direct and semi-direct radiative forcing. The carbonaceous aerosol is one of the most uncertain drivers of radiative forcing. It is made up of two dominant components: black carbon (BC) and brown carbon (OC). Direct radiative forcing (DRF) due to the light-absorbing carbonaceous aerosol, including BC and a fraction of OC (optically defined as brown carbon (BrC)), is one of the least understood aspects of the climate system. Part of the reason for this uncertainty is optical parameters of importance to climate modelers have a complex dependency on the aerosol's microphysical properties, including size distribution, shape, and composition (hence, their refractive index). In this study, we apply a successive order of scattering (SOS) code to simulate remote reflectance signals at the top of the atmosphere (TOA) to a variety of aerosol microphysical inputs. The results show that aerosol's aerosol microphysical properties sensitively affect the polarimetric measurements at TOA. The sensitivity levels are measured by atmospheric reflectance Jacobians to specific aerosol properties. Our quantitative sensitivity analyzes also show that the refractive index of light-absorbing aerosol normally has more significant effects on atmospheric radiative transfer compared to size distribution. This spectral sensitivity of atmospheric reflectance reaches its maximum in the regime where the imaginary refractive index less than 0.1. It implies polarimetric measurements are more effective in tracking the evolution of the absorption capacity of the aerosol which is composed of weakly absorbing material (e.g., BrC). This type of remote sensing technique can be further applied to study the atmospheric aging process of BrC.

16CA.6

Enhanced Formation of Brown Carbon from Photooxidation of 1-Methylnaphthalene in the Presence of Nitrogen Oxides, Ammonia, and Water Vapor. YUMENG CUI, Alexander Frie, Justin Dingle, Stephen Zimmerman, Isis Frausto-Vicencio, Francesca Hopkins, Roya Bahreini, *University of California, Riverside*

Improved understanding of secondary organic aerosol (SOA) particles' optical properties are needed to better predict their radiative impacts. Here, SOA were produced by reacting 1-methylnaphthalene with hydroxyl radicals (OH), under variable ammonia (NH_3), nitrogen oxides (NO_x), and relative humidity (RH) conditions. The resulting single scattering albedo (SSA), mass absorption coefficient (MAC) and refractive index (RI) values at λ=375 nm suggest formation of light-absorbing aerosols. Under intermediate-NO_x and dry conditions, MAC values increased by a factor of two with the addition of NH_3 to 0.24 m^2 g^{-1} while with increased RH MAC further increased ~50%. Under high-NO_x conditions, MAC value increased by 20% to 0.51 m^2 g^{-1} with the addition of NH_3. The highest MAC was reached under high-NO_x, high NH_3 and increased RH (0.69 m^2 g^{-1}). Time series of MAC showed increasing trends only in the presence of NH_3, suggesting continuous formation of chromophores. Composition analysis of SOA suggests that organonitrates (ON) and other nitrogen-containing organic compounds (NOC) are potential chromophores in the 1-methylnaphthalene SOA. Formation of NOCs was observed only in the presence of NO_x and NH_3, and was enhanced under elevated RH. Organic mass spectra obtained by a time-of-flight Aerosol Mass Spectrometer (mAMS) were analyzed with Positive Matrix Factorization (PMF) model. More details about the correlations between 1-methylnaphthalene SOA optical properties and the factors resolved by PMF during different oxidation conditions will be presented.

16CA.7

Tracking the Evolution in Soot Aggregate Optical Properties Concurrently with its Morphology.
OGOCHUKWU ENEKWIZU, Divjyot Singh, Alexei Khalizov, *New Jersey Institute of Technology*

Radiative forcing by soot is strongly dependent on particle morphology and mixing state, which are complex and subject to significant change during atmospheric aging. The constantly evolving nature of soot is often overlooked in atmospheric models, resulting in significant uncertainties in their estimates of regional air quality and global climate. Our previous research has shown that fractal soot aggregates can restructure in the presence of particularly thin coatings. Recently, we developed an algorithm to model aggregate restructuring and found that individual aggregates with the same initial fractal parameters can end up with different levels of compactness. In this study, we examine the impact of structural evolution on the optical properties of thinly coated soot. We apply our restructuring algorithm to an ensemble of fractal aggregates with the same initial morphological parameters. As each aggregate restructures continuously from fractal to compact shape, we extract and save morphologies that match a set of predefined fractal parameters. Using Discrete Dipole Approximation (DDA), we compare the optical properties of our aggregates that were generated fractal and then restructured against those of aggregates that were generated compact. Additionally, we perform optical calculations on those fractal and compact aggregates after adding the coating material, which can be distributed in two different ways: a uniform layer or menisci localized in junctions between individual graphitic spheres in the aggregate. By tracking the evolution in optical properties of coated soot aggregates, the outcome of our findings will help improve the accuracy of radiative forcing by soot in atmospheric models.

16CA.9

Molecular-Specific Optical Properties of Atmospheric Brown Carbon Proxies. ANUSHA P.S. HETTIYADURA, Valeria Garcia, Christopher West, Jay Tomlin, Chunlin Li, Quanfu He, Yinon Rudich, Alexander Laskin, *Purdue University*

This study explores the chemical composition and light absorption properties of biomass tar condensates as proxies of atmospheric brown carbon (BrC) emitted from biomass burning (BB). The condensates were generated from dry-distilling wood pellets simulating oxidative and pyrolysis BB conditions. Both condensates separated into two immiscible, 'darker oily' and 'lighter aqueous', phases. These phases were separately analyzed using reversed-phase high performance liquid chromatography (HPLC) coupled with a photodiode array (PDA) detector and a high-resolution mass spectrometer (HRMS) interfaced with interchangeable electrospray and atmospheric pressure photo ionization sources. Based on HPLC-PDA-HRMS results, two sets of BrC chromophores were identified: 1) less absorbing, polar mono-aromatic species, *common* among different fractions, and 2) more absorbing, non-polar poly-aromatic species, *specific* to oily fractions. Chemical composition of BrC chromophores is inferred from the correlative analysis of the HRMS and PDA records: furans and 2-methoxyphenols are identified as the major *common* chromophores and oxidized diterpenoids and alkyl phenanthrenes are identified as the major *oil-specific* chromophores. The pyrolysis oily (PO) phase showed the highest UV-Vis absorption and was used to generate BrC aerosol, followed by 1) collection of the size-separated aerosol samples using a cascade impactor, and 2) their analysis using the HPLC-PDA-HRMS platform. Aerosolized PO samples showed substantial increase in their corresponding mass absorption coefficient ($MAC_{300\text{-}428\ nm}$) compared to that of the bulk PO sample. We show that the increase of MAC values caused by evaporation and gas-phase partitioning of relatively volatile, low-MW and less-absorbing chromophores. The optical properties of the aerosolized PO were consistent with the reported measurements of ambient BB-BrC aerosol.

16CA.10

Black Carbon Source Apportionment and Fluxes in Delhi Measured Using a Single Particle Soot Photometer (SP2). Rutambhara Joshi, JAMES ALLAN, Ernesto Reyes Villegas, Dantong Liu, Eiko Nemitz, Ben Langford, James Cash, Neil Mullinger, Drysdale Will, James Lee, Chiara Di Marco, Shivani Shivani, Ranu Gadi, Hugh Coe, *University of Manchester*

Black carbon (BC) plays a significant role in climate, human health and the environment. Indian cities, especially its capital Delhi is known to emit a large amount of BC aerosol, and their emissions have been rising due to continuing rapid growth in population. However, the precise emissions from different sources are currently uncertain, which are critical for making effective policies for mitigation. In this study, we measure BC using a Single Particle Soot Photometer (SP2) at an urban location near Old Delhi's Kashmere Gate, at Indira Gandhi Delhi Technical University for Women, measuring both ambient concentrations and also fluxes using the eddy covariance (EC) technique. During pre-Monsoon (25th May - 2nd June) and post-Monsoon (12th Oct - 23rd Nov) of 2018, which included the Diwali festival (known for lighting fireworks) and is a period associated with crop residue burning across the region. The measurements were made as part of large UK–India fieldwork, part of Air Pollution and Human Health (APHH) programme. We focus on characterising BC properties for pre-monsoon and post-monsoon periods, particularly its mixing state, through analysis of the size and coating content of individual particles. This allows us to attribute individual particles to potential sources. In the last two weeks of the post-monsoon period, we additionally include BC flux measurements from a 33 m tower. BC emission fluxes were calculated over flux footprints of up to ~ 1 km. Very high levels of BC concentrations were observed with half-hourly averaged concentrations routinely above 10 mg m^{-3} during both seasons. The campaign wide mean BC concentrations were 4.2 mg m^{-3} (Pre-monsoon) and 10.7 mg m-3 (Post-monsoon), and mean BC mass flux was 16 ng m^{-2} s^{-1}.

16CA.11

Impact of Organic Carbon on Soot Light Absorption. GEORGIOS A. KELESIDIS, Alexander Bruun, Sotiris Pratsinis, *ETH Zurich*

The impact of organic carbon (OC) on the light absorption of soot is determined by discrete element modeling coupled with the discrete dipole approximation for computing the scattering of radiation by soot particles. The mass absorption cross-section (MAC) of soot is used widely to determine its light absorption. Typically MAC is obtained from the mass average refractive index of OC and elemental carbon (EC) with large C/H that make up mature soot. As such, MAC can be overestimated by a factor of 3 in fuel-rich flames where newly-formed young soot contains EC with small C/H and OC that predominantly scatters light reducing its absorption by soot. Here a relation for the soot refractive index is derived accounting for soot morphology, maturity and OC content through its band gap at wavelength, λ = 266 - 1064 nm. Using this relation, the MAC of soot containing OC (up to 50 wt%) is in excellent agreement with carbon black, graphene and soot data at λ = 300 - 840 nm. This confirms that soot morphology, maturity and OC content greatly influence light absorption during characterization of in-flame and freshly-emitted soot by laser induced incandescence and light extinction, especially in fuel-rich flames, and need to be properly accounted for in the soot refractive index.

16CA.12

Health Impacts of Regional Open and Agricultural Fires in Northern South America. KAREN BALLESTEROS, Amy P. Sullivan, Ricardo Morales Betancourt, *Universidad de los Andes*

Smoke from open biomass burning (BB) significantly deteriorates air quality globally and negatively impacts human health. Exposure to BB smoke has been associated with increased incidence of premature mortality and morbidity outcomes. Recent work indicates a strong correlation between the number of fires in Northern South America (NSA) and smoke tracers such as brown carbon and levoglucosan measured at densely populated areas in Colombia. This suggests there is a strong influence of open BB on the seasonality of air pollution in the region. In this work we used the Weather Research and Forecasting Model coupled with Chemistry (WRF-Chem) to estimate the contribution from open BB to excess fine particulates ($\Delta PM_{2.5}$) and quantified short-term effects associated with BB during a peak of fire season in NSA. Three nested modeling domains that cover the northern half of South America at a horizontal resolution of 27, 9, and 3 km, respectively, centered in Colombia (lat. 5.194 – long. -73.522) were used. Aerosols were described with the two-moment sectional aerosol scheme MOSAIC. $\Delta PM_{2.5}$ was quantified by carrying out a sensitivity analysis in which two scenarios were defined. A FIRE scenario including biogenic, anthropogenic, and BB emissions input from the FINN BB emission inventory and a NO_FIRE scenario in which BB were not included. Our simulations results estimate a monthly-mean $\Delta PM_{2.5}$ of 4 µg m^{-3} over, with a maximum daily mean of 200 µg m^{-3} in regions near the most intense open BB sources. The corresponding short-term PM2.5-related all-cause, cardiovascular, and respiratory mortality outcomes estimates were calculated using a log-linear concentration-response function (CRF). We also estimated Chronic Obstructive Pulmonary Disease (COPD) cases due to $\Delta PM_{2.5}$ and calculated the increase in emergency visits associated to respiratory symptoms in the most populated Colombian cities. Results estimated mortality were higher in densely populated areas, especially over Colombia with about 70% of cases in NSA.

16CA.13

Predicting the Influence of Particle Size on the Glass Transition Temperature and Viscosity of Secondary Organic Material.

MARKUS PETTERS, Sabin Kasparoglu, *North Carolina State University*

Atmospheric aerosols can assume liquid, amorphous semi-solid or glassy, and crystalline phase states. Particle phase state plays a critical role in understanding and predicting aerosol impacts on human health, visibility, cloud formation, and climate. Melting point depression increases with decreasing particle diameter and is predicted by the Gibbs-Thompson relationship. This work reviews existing data on the melting point depression to constrain a simple parameterization of the process. The parameter ξ describes the degree to which particle size lowers the melting point and is found to vary between 300 and 1800 K nm for a wide range of particle compositions. The parameterization is used together with existing frameworks for modeling the temperature and RH dependence of viscosity to predict the influence of particle size on the glass transition temperature and viscosity of secondary organic aerosol formed from the oxidation of α-pinene. Literature data are broadly consistent with the predictions. The model predicts a sharp decrease in viscosity for particles less than 100 nm in diameter. It is computationally efficient and suitable for inclusion in models to evaluate the potential influence of the phase change on atmospheric processes.

16CA.14

Determination of the Volume Fraction of Soot Accounting for Its Composition and Morphology.

GEORGIOS A. KELESIDIS, Sotiris Pratsinis, *ETH Zurich, Switzerland*

The soot volume fraction, f_v, is essential for combustion engineering, air quality and climate modeling. It is commonly obtained from mobility or optical data assuming soot spheres of constant composition that tend to overestimate f_v by up to an order of magnitude. Here, a method is presented for estimation of the f_v from soot mobility or optical diagnostics data accounting for the realistic soot morphology and composition. With mobility data, the f_v is determined by a power law for soot morphology (fractal-like structure) and the average primary particle diameter from microscopy, gas adsorption or power laws [1]. Such f_v and the corresponding soot volume/mass size distributions are in excellent agreement with accurate but tedious soot mass-mobility measurements in premixed flames along various heights above the burner (HAB) as well as from the exhaust of diffusion flames and diesel engines. With light extinction data, the f_v is obtained by explicitly accounting for soot composition (through its optical band gap and refractive index, RI) and the light absorption enhancement (due to multiple light scattering within soot agglomerates) in the absorption function, E(RI) [2]. So as nascent soot matures by surface growth and agglomeration, its optical band gap decreases while its mobility diameter, carbon to hydrogen (C/H) ratio and f_v increase, increasing the soot E(RI) from 0.22 to 0.40, in excellent agreement with laser induced incandescence data from flat premixed ethylene flames. Using this variable E(RI), the soot f_v from light extinction data in these flames is up to 50 % lower than that using standard constant E(RI) for soot spheres.

[1] G.A. Kelesidis, E. Goudeli, S.E. Pratsinis, Morphology and mobility diameter of carbonaceous aerosols during agglomeration and surface growth, Carbon 121 (2017) 527-535.
[2] G.A. Kelesidis, S.E. Pratsinis, Soot light absorption and refractive index during agglomeration and surface growth, Proc. Combust. Inst. 37 (2019) 1177-1184.

16CA.16

Using Aerosol Instruments to Characterize Soot Particles Generated by Spark Discharge. ROBERT VANGUNDY, Vaithiyalingam Shutthanandan, David Bell, Dan Imre, Alla Zelenyuk, *Pacific Northwest National Laboratory*

Black carbon particles are formed through incomplete combustion of materials and are important to a wide variety of atmospheric processes. To study the effects of atmospheric black carbon in the laboratory, reliable and reproducible sources are necessary. Soot particles generated by graphite spark discharge (GSD) generators are commonly used as proxy for fractal combustion soot for instrument calibration, and studies of soot reactivity, inhalation toxicity, and optical properties.

I will present the results of a recent study, in which we characterized two distinct types of soot particles generated by GSD. The first type is well-documented in literature as small, stringy, fractal like agglomerates that comprise the majority of generated particles. The second type of particles are compact agglomerates with very different shapes and morphologies.

Using a suite of state-of-the-art aerosol instruments, which include single particle mass spectrometer, scanning mobility particle sizer, centrifugal particle mass analyzer, and aerodynamic aerosol classifier, we separated in situ two types of soot particles and comprehensively characterized their properties (number concentrations, size, composition, mass, morphology, and effective density) as a function of particle size. Additionally, the separated particles were collected for microscopic analysis, confirming their distinct morphologies.

We find that compact agglomerates, comprising up to 20% of particle number concentration, have significantly higher effective densities and significantly contribute to particles mass loadings. We demonstrate the presence of compact agglomerates can lead to an apparent discontinuity in particle effective density, based on the measured particle mass and mobility diameter depending on the order of these measurements.

16CA.17

Observations of Aerosol Absorption and Attribution to Black Carbon, Brown Carbon, and Coating Enhancement in Wildfire Smoke during the FIREX-AQ Mission. NICK WAGNER, Adam Ahern, Charles Brock, Daniel Murphy, Ming Lyu, Joshua P. Schwarz, Joseph Katich, Anne Perring, Braden Mediavilla, Richard Moore, Elizabeth Wiggins, Rodney J. Weber, Linghan Zeng, Jack Dibb, Eric Scheuer, Edward Winstead, Claire Robinson, *CU CIRES - NOAA ESRL*

Particulate emissions from wildfires are expected to increase in the future and to account for a larger fraction of overall particulate emissions. The climatic impact (specifically the direct radiative effect) of the smoke depends on microphysical and optical properties of the smoke particles and the evolution of these particles downwind of the fires. We present airborne measurements of aerosol absorption in fresh wildfire plumes sampled in a quasi-Lagrangian manner one hour to one day downwind of wildfires over the western North American in summer of 2019 during the FIREX-AQ mission. The total aerosol absorption is attributed to black carbon (BC), brown carbon (BrC) and the coating enhancement of BC absorption (“lensing”). The relative absorption due to each of these absorbers evolves downwind of the wildfires and varies between plumes depending on burning conditions. Brown carbon absorption derived from the wavelength dependence of the total absorption and direct measurements of soluble BrC absorption are compared. The observations during FIREX-AQ are also compared to similar airborne datasets collected over the last decade.

16CA.18

Molecular Composition and the Optical Properties of Brown Carbon Generated by the Ethane Flame. CHRISTOPHER WEST, Anusha P.S. Hettiyadura, Andrew Darmody, Gaurav Mahamuni, Justin Davis, Igor Novosselov, Alexander Laskin, *Purdue University*

Atmospheric ‘Brown Carbon’ (BrC) is a complex mixture of organic compounds with diverse molecular composition and variable light-absorbing properties. Previous reports provided substantial molecular-specific information of BrC related to biomass burning emissions; however, very few studies describe BrC generated from hydrocarbon fuel combustion. The work presented here is the first study that identifies and characterizes BrC formed in the controlled flame combustion of ethane – one of the most basic hydrocarbon fuels. To understand the molecular composition and optical properties of BrC, we used an analytical platform that includes high-performance liquid chromatography (HPLC) coupled to photodiode array (PDA) detection, followed by dopant-assisted atmospheric pressure photoionization (APPI) and high-resolution mass spectrometry (HRMS). For this study, six soot samples were generated in a custom-built inverted gravity flame reactor (IGFR) at different combustion settings. The temperature of the diffusion flame was controlled by fuel dilution with Argon (up to 80% v/v) and was measured to be in the range of 1750-1950K. Basic characterization of the samples (i.e., mass loading, OC/soot ratio) was employed, followed by molecular speciation of BrC chromophores. A vast majority of BrC chromophores identified in these samples are oxygenated polycyclic aromatic hydrocarbons (O-PAHs) and unsubstituted PAHs. Nearly 90% of the total BrC absorbance was attributed to approximately equal contributions from the groups of O-PAHs, low and high molecular weight PAHs referred as PAHBaP (i.e., smaller and larger than Benzo[a]pyrene (BaP), respectively). The mass absorption coefficient (MACbulk) measured at λ350nm for the BrC fraction of aerosol emitted from hottest flame (Tmax=1946 K) was 0.49 m2/g.

16CA.19

Brown Carbon Global Direct Radiative Effects. LINGHAN ZENG, Aoxing Zhang, Yuhang Wang, Nick Wagner, Joseph Katich, Joshua P. Schwarz, Gregory Schill, Charles Brock, Karl D. Froyd, Daniel Murphy, Christina Williamson, Agnieszka Kupc, Eric Scheuer, Jack Dibb, Rodney J. Weber, *Georgia Institute of Technology*

Organic aerosols (OA) mostly scatter solar radiation cooling the planet. However, a portion of organic species, brown carbon (BrC), absorbs light at shorter visible and near-ultraviolet wavelengths. BrC is emitted directly by the incomplete combustion of fuels, especially biomass and biofuel burning, or from secondary formation processes. Globally, the radiative impacts of BrC are difficult to assess due to the lack of BrC observational data. To address this, filter samples were collected on the NASA DC-8 research aircraft with near pole-to-pole latitudinal coverage over the Pacific and Atlantic basins in three seasons as part of the Atmospheric Tomography Mission (ATom). These filters were sequentially extracted into water then methanol and the light absorption of the solutes measured with a spectrophotometer. The results provide the first data set of BrC on a global scale. We find that BrC concentrations were highly spatially heterogeneous with levels below the detection limits (0.05 to 0.15 Mm^{-1}) in most of the remote atmosphere, whereas levels above the detection limit were observed in air masses that had been transported from regions of biomass burning. The impact of BrC was assessed with a radiative transfer model for the measurement regions. The direct radiative effect due to BrC absorption accounted for approximately up to 48% of top of the atmosphere clear sky instantaneous forcing due to absorbing carbonaceous aerosols. These results show that BrC from biomass burning is an important component of the global radiative balance.

16CA.20

Garbage Burning Contribution to Ambient Particulate Pollution. MD. ROBIUL ISLAM, Tianyi Li, Nita Khanal, Khadak Mahata, Siva Praveen Puppala, Narayan Babu Dhital, Michael Giordano, Benjamin Werden, Anobha Gurung, Arnico Panday, Robert J. Yokelson, Peter F. DeCarlo, Elizabeth Stone, *University of Iowa*

An estimated 1 to 2 billion metric tons of solid waste is produced globally per year. Much of this waste is disposed of by open burning which produces hazardous gases and particulate matter (PM). Among the PM are antimony (Sb) and 1,3,5-triphenylbenzene (TPB) that are associated with plastic, which comprises approximately 10% of waste. During the Nepal Ambient Monitoring and Source Testing Experiment (NAMaSTE), emission factors (EF) of $PM_{2.5}$ ranged from 7.4 g/kg for dry mixed waste to 124 g/kg for damp mixed waste burning. EFs of TPB and Sb were also measured to estimate garbage burning contributions to ambient PM. In the Kathmandu Valley, source apportionment of $PM_{2.5}$ organic carbon (OC) indicated garbage burning contributions of 3.1±1.3 $\mu gC/m^3$ (18%) at Bode in the pre-monsoon season in 2015, and 11±5 $\mu gC/m^3$ (29%), 12±6 $\mu gC/m^3$ (33%), and 6.1±2.0 $\mu gC/m^3$ (40%) at Kathmandu, Lalitpur, and Dhulikhel in the winter of 2017-18. These results indicate higher wintertime contributions of garbage burning to PM as well as spatial heterogeneity within the Valley. In the Terrai region, garbage burning contributions to $PM_{2.5}$ OC were lower in the winter of 2017-18 at 2.7±2.2 $\mu gC/m^3$ (5%). Two tracers of garbage burning—TPB and Sb—moderately correlated at the Kathmandu site, supporting their originating from the same source. Together, these studies demonstrate that garbage burning is an important source of $PM_{2.5}$ in South Asia, with potentially significant impacts on the environment and human health. Considering the importance and yet large variability in emissions due to variation of garbage types, further investigations are needed to better constrain its contribution to ambient PM.

16CA.21

An Overview of NASA Langley Aerosol Research Group (LARGE) Airborne Measurements during the 2019 FIREX-AQ Field Campaign. RICHARD MOORE, Elizabeth Wiggins, Claire Robinson, Kenneth Thornhill, Edward Winstead, Kevin Sanchez, Luke Ziemba, Bruce Anderson, John Barrick, Matthew Brown, Gao Chen, Ewan Crosbie, Carolyn Jordan, Taylor Shingler, Michael Shook, *NASA*

We present a summary of observations made by the LARGE airborne instrument suite (https://science.larc.nasa.gov/large/) as deployed on the NASA DC-8 aircraft during the recent, Fire Influence on Regional to Global Environments and Air Quality field campaign (FIREX-AQ; https://www.esrl.noaa.gov/csl/projects/firex-aq/). FIREX-AQ consisted of a series of flights sampling both western wildfires and smaller, agricultural burning in the eastern United States that were carried out in July-September, 2019. The LARGE instruments focused on measurements of aerosol concentration and size distribution, CCN concentrations, dry and humidified submicron particle scattering at three wavelengths, and filter-based particle absorption at three wavelengths. One set of particle counters and optical particle sizers was thermally-denuded at 350 degrees Celsius in order to examine the contribution non-volatile aerosol fraction. Finally, quartz filters were collected for offline elemental/organic carbon (EC-OC) analysis. The LARGE instruments, as well as those from collaborating research groups, shared a common isokinetic inlet and bridge dilution system in order to reduce disparities across inlet sampling systems. Carbon dioxide measurements were also made from the aerosol inlet in order to account for possible fire plume heterogeneity across the aircraft fuselage spatial scales. A detailed description of the research flights, LARGE instrument suite, and instrument performance during FIREX-AQ will be discussed.

16CA.22

Chemical Imaging of Atmospheric Biomass Burning Particles from North American Wildfires. FELIPE RIVERA-ADORNO, Jay Tomlin, Kevin Jankowski, Rebecca Washenfelder, Ann M. Middlebrook, Swarup China, Daniel Knopf, Ryan Moffet, Lisa Azzarello, Alessandro Franchin, Alexander Laskin, *Purdue University*

Smoke emissions impact atmospheric chemistry, visibility, human health, and climate. Specific effects of biomass burning aerosols (BBA), such as radiative forcing alterations and cloud formation propensity are highly influenced by variability in the chemical composition and internal structures of individual particles within smoke plumes. To improve our understanding of the chemical and physical properties of BBA and how these change during atmospheric aging, samples were collected onboard NOAA research aircraft during the 2019 FIREX-AQ field study. A time-resolved aerosol collector was used to collect BBA particles for later chemical imaging of ambient particles. We use synchrotron-based soft X-ray spectro-microscopy to visualize particles and their internal components. This provides advanced chemical speciation and mapping of carbon, allowing us to distinguish between organic carbon and elemental carbon (soot). Electron microscopy and elemental microanalysis, on the other hand, provides information on the size and morphology of particles by providing high resolution images and elemental composition on a particle-by-particle basis. Our results suggested notable differences in the internal and external mixing of particles collected during daytime and nighttime. While daytime-collected samples were dominated by organic carbon, nighttime samples were notably rich with inorganic material. Microscopy images showed that there are also differences between the morphology and consistency of daytime and nighttime-collected particles. Daytime particles were seen to be of spherical shape consistent with viscous or “glassy” composition. In contrast, nighttime particles appear to be of a more liquid consistency and had internal arrangements of inorganic cores with organic coatings. Ongoing work involves the correlation of our data with real-time records from co-deployed instruments that measured concentrations of trace gases, aerosol mass concentrations and optical properties.

16CA.23

Characterization of Benzene Polycarboxylic Acids and Nitroaromatics in Atmospheric Aerosols and Vehicular Emitted Particulate Matter using UPLC-ESI-QqQ-MS. MAHMOUD YASSINE, Michal Suski, Ewa Dabek-Zlotorzynska, *AAQS, AQRD, Environment Canada*

The impact of atmospheric $PM_{2.5}$ in urban areas on human health, visibility degradation, and global climate change has prompted an increased scientific focus on identifying the components and sources of $PM_{2.5}$ that are most directly responsible for such effects. Of great interest is the organic fraction, in particular, the water-soluble organic carbon (WSOC), which is composed of a multitude of individual polar oxygenated compounds generated from a variety of sources. Many studies on WSOC speciation have identified several classes of organic species, i.e., mono-, di-, and polycarboxylic acids along with additional functional groups, such as hydroxy-, methoxy-, and/or nitro-groups. Yet, improved molecular characteristics and distribution of WSOC constituents are critically important to gain insights into the sources and the underlying mechanisms of secondary organic aerosol formation and transformation.

This study describes an efficient and reliable ultrahigh pressure liquid chromatography-electrospray ionization-triple quadrupole mass spectrometry (UPLC-ESI-QqQ-MS) method for the simultaneous quantitative determination of 28 analytes distributed among three classes of compounds: (i) benzene polycarboxylic acids; (ii) nitroaromatic acids and (iii) nitrophenols (NPs) in urban $PM_{2.5}$.and vehicular-emitted samples. Of all samples tested, the highest concentrations of both benzene polycarboxylic and nitroaromatic acids with much lower abundance of NPs were found in the diesel-emitted $PM_{2.5}$. There were fewer target analytes observed in gasoline-emitted $PM_{2.5}$. Clear differences in distribution of target species were observed between urban $PM_{2.5}$ affected by the traffic and biomass burning emissions. This study also focuses on identifying potential compounds that may be used as tracers for specific sources.

16CC.1

Determination of the Water-polymer Interaction Parameter and Hygroscopicity of Particles. Chun-Ning Mao, AKUA ASA-AWUKU, *University of Maryland*

Hygroscopicity determines the ability of a particle to swell or contract in the presence of water vapor. The hygroscopicity for organic nano-particles is a known function of the solute molar volume. This is particularly true for low-molecular weight (< 200 g mol $^{-1}$) organic compounds used for drug delivery. In this work, four commonly used biodegradable hydrophilic compounds, mannitol, lactose, gelatin and polyethylene glycol are measured with a fast and unique hygroscopicity-cloud condensation nuclei activation technique. Flory-Huggins Köhler theory is used to estimate the single parameter hygroscopicity. Results show that for the high molecular weight compounds, a water-polymer interaction parameter must also be considered and the water-polymer interaction parameter for nanoparticles can be determined in the supersaturated regime. The water affinity becomes essential for nanoparticle hygroscopicity, and the organic molar volume contribution starts to decrease as the molecular weight increases. In summary, the water affinity of the interaction parameter can be measured for nano-particles and plays an important role in the water uptake of biodegradable organic nano-particles.

16CC.2

Effects of Dry Intrusion Events across the North Atlantic on Composition of Atmospheric Particles around the Azores Islands. Jay Tomlin, KEVIN JANKOWSKI, Daniel Veghte, Matthew Fraund, Swarup China, Benny Wong, Peiwen Wang, Josephine Aller, Guangjie Zheng, Jian Wang, Daniel Knopf, Shira Raveh-Rubin, Ryan Moffet, Alexander Laskin, *Purdue University*

Our project investigates the physicochemical properties of atmospheric particles collected during the Aerosol and Cloud Experiment in the Eastern North Atlantic field campaign conducted at Azores Islands in 2017-2018. The campaign employed both ground and aircraft measurements designed to characterize the difference in contributions from various sources with respect to atmospheric particles typical for the marine boundary layer (MBL) and free troposphere (FT). The MBL can become mixed with air from the FT during a meteorological event known as ‘dry intrusion’. Dry intrusions are events of cold, dry, rapid descending airflow from the upper troposphere down toward the lower troposphere. Aerosols carried during these events experience long range transport and aging where they undergo substantial changes in size, morphology, and composition. We used computer-controlled scanning electron microscopy and X-ray microanalysis for elemental analysis of statistically significant number of particles. Scanning transmission X-ray microscopy was used to probe of chemical bonding of carbon, nitrogen, oxygen, and sulfur. The particle composition, mixing state, and morphology is then combined with real-time measurement of aerosol size distribution, CCN concentration, hygroscopicity, aerosol bulk composition, and back trajectory calculations. Combined, these results allow us to assess the sources of dominant particles observed at the eastern north Atlantic (e.g. biogenic vs. anthropogenic, primary vs. secondary) and gain insight into the atmospheric processing of aerosol particles resulting from condensation, coagulation, oxidative aging, and cloud processing.

16CC.3

Effects of Cloud Conditions on Particle Size Distributions in the Southeast US.

STEPHEN NOBLE, *Savannah River National Laboratory*

Clouds can alter atmospheric particle concentrations and size through physical and chemical processing. This aerosol-cloud interaction is understudied but has implications for short wave cloud albedo. Bimodal distributions associated with cloud processing are prevalent in the marine environment (Hoppel et al. 1986; Hudson et al. 2015). Clouds have also been shown to influence particle size distributions (PSD) in continental air masses at the Southern Great Plains site in the central US (Noble & Hudson 2019). In the Southeastern US where influences from both maritime and continental airmasses are prevalent, PSDs were measured using a Scanning Particle Mobility Sizer at the Savannah River Site (near Aiken, SC). Preliminary data show PSDs vary with differing conditions. Bimodal PSDs with lower concentrations and larger accumulation mode sizes were found with persistent status clouds with cloud bases near 600 m above ground level. During a period of scattered shallow cumulus clouds with bases near 1100 m, PSDs were found to be only slightly bimodal with smaller accumulation mode sizes and higher total concentrations. PSD taken during clear skies showed the highest PSD total concentrations with a single mode peaking in the Aiken range (<100 nm). These measurements are consistent with Noble & Hudson (2019) which found PSDs associated with high cloud fractions and low cloud bases had reduced total concentrations, larger mean sizes, and increased concentrations in the accumulation mode. Thus, cloud processing of aerosols through widespread aerosol-cloud interactions is not limited to the marine environment. The tendency of clouds to modify particles that act as cloud condensation nuclei impacts subsequent cloud formation and cloud radiative properties.

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16CC.4

Rethinking of Black-Carbon Associated Organic Particles: Insights into Aged Biomass Burning Organic Aerosol.

JUNFENG WANG, Jianhuai Ye, Dantong Liu, Yangzhou Wu, Jian Zhao, Weiqi Xu, Conghui Xie, Fuzhen Shen, Jie Zhang, Paul Ohno, Yiming Qin, Scot T. Martin, Alex Lee, Pingqing Fu, Daniel Jacob, Qi Zhang, Yele Sun, Mindong Chen, Xinlei Ge, Xiuyong Zhao, *Harvard University*

Black carbon (BC) particles in Beijing summer haze pollution play an important role in the regional radiation balance and related environmental processes, yet understanding the factors that lead to variability in those effects remains limited. The role of BC particles can vary with the aerosol mixing state (i.e., internally compared to externally mixed) as well as with other chemical species that can coat the BC cores. Here, we present observations by a soot-particle aerosol mass spectrometer of BC-containing submicron particulate matter (BC-PM1) in the summer of 2017 in Beijing, China. These observations were compared to concurrently measured total non-refractory submicron particulate matter (NR-PM1) by a high-resolution aerosol mass spectrometer (HR-AMS). There were important differences between NR-PM1 and BC-PM1 related to organic aerosol (OA) composition. Hydrocarbon-like OA (HOA) in BC-PM1 was up to two-fold higher than that in NR-PM1 in fresh plumes of vehicle emissions, indicating that a part of HOA in BC-PM1 may be undetectable by HR-AMS. The implication is that the factorization analysis for the bulk NR-PM1 may be misinterpreted. Cooking-related OA was only identified in NR-PM1, while aged biomass burning OA (A-BBOA) was a unique factor only identified in BC-PM1. The A-BBOA was linked to those heavily coated BC characterized by coating-to-BC mass ratios RBC > 9 and particle mode size > 300 nm. These particles may lead to enhancement of the light absorption ability of BC by a factor of two via the "lensing effect". Furthermore, the fractions of less-oxidized oxygenated OA (LO-OOA) were similar in both types of particles. More-oxidized oxygenated OA (MO-OOA) identified in BC-PM1 was found to be slightly different from that observed by HR-AMS, mainly due to the influences of A-BBOA. Overall, these findings highlight that a unique biomass-burning related OA associated with BC may be ubiquitous in transported BC-PM1, and this OA may play a role in regional energy balance that has not previously been fully considered.

16CC.5

Airborne Observations of Aerosol Properties in Southeast Asia: Overview of Emissions, Cloud Processing, and Long Range Transport during NASA CAMP2Ex. LUKE ZIEMBA, Ewan Crosbie, Claire Robinson, Michael Shook, Edward Winstead, Jian Wang, Josh DiGangi, Glenn Diskin, Allison Collow, Arlindo Da Silva, Richard Ferrare, Chris Hostetler, *NASA Langley Research Center*

The Southwest Monsoon is an important synoptic scale forcing that modulates precipitation and air quality throughout Southeast Asia. Diverse aerosol sources exist throughout the region. Understanding interactions between these particles and clouds is important for future climate predictions and societal response to more frequent periods of extreme flood and drought. Here we present airborne observations made in support of the NASA CAMP2Ex (Cloud and Aerosol Monsoonal Processes-Philippines Experiment) mission aboard the Wallops Flight Facility P-3 research aircraft, based at Clark International Airport in the Luzon region of Northern Philippines. Nineteen research flights were conducted in August-October of 2019.

An extensive suite of aerosol microphysical, optical, and chemical instrumentation was deployed, along with trace gas and remote sensing measurements, to characterize aerosol emissions and their vertical/spatial variability associated with moderately convective marine cloud systems in the region. Analysis will focus on the evolution of aerosols from Indonesian agricultural biomass burning activities, compared with urban emissions from the megacity Manila and transported air masses from mainland Asia. Dry mass scattering and absorption efficiencies are derived to assess optical treatments by global circulation models in this complex meteorological environment.

16CC.6

Differences in Fine Particle Chemical Composition, Hygroscopicity, and Aerosol Liquid Water on Clear and Cloudy Days. AMY CHRISTIANSEN, Annmarie Carlton, Barron Henderson, *University of California, Irvine*

Clouds are abundant and alter fine particulate matter ($PM_{2.5}$) mass and chemical composition, yet they are sampled infrequently for chemical composition. This leads to a persistent, yet implicit clear sky bias in the characterization of tropospheric composition. For example, satellite retrievals of aerosol properties impacted by clouds are often screened from final data products to avoid measurement artifacts, hindering quantitative estimates of tropospheric chemical composition during cloudy times. Although previous studies have focused on quantitative differences in $PM_{2.5}$ mass between cloudy and clear sky times, little attention has been given to differences in $PM_{2.5}$ chemical composition, especially regarding particle hygroscopicity and water uptake. Aerosol mass concentrations and chemical speciation including aerosol liquid water (ALW) influence aerosol radiative properties, cloud microphysics, and mesoscale convective systems. A quantitative understanding of aerosol-cloud interactions, currently a critical uncertainty in atmospheric models, is necessary to improve model representation of aerosol impacts. Here, we investigate differences in surface particle chemical components, particle hygroscopicity, and associated ALW between cloudy and clear sky time periods in the context of satellite cloud flags. We examine surface data from the Interagency Monitoring of PROtected Visual Environments (IMPROVE) network across the contiguous US (CONUS) during cloudy and clear sky times using satellite cloud flag data from the Moderate Resolution Imaging Spectroradiometer (MODIS). We estimate ALW concentrations from inorganic and organic components using the thermodynamic model ISORROPIA and κ-Kohler theory. We find that ALW concentrations and hygroscopic growth factors are on average 31% and 14% larger during cloudy times, when satellites are unable to remotely sense particle properties and impacts. Further, particle chemical composition is significantly altered between cloudy and clear sky times across the CONUS. This suggests that the clear sky bias may hinder accurate model representation of particle chemical constituents, especially ALW, and associated impacts.

16CC.7

Relationship between Aerosol and Precipitation Composition at a Coastal Site in the Southeast United States.

ANDREA F CORRAL, Hossein Dadashazar, Connor Stahl, Eva-Lou Edwards, Paquita Zuidema, Armin Sorooshian, *University of Arizona*

This study combines field data and modeling to characterize temporal trends and interrelationships between aerosol and precipitation chemistry as an alternative and indirect method to gain insight on aerosol-cloud interactions. Long-term aerosol and precipitation chemistry measurements from co-located monitoring sites in southern Florida between 2013 and 2018 were used for this analysis. A positive matrix factorization (PMF) model identified six potential emission sources impacting the study area. The PMF model solution yielded the following source profiles with varying monthly concentration profiles: (i) combustion; (ii) fresh sea salt; (iii) aged sea salt; (iv) secondary sulfate; (v) shipping emissions; and (vi) dust. Based on these results, concentration-weighted trajectory maps were developed to identify possible sources contributing to the PMF factors. Sea salt is shown to be the main source of cloud condensation nuclei (CCN), even during summertime, when African dust is an important aerosol source. This was likely due to sea salt particles larger than 2.5 µm participating in cloud processes and the site’s proximity to the coast (~25 km). Fresh sea salt rather than aged sea salt (depleted in Cl^- due to NO_3^-) was more influential for aerosol and cloud processes. The highest mean annual deposition fluxes were attributed to Cl^-, NO_3^-, SO_4^{2-}, and Na^+ between April – October, which were the more strongly precipitating months. The results of this study provide findings with regard to the combination of the following: (i) composition of particles serving as either the cloud condensation nuclei (CCN) or ice nuclei (IN) that eventually fall to the surface via wet deposition; (ii) uptake of species into existing droplets in cloud; and (iii) sub-cloud scavenging of different constituents.

16CC.8

Impact of Climate Uncertainty on Projections of PM2.5 Pollution over the US.

JAMES EAST, Erwan Monier, Fernando Garcia-Menendez, *North Carolina State University*

Projections of climate change impacts on air quality show that climate and air quality are connected, beyond anthropogenic emissions, and that a warming climate can lead to a "climate penalty" on $PM_{2.5}$ levels over the US. However, these projections are subject to considerable uncertainty derived from climate modeling. Despite significant advancements in understanding the role of major sources of uncertainty in climate change simulations (internal variability, greenhouse gas emissions scenario, and model response), these uncertainties have not been systematically analyzed for air quality impacts. Using a coupled climate-air quality modeling framework designed to account for these uncertainties, we simulate over 3900 years of atmospheric chemistry driven by climate projections at the beginning, middle, and end of the 21st century to assess the contribution of each source to total uncertainty in air quality projections. We show that uncertainty in $PM_{2.5}$ projections due to internal variability increases slightly from beginning to end century, but is surpassed by scenario and climate model response uncertainty at mid-century. By end-century, scenario uncertainty dominates, followed by climate model response and internal variability. Uncertainty in internal variability, emissions scenario, and model response lead to US average uncertainties of 0.2, 0.5, and 0.6 ug/m^3 for the $PM_{2.5}$ air quality penalty at end century and reach 4.0 ug/m^3 in polluted regions in the Midwest and Northeast. The climate penalty on $PM_{2.5}$ increases with climate sensitivity and with less restrictive policy, reaching 2 ug/m^3 under a no-policy and high climate sensitivity scenario. These results give clarity to the role of climate uncertainty in projections of $PM_{2.5}$.

16CC.9

Cloud Chemical Speciation Measurements Conducted On-Line with a mini-AMS during the CAIPEEX Seeding Study.

SUBHARTHI CHOWDHURI, Edward Fortner, Benjamin Werden, Mahen Konwar, Sachin Patil, Mercy Varghese, Sudarsan Bera, P Murugavel, Philip Croteau, John Jayne, Manjula Canagaratna, Kurt Hibert, Neelam Malap, Sandeep J, Duncan Axisa, Peter F. DeCarlo, Douglas Worsnop, Thara Prabhakaran, *Aerodyne Research, Inc.*

A mini-AMS (aerosol mass spectrometer) was flown during the Cloud Aerosol Interaction and Precipitation Enhancement Experiment (CAIPEEX), a project for examining the effects of seeding on clouds conducted by the Indian Institute of Tropical Meteorology, Pune. Various chemical and meteorological parameters involving cloud condensation nuclei (CCN) and cloud processing were measured during the experiment, during the monsoon season in the rain shadow region of the Western Ghat in Solapur India. The instrumented research aircraft used in the experiment had both isokinetic and CVI inlets to allow for characterizing either total non-activated submicron aerosol in or out of clouds (isokinetic inlet) or alternatively cloud droplet residuals from in-cloud measurements (CVI inlet).

The mini-AMS was operated on the research aircraft from 25 July – 10 September 2019 to examine the chemical speciation of cloud and background aerosols. The mini-AMS acquired data on 37 research flights. During these flights, measurements were focused on cumulus cloud development, stratus clouds, and regional air quality. The mini-AMS provided 1 Hz measurements of various chemical loadings in aerosol including NO3, SO4, Chl and Organics. Cloud seeding was conducted using CaCl2 burn in place hygroscopic flares and the mini-AMS detected chemical signatures in the seeded clouds consistent with CaCl2. Other non-seeded Cl species were also observed in cloud residuals and are compared with the seeded CaCl2 signature. Aircraft passes through both seeded and unseeded clouds provide framework for comparing the variability of chemical composition in these different cloud types. Finally, measurements of aerosol composition and size with the mini-AMS outside of clouds also provide additional comparison points for cloud residual composition.

16CC.10

Emissions and Radiative Impacts of Sub-10 nm Particles from Biofuel and Fossil Fuel Cookstoves.

SHANTANU JATHAR, Naman Sharma, Kelsey Bilsback, Jeffrey R. Pierce, Joonas Vanhanen, Timothy Gordon, John Volckens, *Colorado State University*

Combustion sources have been shown to directly emit particles smaller than 10 nm. The emission of 1-3 nm particles from biofuel or fossil-fuel cookstoves has not been studied previously, nor have the radiative impacts of these emissions been investigated. In this work, emissions (number of particles) were measured during a water boiling test performed on five different cookstoves (three-stone fire, rocket elbow, gasifier, charcoal, and liquefied petroleum gas [LPG]) for particle diameters between ~1 and ~1000 nm. We found significant emissions of particles smaller than 10 nm for all cookstoves ($>5\times10^{15}$ # kg-fuel^{-1}). Furthermore, cleaner (e.g., LPG) cookstoves emitted a larger fraction of sub-10 nm particles (relative to the total particle counts) than traditional cookstoves (e.g., three-stone fire). Simulations performed with the global chemical transport model GEOS-Chem-TOMAS that were informed by emissions data from this work suggested that sub-10 nm particles were unlikely to significantly influence number concentrations of particles with diameters larger than 80 nm that can serve as cloud condensation nuclei (CCN) (<0.3%, globally averaged) or alter the cloud-albedo indirect effect (absolute value <0.005 W m^{-2}, globally averaged). The largest, but still relatively minor, localized changes in CCN-relevant concentrations (<10%) and the cloud-albedo indirect effect (absolute value <0.5 W m^{-2}) were found in large biofuel combustion source regions (e.g., Brazil, Tanzania, Southeast Asia) and in the Southern Ocean. Enhanced coagulation-related losses of these sub-10 nm particles at sub-grid scales will tend to further reduce their impact on particle number concentrations and the aerosol indirect effect, although they might still be of relevance for human health.

16CC.11

Predicting Effect of Organic-Inorganic Internally Mixed Particles on Water Uptake and Optical Properties of Atmospheric Aerosols. LUCY NANDY, Yu Yao, Nicole Riemer, *University of Illinois at Urbana-Champaign*

To study the impact of aerosol particles on Earth's climate, there are important parameters like, the particle size, water content, chemical composition, to consider when estimating their optical properties. This study while considering these factors, assumes that the particles are spherical in shape and are internally mixed. The aim is to predict the water uptake by submicron dry particles at water sub-saturation, determining the size distribution of the dry and wet particles, and the optical properties with and without hydrophobic black carbon in the particle core, focusing on the absorption enhancement by black carbon. The hygroscopic growth determined by using a lattice-based adsorption isotherm model in this study is found to differ by upto 50% for particles containing high fractions of organic matter than using existing aerosol models (e.g. MOSAIC, κ-Köhler parameterization) generally used in regional/global climate models. It is also found that the particles scatter and absorb more solar radiation in the visible spectrum than most predictions. To study absorption properties, black carbon is assumed to be in the core of these particles, and we have found that the single scattering albedo (ω) is higher by upto 1 - 2% than the other model calculations at high relative humidities and organic mass fractions. This study while elucidating the discrepancies, could reduce uncertainty in radiative forcing by improved aerosol water uptake estimations/parameterization required by the climate models.

16CC.12

Laboratory Exploration of the Effect of Mean and Fluctuations in Saturation Ratio on Activation in a Turbulent Cloud. ABU SAYEED MD SHAWON, Prasanth Prabhakaran, Gregory Kinney, Jesse C. Anderson, Raymond Shaw, Will Cantrell, *Michigan Technological University*

The aerosol indirect effect is notably dependent on the inextricable interaction between aerosol and cloud. The prerequisite to form a cloud droplet is the preexistence of an aerosol in the atmosphere. This cloud forming process (i.e. aerosol activation) is also the primary removal mechanism for the accumulation mode aerosol (diameter ranges from 0.1 to 1 µm). From a conventional point of view, the possibility of an aerosol to become a cloud droplet depends on its size, chemical composition, and the ambient supersaturation. However, field campaigns, laboratory measurements, and simulation results suggest that the knowledge of only size and chemical composition does not provide enough information to predict which particles (or fraction of particles) will activate. The knowledge of fluctuations in the saturation ratio, induced by turbulence, is also necessary to get a complete picture of the activation process.

We report a series of targeted experiments, performed in the controlled environment of Michigan Tech's cloud chamber to better perceive how the mean saturation ratio and its fluctuations affect the activation process. A protocol was developed and implemented to study the effect of mean and fluctuations independently. In steady state conditions, measurements from the chamber show coexistence of monodisperse aerosols with homogeneous chemical composition in both interstitial and cloud droplet residual distributions, suggesting the absence of one to one correspondence of size, chemistry, and activation. Different regimes of activation were achieved only by changing the saturation ratio which suggests that the fluctuation in saturation ratio can mimic the effect of heterogeneity in size and chemical composition on the aerosol activation process.

16CC.13

Influence of Various Surfactants of Hygroscopic Growth of Course Mode Aqueous Aerosol Particles. BENJAMIN SWANSON, Amanda Frossard, Rachel Bramblett, *University of Georgia*

Aerosol particles have a myriad of influences on the global climate budget, but significant uncertainties in their effects remain. The constituents of sea spray aerosols from open-ocean sources may be influenced by organic and surfactant materials on the ocean surface. Surfactants present in aerosol particles, whether natural or anthropogenic, have largely been ignored within large-scale climate modeling. Examinations of the effects of surfactants present in droplets have shown that both the surface tension and hygroscopic growth of droplets can be drastically affected. Here, we compare the effect of different surfactants, including various surfactant ionic classes, structures, and sizes, on the hygroscopic growth and surface tension of aqueous course mode particles. We also examine the effect of these surfactant classes as a function of particle size for these individual aqueous particles. These growth parameters were measured using an Aerosol Optical Trap (AOT) combined with Raman spectroscopy, which traps and sizes individual aqueous aerosol particles. For a relative humidity (RH) shift from 70% to 80% RH, addition of surfactants of all types causes deviations in growth factors of aqueous particles compared to those containing only NaCl. These deviations vary based on surfactant size and structure. Depending on the surfactant concentrations and types present in atmospheric aerosol particles, there may be deviations in the size and composition dependent growth factors of sea-spray aerosols from what current models represent.

16CC.14

Constraints on the Importance of Mineral Dust and Proteinaceous Ice Nucleating Particles in the Canadian High Artic during the Fall of 2018 Based on Heat and Ammonium Sulfate Treatments. JINGWEI YUN, Erin Evoy, Soleil Worthy, Melody Fraser, Daniel Veber, Andrew Platt, Allan Bertram, *University of British Columbia*

Ice nucleating particles (INPs) can trigger the heterogeneous freezing of cloud droplets at warm temperatures. Constraints on the concentration and composition of INPs are essential to predict ice formation in clouds. Despite previous INP measurements in the Arctic, our understanding of the concentrations, composition, and sources of Arctic INPs is far insufficient, especially in the fall. Here we report daily concentrations of INPs at Alert, Nunavut, a ground site in the Canadian High Arctic, during the fall of 2018 (from October to November). The contributions of mineral dust and proteinaceous particles to the total INP population were evaluated by testing the responses of INP concentrations for the samples to heat and ammonium treatments. Possible source locations of the effective INPs were investigated by combining the results for the surface coverage type in the Arctic, correlations of INP concentrations with concentrations of tracer chemical species, and simulations with a Lagrangian particle dispersion model. The results show that the INP concentrations of the samples collected in October were higher than the INP concentrations of the samples collected in November. Combining our results with previous INP measurements at Alert, a seasonal trend was observed, with an increase of the INP concentrations at Alert from spring to summer and then a decrease from summer to winter. For the samples collected in October, at T>-21 °C 60 % to 90 % of the total INPs was proteinaceous. At T-19 °C 30 % to 85 % of the total INPs was proteinaceous. At T3^{-} suggest that South China and California are the possible sources of INPs through long range transport.

16CC.15

Error in Aerosol Mixing State Induced by Aerosol Representation Assumptions. ZHONGHUA ZHENG, Matthew West, Nicole Riemer, *University of Illinois at Urbana-Champaign*

Modal aerosol models are a popular choice to represent aerosols in regional chemical transport models and earth system models because they are computationally efficient while capturing aerosol size distribution and composition. Modal models are, to some extent, “mixing state-aware,” since they represent the aerosol by several overlapping modes (subpopulations), and hence resolve composition differences within given size ranges. However, choices need to be made regarding the number of modes and which chemical species they contain, as well as regarding the rules to transfer aerosol number and mass between modes. These choices may introduce considerable yet poorly-characterized structural uncertainty in aerosol simulations. This raises the question: how well do modal models represent mixing state? This study aims to verify the global distribution of aerosol mixing state represented by modal models by using benchmark simulations from the particle-resolved stochastic aerosol model PartMC-MOSAIC. We used the aerosol mixing state index χ as a metric to quantify aerosol mixing state. To achieve a spatiotemporal comparison, we calculated the mixing state index using output from the Community Earth System Model with the modal MAM4 aerosol module, and compared the results with the mixing state index from a machine learning-enabled surrogate model based on high-detail particle-resolved simulations. The two methods yielded very different spatial patterns of mixing state index. In some regions, the yearly-averaged χ value computed by the modal model was up to 70 percentage points different than the benchmark values. These errors tended to be zonally structured, with the modal method predicting a more internally mixed aerosol at low latitudes, and a more externally mixed aerosol at high latitudes, compared to the benchmark.

16CC.16

Role of Organic Acid-Amine Reactions in Atmospheric New Particle Formation. SANDRA FOMETE, Coty Jen, *Carnegie Mellon University*

Atmospheric New Particle Formation (NPF) plays a critical role in climate, air quality and human health. Though aerosols play an important role in climate change, the mechanisms behind aerosol particle formation in the atmosphere are still not well understood. Studies have identified sulfuric acid, water, oxidized organics, and ammonia/amines as main precursors to nucleation of freshly formed aerosol particles in the atmosphere. However, the role of organic diacids such as oxalic and malonic acids on atmospheric NPF has not been extensively explored. Oxalic (OxA) and malonic acids (MaA), which are naturally and anthropogenically produced, are much higher in concentration than sulfuric acid (~10^{10} vs ~10^{6}-10^{8} cm-3 respectively) in the atmosphere. In addition, computational chemistry studies predicts that organic diacids can react with amines in the atmosphere to form stable organic salts in the absence of sulfuric acid. In this study, we examined nucleation reactions of malonic and oxalic acids with mono and diamines at various relative humidity values. These nucleation reactions were carried out in a clean laminar flow reactor operated at ~298-300K. The chemical composition of the freshly nucleated clusters in the flow reactor were analyzed using a custom-built, transverse chemical ionization atmospheric pressure interface long time of flight chemical ionization mass spectrometer (Cluster CIMS). A nanoparticle sizer and counter, which can measure down to ~1 nm in diameter, was used to analyze the effect of OxA and MaA on the rate of formation and growth of particles in the flow reactor. Contrary to computational predictions, no new particles form from diacid-amine nucleation reactions. However, addition of sulfuric acid to the dicarboxylic acid-amine reaction system leads to a higher particle formation rate and growth rate compared to the previously studied sulfuric acid-diamine binary nucleation system. Results from this study improves current understanding of how new particles form in the atmosphere and will enable improvements in current regional and global models that predict climate change.

16CC.17

Analysis of Cloud Condensation Nuclei Number, Hygroscopicity and Cloud Formation Over the Swiss Alps. PARASKEVI GEORGAKAKI, Aikaterini Bougiatioti, Jörg Wieder, Zamin A. Kanji, Fabiola Ramelli, Jan Henneberger, Claudia Mignani, Maxime Hervo, Alexis Berne, Ulrike Lohmann, Athanasios Nenes, *LAPI, EPFL (Switzerland) / ICE-HT, FORTH (Greece)*

Orographic mixed-phase clouds (MPCs) provide a natural laboratory to investigate the complex web of interactions and feedbacks between atmospheric dynamics, cloud microphysics and terrain. Due to their frequent occurrence over mountain barriers, orographic MPCs play a major role in alpine weather, hydrology and climate. Here we analyze observations collected in the Alpine region of Davos, Switzerland during the Role of Aerosols and Clouds Enhanced by Topography on Snow (RACLETS) field campaign during February and March 2019. Observations of aerosol size distributions, cloud condensation nuclei, hygroscopicity and lidar-derived vertical velocities coupled with a state-of-the art droplet activation parameterization are used to quantify how changes in aerosol and dynamical parameters modulate the predicted droplet number and maximum supersaturation developed in the MPCs. The proposed method performed remarkably well yielding a droplet closure within ~25%. Strongly influenced by the velocity distribution (expressed by its standard deviation, σw) that ranges from 0.1 to 0.6 ms^{-1}, droplet formation is driven by aerosol variability (aerosol-limited regime) when aerosol levels are between 300 and 1500 cm^{-3}. We also find that droplet number never exceeds a characteristic limit of ~150-450 cm^{-3}, which depends solely on the value of σw. The mean CCN-derived hygroscopicity parameter value is ~0.25, which is representative of continental aerosol. Fresh emissions from anthropogenic activities in the valley floor in Davos, apart from increasing cloud droplet number, reduce cloud supersaturation and make the clouds insensitive to aerosol and sensitive to vertical velocity variations. The hourly mean values of σw at the high mountaintop site are greater by 0.1 ms^{-1} than the corresponding values recorded at the valley site, indicating that clouds forming are less susceptible to aerosol fluctuations. Identifying regimes where dynamics can potentially overshadow variations in aerosol concentration is key for interpreting and constraining the aerosol indirect effects.

16CC.18

The North Atlantic Aerosols and Marine Ecosystems Study – A Multi-Year Data Set of Aerosol-Cloud Observations. RICHARD MOORE, NAAMES Science Team, *NASA*

This poster summarizes the combined aerosol and cloud observations obtained from the recently concluded, 5-year NASA NAAMES Earth Venture Suborbital field campaign (https://naames.larc.nasa.gov/). The NAAMES dataset is permanently archived in the NASA Atmospheric Science Data Center (ASDC; https://doi.org/10.5067/Suborbital/NAAMES/DATA001) and the SeaWiFS Bio-Optical Archive and Storage System (SeaBASS; https://doi.org/10.5067/SeaBASS/NAAMES/DATA001). The data set includes ship-, aircraft-, and satellite-based observations of the remote North Atlantic that were carried out during four, approximately-month-long deployments in November 2015, May 2016, September 2017, and March 2018. Here, we focus on the combined subset of data from the first three deployments that focused on sampling boundary layer aerosols and clouds, as, unfortunately, an aircraft engine failure prevented data from being obtained during the 2018 deployment. The aircraft completed twenty cloud modules, each consisting of a series of vertically-stacked, horizontal legs: near-surface 100-meter-altitude leg, below cloud, above cloud base, below cloud top, above cloud top, and a high-altitude remote sensing leg. Each was designed to provide in situ and remote sensing information regarding the vertical structure of the remote marine cloudy atmosphere. Additional information is provided from ship-based radiosonde and ceilometer measurements, while in situ instruments on the ship capture the atmospheric composition at roughly 10 m above the sea surface. We present a description of the key observational variables, summary statistics of the dynamic range of aerosol and cloud variability encountered during NAAMES, and contextual information for those interested in exploring and analyzing the NAAMES data set in the future.

16CC.19

Assessing the Role of Surface Tension Depression in Sesquiterpene Organic Aerosol CCN Activity.

BENJAMIN SCHULZE, Ryan Ward, Yuanlong Huang, Andreas Zuend, John Seinfeld, *California Institute of Technology*

Numerous studies suggest that low-solubility, surface-active organic species can depress the surface tension of activating cloud droplets. Detailed understanding of this process is needed to accurately represent CCN activation, as particle critical supersaturation depends on surface tension variation during droplet growth. Sesquiterpene oxidation products, which constitute a particularly hydrophobic class of biogenic SOA, may reduce surface tension when present in activated particles. However, the existence of such surface tension effects, as well as their dependence on factors such as dry particle size, chemical composition, and the presence/absence of inorganic solutes, is largely unknown. Here, we evaluate experimentally the CCN activity of mixed β-caryophyllene SOA-ammonium sulfate (SOA-AS) particles of varying size, organic mass fraction, and oxidative age generated in the Caltech Photooxidation Flow Tube reactor (CPOT). We use multiple droplet activation models, including the Aerosol Inorganic–Organic Mixtures Functional groups Activity Coefficients (AIOMFAC) model and its gas–particle equilibrium variants to interpret the observations. These analyses permit evaluation of the extent to which simplified parameterizations of CCN activity, such as the κ-Kohler model, reasonably describe sesquiterpene SOA activation across the broad range of particle sizes, oxidative ages, and organic:inorganic mass ratios found in the atmosphere. Simultaneous measurements of aerosol composition using an Aerodyne AMS and filter-based thermal-desorption CIMS allow linkage of CCN properties to changes in the abundance of specific organic species. Using an aerosol cloud parcel model, we evaluate changes in cloud droplet number concentrations produced as a result of different assumptions regarding the SOA-AS CCN activation properties. Our results provide insight into the physicochemical detail needed to accurately represent biogenic SOA CCN activation in regional and global models.

16RA.1

The Optical and Molecular Characteristics of Water-soluble Organic Carbon in Seasonal Snow across Northern Xinjiang, Northwestern China.

YUE ZHOU, Christopher West, Anusha P.S. Hettiyadura, Xiaoying Niu, Tenglong Shi, Wei Pu, Xin Wang, Alexander Laskin, *Purdue University*

The deposition of light-absorbing aerosol on snow lowers the surface albedo and therefore influences the regional and global climate. In this study, snow samples were collected across regional area of northern Xinjiang, Northwestern China to investigate the optical and molecular characteristics of water-soluble organic carbon (WSOC), and to estimate effects of deposited aerosol on radiative forcing. For samples collected from the industrial region (IND) in Xinjiang, the concentrations of WSOC were higher than those from remote region (REM) (1.97 mg L-1 vs. 0.92mg L-1). The average absorption coefficient of the IND samples was approximately twice higher than that of the REM samples, however values of their characteristic mass absorption coefficients (MACs) showed no substantial difference. Based on the Excitation-Emission Matrices (EEMs) of WSOC samples and parallel factor (PARAFAC) analysis, two humic-like (HULIS-1 and HULIS-2) and one protein-like (PRLIS) components were identified. IND samples exhibited higher relative intensities of HULIS-2 (46%), but lower PRILS contributions (30%) compared to those of REM samples (36% and 42%, respectively). Molecular-level characterization of WSOC samples using high-resolution mass spectrometry provided further insights into differences between IND and REM collected WSOC samples. Generally, the IND samples were characterized by lower H/C and O/C elemental ratios, but higher unsaturated degree compared to REM samples. Much more CHOS and CHONS compounds were detected in IND samples, indicating different sources of snow WSOC from these two regions. The averages of WSOC-induced radiative forcing (RF) were estimated as 0.21 and 0.14 W m-2 in IND and REM regions, respectively, and contributed to 7% and 10% of the BC-induced RF. This study presents a comprehensive overview of WSOC in seasonal snow of Northwestern China, which helps to better understand their characteristics, sources, and climatic effects.

16RA.2

Influence of Small-scale Agricultural Activity on Local Particle- and Gas-phase Organic Composition. GRAHAM FRAZIER, Chenyang Bi, Namrata Shanmukh Panji, Gabriel Isaacman-VanWertz, *Virginia Tech*

Localized human activity can have a wide range of atmospheric impacts, from direct emissions of gas- and particle-phase reactive carbon, to influencing the chemical transformations of dominant biogenic emissions. The Covid-19 pandemic-related lockdown lowers community emission and enables us to better examine localized anthropogenic emissions. We present data from a new month-long field deployment to characterize changing biogenic and anthropogenic emissions during the aforementioned time period. The composition of organic aerosol and aerosol-forming organic gases were measured by a semi-volatile thermal desorption aerosol gas chromatography (SV-TAG) at a small farm at the western edge of the Richmond, VA, metropolitan area, representative of rural suburb interface in the southeastern US. Particle and semi-volatile gases were collected and analyzed by gas chromatograph/mass spectrometry with hourly time resolution for a one-month period in the late spring during the pandemic-driven stay-at-home orders. This work focuses on understanding the influence of local agricultural activity on particle chemistry, direct particle emissions, and changes to emissions from vegetation. We present concentrations of oxidation products and their precursors and discuss them in the context of meteorological conditions and changing human activity.

16RA.4

Per- and Polyfluoroalkyl Substances (PFASs) in Ambient Fine Aerosol (PM2.5) in North Carolina. JIAQI ZHOU, Karsten Baumann, Jason Surratt, Ralph Mead, Stephen Skrabal, Robert Kieber, Gene Avery, Megumi Shimizu, Wanda Bodnar, Zhenfa Zhang, Jamie DeWitt, Mei Sun, Leonard Collins, Barbara Turpin, *UNC-Chapel Hill*

While per- and polyfluoroalkyl substances (PFASs), especially legacy compounds, have been measured in ambient air in urban and rural environments at several locations globally, PFASs concentrations, source contributions and atmospheric transformations remain poorly understood. North Carolina (NC) is a good place to study these, given the existence of a fluoropolymer and specialty chemicals manufacturing plant (Chemours) and large military bases, as well as more typical sources of environmental PFASs contamination (e.g., fluorinated fire-fighting foam use, urban waste streams). In addition to ingestion of PFASs as a result of direct contamination of drinking water supplies via atmospheric deposition, potential human exposure to PFASs occurs also through inhalation. For these reasons, we initiated a one-year sampling campaign involving 5 NC locations and seasonally-composited 6-day duration ambient fine particulate matter ($PM_{2.5}$) samples collected on pre-baked quartz fiber filters downstream of a multiple-jet 2.5 mm cut-point impactor. Quarterly composited samples were analyzed for 34 targeted PFASs by LC-MS/MS on an AB SCIEX Triple Quad™ 6500 mass spectrometer system. In all, 7 PFASs were above detection limits (perfluoro-n-octanoic acid (PFOA), sodium perfluoro-1-octanesulfonate (PFOS), sodium perfluoro-1-heptanesulfonate (PFHpS), perfluoro-n-dodecanoic acid (PFDoA), perfluoro-n-heptanoic acid (PFHpA), perfluoro-n-undecanoic acid (PFUnA), ethanesulfonic acid, 2-[1-[difluoro(1,2,2,2-tetrafluoroethoxy)methyl]-1,2,2,2-tetrafluoroethoxy]-1,1,2,2-tetrafluoro- (Nafion BP2)) and mostly below 1 pg/m^3 in respirable $PM_{2.5}$. PFOA and PFOS were most frequency detected. Elevated PFOA and PFOS concentrations were observed in warmer months at Charlotte (14.1 pg/m^3 for PFOA) and Wilmington (4.75 pg/m^3 for PFOS), respectively. Concentrations will be placed in context and plausible explanations for the elevated concentrations will be discussed.

16RA.5

Evaluation of MODIS MAIAC AOD Retrievals against AERONET AOD over Different Land Cover Types.

SOMAYA FALAH, Alaa Mhawish, Meytar Sorek-Hamer, David Borday, *Technion*

The Multi-Angle Implementation of Atmospheric Correction (MAIAC) algorithm enables retrieving aerosol and surface bidirectional reflectance products over the land from the Moderate Resolution Imaging Spectroradiometer (MODIS) measurements. We performed critical assessment of MAIAC AOD550nm at 1km spatial resolution using ground-truth AOD550nm data from 21 Aerosol Robotic Network (AERONET) sites in Northern Africa (NA), California (CA) and Germany (GR) from the years 2007-2017. For this, we centered the MAIAC AOD, spatially averaged over 1, 9, 25 and 81 km2 (corresponding to 1x1, 3x3, 5x5 and 9x9 pixels of 1x1 km), around the AERONET stations. AERONET Version 3, Level 2 (V3, L2) Direct Sun AOD retrievals were averaged over 5, 15 and 30 min around the satellite overpass time. This enabled us to investigate the effect of different spatial and temporal averaging windows on the MAIAC performance.

The MAIAC accuracy was found to depend on the surface properties, with ~70% of the retrievals falling within the expected error, EE = ±(0.05 + 0.05 × AOD), and the correlation coefficient, R2, exceeding 0.897 over highly vegetated (i.e. dark) regions (NDVI > 0.6). However, the accuracy of AOD retrievals over bright surfaces was poorer, with EE = 58% and R2 = 0.772. In addition, the MAIAC accuracy is also affected by the aerosol loading in the atmospheric column, estimated in terms of high/low AOD, and by the aerosol type. The retrieval bias found higher at high aerosol loading (high AOD) and coarse aerosol types (low AE).

In general, Aqua MAIAC AOD retrievals showed good agreement with the AERONET measurements, with correlation coefficients of 0.768, 0.634 and 0.747, and expected errors of 50.3%, 73.54% and 60.4%, for North Africa, California and Germany, respectively.

The results contribute to a comprehensive evaluation of MAIAC AOD retrievals, with the latter being used for estimation particulate matter over different land cover types.

16RA.6

Shipborne Measurements of Fine Particles over the Yellow Sea during Spring (2015-2018).

NOHHYEON KWAK, Hyunok Maeng, Seojong Kim, Kwangyul Lee, Arom Seo, Jihyo Chong, Jo Wan Cha, Sang-bum Ryoo, Kihong Park, *Gwangju Institute of Science and Technology*

Atmospheric environment over the Yellow Sea located between China and Korea was often affected by the continental air masses transported from the two countries. In this study, shipborne measurements were carried out on board the GISANG 1 (Research Vessel of the Korea Meteorological Administration) every spring from 2015 to 2018 to examine chemical and physical characteristics of fine particles over the Yellow Sea. For chemical composition, ionic species (NH4+, Na+, K+, Mg2+, Ca2+, Cl-, NO3- and SO42-), elements (Mg, Al, V, Cr, Mn, Co, Ni, Cu, Zn, As, Se, Sr, Cd, Ba and Pb), organic carbon (OC) and elemental carbon (EC) were analyzed. Transmission electron microscopy/energy dispersive spectroscopy (TEM/EDS) was used to look into the morphology and elements of fine particles. Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model of National Oceanic and Atmospheric Administration (NOAA) was applied to investigate the origins and pathways of air masses arriving at the sampling location. During shipborne measurement in 2018, the percentage of air masses that passed the Sea, China and Korea were 53.3%, 25.5% and 9.2%, respectively. Averaged mass concentration of PM2.5 was 18.6 ± 10.6 µg /m3. Three high PM2.5 episodes were identified, having concentrations over 25 µg/m3. The highest concentration of 32.1 µg/m3 was observed on May 24 possibly related to long-range transported dust. During the high PM2.5 episodes, higher fraction of Al, Sr, Zn, Ba and Cd, and lower fraction of Na+, Cl-, NO3-, SO42-, Mn, Co, Ni and Cu in PM2.5 were observed relative to non-event periods. Further discussion on morphology and chemical data of PM2.5 will be presented.

16RA.7

Identifying the Influence of Wildland Fires on Air Quality Monitoring Data. R BYRON RICE, Stephen McDow, Katie Boaggio, Mckayla Lein, *U.S. EPA*

Identifying and quantifying the influence of wildland fires on ambient air quality is an emerging topic of interest relevant to the assessment of public health and environmental impacts of air pollution. The influence of wildland fires on monitor concentrations is generally established by the demonstration of unusually high concentrations compared to typical seasonal levels, combined with clear evidence that fire emissions were transported to the monitor, such as wind trajectory analysis or satellite imagery. However, the application of these approaches has been largely limited to the most extreme events. By linking known wildland fires to air quality monitoring station locations over a broad range of concentrations using the Monitoring Trends in Burn Severity (MTBS) database and other fire location data sources, we will analyze common trends in the composition of air quality monitoring data and determine if these trends can indicate the likelihood of influence from wildland fires. Ultimately, we seek to develop a systematic and reproducible method for identifying instances of wildland fire influence on air quality monitoring data. 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.

16RA.8

Mixing State of Secondary Species in Alaskan Arctic Aerosol Using Single-Particle Mass Spectrometry. JUDY WU, Jun Liu, Jamy Lee, Lucia Upchurch, Patricia Quinn, Kerri Pratt, *University of Michigan*

Atmospheric aerosol particles are complex chemical mixtures that play a significant role in impacting climate and the environment. The distribution of chemical species across the aerosol population (i.e. chemical mixing state) impacts particle properties, including the ability to take up water and to scatter or absorb light. Few measurements exist of the mixing states of aerosol particles in the Arctic, particularly in the fall and winter. To better understand atmospheric processes in the Arctic, the APUN (Aerosols during the Polar Utqiaġvik Night) field campaign during November to December 2018 included deployment of an aerosol time-of-flight mass spectrometer (ATOFMS) to measure the chemical composition of individual particles in Utqiaġvik, AK. These measurements provide information about the sources of aerosol particles and the chemical processes they have undergone in the atmosphere. Based on the presence of specific marker ions, which act as a chemical fingerprint, the particle mass spectra were sorted into groups, including sea spray aerosol (both aged and fresh), organic carbon, biomass burning, and other minor types. For each of these aerosol particle categories, the presence or absence of certain species can shed light on how the aerosol particles were impacted by atmospheric processes such as chemical aging and long-range transport. For instance, numerous aerosol particle spectra contained sulfate or nitrate species, which indicated that chemical aging of the particles occurred. By combining bulk aerosol chemical composition data obtained by the National Oceanic and Atmospheric Administration and single-particle ATOFMS data at Utqiaġvik, the distribution of chemical species measured by the long-term monitoring site across individual particles can be identified and thereby improve the understanding of the atmospheric processes in the Arctic.

16SA.1

Elucidating Ambient and Indoor Sources of VOCs in Dhaka, Bangladesh. Md. Aynul Bari, SANCHITA PAUL, Nisha Ahamed, Christophe Walgraeve, Herman Van Langenhove, *University at Albany, SUNY*

Exposure to important ozone precursors i.e., VOCs is of interest because of their potential carcinogenic and other adverse effects on public health. Limited studies are available about ambient VOC levels in Dhaka, the Capital of Bangladesh. To our knowledge, this is the first exploratory study to understand ambient and indoor sources of VOCs in Bangladesh. The data used in this study was obtained from the Ghent University VOC study for Dhaka. Ambient and indoor concentrations of VOC were measured in urban and industrial locations during 2011 and 2013. Both ambient and indoor VOC samples (n = 54) were collected for three separate days (two during weekdays and one at weekend) at two durations (morning and evening) using Tenax TA tubes. A total of 84 VOC species were analyzed by thermal desorption-gas chromatography-mass spectrometry (TD-GC-MS). Median ambient and indoor concentrations of total VOCs were 101 $\mu g/m^3$ and 237 $\mu g/m^3$, respectively. A multivariate receptor model positive matrix factorization (PMF) was applied to better interpret the complex nature of VOC sources. Traffic was identified as the dominant ambient source followed by industrial/vehicular evaporative and biomass emissions. Indoor sources include fragranced consumer products, floor and wall coverings, and deodorizers. Source-specific carcinogenic and non-carcinogenic health risk values were also calculated. Despite limited sample size, these findings offer preliminary information about different emission sources that influence VOC levels in Dhaka and this information can support policymakers in the development of appropriate plans or actions for controlling VOCs in the air.

16SA.2

Ozone Source Apportionment in the Year 2050 under Different Energy Scenarios. YUSHENG ZHAO, Michael Kleeman, *University of California, Davis*

Previous studies that simulated air quality in California under GHG emissions reductions scenarios noted declines in predicted PM2.5 concentrations but increases in predicted ozone concentrations within major cities. Understanding the source of ozone formation and the optimal control measures will improve public health outcomes in those future scenarios.

Here we simulate the air quality in California in 2050 using different energy portfolios that optimize the economic outcomes under different assumptions about available technology and climate change. The chemical transport model used for each simulation was equipped with an ozone source apportionment technique to reveal NOx and VOC sources that contribute to ozone formation. The model spatial resolution allows separate analysis from different geographical regions to focus on the urban cores where high ozone concentrations are most persistent. Ozone source contributions are quantified from nine source types: onroad gasoline vehicles, onroad diesel vehicles, offroad gasoline vehicles, offroad diesel vehicles, woodsmoke, food cooking, aircraft, natural gas, and others (including biogenic emissions). Simulations are conducted at 24km and 4km resolution. The results identify the dominant source of ozone formation in California in the year 2050 and suggest mitigation plans that can be used to reduce the ozone concentration to the level that meets the air quality standards.

16SA.3

Relative Impact of Schiphol Airport Activities in Comparison to Local Freeways on the Increased Particle Number Concentrations (PNCs) in the Nearby Communities.

MILAD PIRHADI, Amirhosein Mousavi, Mohammad Sowlat, Nicole Janssen, Flemming Cassee, Constantinos Sioutas, *University of Southern California*

In this study, we utilized the positive matrix factorization (PMF) source apportionment model to quantify the impact of the Schiphol airport major activities and other local sources on total particle number concentrations (PNCs) in the nearby urban areas affected by the airport. Time-and size-resolved PNCs in parallel with the concentrations of auxiliary variables, such as black carbon, PM2.5, gaseous pollutants (CO and NOx), and number of departures/arrivals were measured over a 6-month period near the Schiphol airport to be employed in the model. Our results demonstrated that the airport activities, collectively, accounted for 79.3% of total PNCs in the area. “Aircraft departures” and “Aircraft arrivals” were characterized with mode diameters <20 nm and contributed to 46.1% and 26.7% of PNCs, respectively. “Ground service equipment (GSE)”, with a mode diameter of 60-90 nm, accounted for 6.5% of the PNCs. “Road traffic”, mainly associated with the surrounding freeways, was characterized with a mode diameter of 30-40 nm, and contributed to 18.0% of total PNCs although its absolute contribution to PNCs was close to that of areas extensively affected by traffic emissions. Finally, “Urban background” with a mode diameter at 150-225 nm, showed a negligible contribution (2.7%) to total PNCs; while it dominated the particle volume/mass concentrations with a contribution of 58.2%. The PNC pollution roses plotted for the identified factors corroborated their origin by providing critical information on the directionality of each identified source to the sampling site. We illustrated that each of the airport major activities as well as other sources present in the area (e.g., road traffic) are characterized by a single mode diameter. More importantly, our findings highlight the dominant role of the Schiphol airport activities in ambient PNCs in the surrounding areas, which could adversely affect the public health.

16SA.4

Effect of Gas-Particle Partitioning on Source Apportionment of Ambient Mass Spectrometry Data.

SAHIL BHANDARI, Andrew Dinh, Gazala Habib, Joshua Apte, Lea Hildebrandt Ruiz, *University of Texas at Austin*

As a part of the Delhi Aerosol Supersite (DAS) campaign, submicron organic aerosol (OA) was measured in spring 2018 in Delhi, India using an Aerodyne aerosol chemical speciation monitor. Previously, we conducted positive matrix factorization (PMF) on this particle-only dataset. We obtained three factors: a hydrocarbon-like OA (HOA) factor, a biomass burning OA factor, and an oxidized organic aerosol (OOA) factor. Recent research suggests that the inclusion of measured or modeled gaseous organic compounds allows improved characterization of sources by accounting for the non-linearity effects of gas-particle partitioning (Xie et al., 2014).

Here, we estimated gas-phase concentrations corresponding to HOA, BBOA, and OOA by using volatility basis set (VBS) parameters for particle-only PMF factors and assuming equilibrium. We applied PMF to the combined gaseous and particle-phase data using the EPA PMF tool. This combined PMF yielded three factors similar in mass spectra to the particle-only analysis but different in contributions. Particularly, compared to the particle-only analysis, the combined analysis amplifies the contributions of the HOA and BBOA factors, especially during nighttime. This combined particle-gas phase source apportionment of mass spectrometry data may more accurately reflect the relative importance of different sources contributing to particulate matter formation.

Reference:

Xie, M., Hannigan, M.P., and Barsanti, K.C., 2014. Impact of gas/particle partitioning of semivolatile organic compounds on source apportionment with positive matrix factorization. Environmental Science & Technology, 48(16), pp.9053-9060.

16SA.5

Aerosol Concentration in Northern South America: Attribution to Economic Sectors Using Chemical Transport Modeling. SEBASTIAN ESPITIA, Alejandra Montejo-Barato, Ricardo Morales Betancourt, Jorge A. Bonilla, Claudia Aravena, *Universidad de los Andes*

Air quality modeling is a widely used tool to represent the complex meteorological and chemical processes that take place in the atmosphere and ultimately determine air quality at a given location. These tools, however, have not been thoroughly utilized in Colombia to inform the design of environmental public policy. In this work, we use the chemical transport model WRF-Chem version 3.9.1 to evaluate the impact of different economic sectors on aerosol particles and gas-phase pollutants in Colombia and its capital, Bogotá. Three nested domains located in northern South America were used with resolutions of 27 km, 9 km, and 3 km, with 120x120, 126x126 and 132x132 grid-cells in each domain, respectively. All domains had 41 vertical sigma-pressure levels. Anthropogenic emissions from the global emissions inventory EDGARv4.3.1 were merged with a local emissions inventory for the city of Bogota. Biogenic emissions are also included using MEGAN. Aerosols are described with the two-moment, modal aerosol scheme MADE-VBS. A base case simulation was generated for the three domains. To evaluate the regional contribution five scenarios were defined disaggregating anthropogenic emissions into Agricultural, Electric Power Generation, Industrial, Mobile, Commercial, and other´s sectors. At the national scale, our results show that the sectors with the greatest contribution to PM2.5 concentrations are Mobile and Industrial, contributing 2.8 and 2.3 µg m^{-3} respectively, to the monthly-mean surface concentration. To establish contributions at the city level, only the sectors relevant for urban areas were evaluated (Industrial, Mobile and Resuspended Particulate Matter). For the city of Bogota, it was found that the paving of unpaved roads, the heavy-duty vehicles renewal and technology change in the industry can generate a maximum reduction of 8.0, 2.0 and 1.6 µg m^{-3} respectively, benefiting low and middle income areas of the city.

16UA.1

Estimation of Effective Particle Mass Emission Indices from In-use Commercial Aircraft based on Field Observations. KENTARO MISAWA, Yuji Fujitani, Akihiro Fushimi, Yoshiko Murashima, Hiromu Sakurai, Nobuyuki Takegawa, *Tokyo Metropolitan University*

Particle number size distributions in exhaust plumes from in-use commercial aircraft were observed using a scanning mobility particle sizer (SMPS) and an engine exhaust particle sizer (EEPS) at an observation point near the major runway of Narita International Airport from February 5 to 26, 2018. The mixing ratios of carbon dioxide (CO_2) were also measured simultaneously. We found reasonably good agreement between the SMPS and EEPS data for selected time periods. We used the EEPS data for estimating the particle mass concentrations because of its fast response time. The majority of particle number concentrations were found at diameters smaller than 50 nm in aircraft exhaust plumes. The mass concentrations of particles in the diameter range of 6-560 nm (referred to as the submicron size range) did not exhibit significant diurnal variations, whereas those with diameters smaller than 50 nm (referred to as the nanoparticle size range) showed significant enhancements in the morning and evening, corresponding to a time slot with frequent aircraft traffics (rush hours). The “effective” particle mass emission indices (EIs) from an ensemble of aircraft plumes were estimated by using the EEPS and CO_2 data obtained during the evening rush hours on each day. The average EIs were found to be 31-107 mg $(\text{kg-fuel})^{-1}$ for the submicron size range and 14-75 mg $(\text{kg-fuel})^{-1}$ for the nanoparticle size range. The effective particle mass EIs derived in this study were found in the lower bound of the range of particle mass EIs reported by earlier studies.

16UA.2

Apportionment of Metals and Particulate Matter at an Environmental Justice School in Maywood, California.

STEVEN G. BROWN, Olivia Ryder, Jennifer DeWinter, Hilary Hafner, Jenny Lentz, Joe Lyou, Felipe Aguirre, *Sonoma Technology, Inc*

The community of Maywood in Los Angeles County, California, is surrounded by freeways with heavy truck traffic, a major railyard, and industrial facilities. Maywood is in the highest (1st) percentile of the environmental justice index for air pollution. During May-July 2019, we collected measurements at Heliotrope Elementary School in Maywood to determine sources and concentrations of metals, chromium-6, and diesel particulate matter (DPM), as well as to estimate associated health risks to the community. We collected hourly speciated metals via an Xact 625i, black carbon via an AE33 Aethalometer, PM2.5 via a T640 instrument, plus chromium-6 and meteorological measurements. Chromium-6 concentrations were, on average, 0.065 ng/m3, typical of urban Los Angeles levels, and associated with cancer risk of 2-in-a-million. Arsenic was the metal with the highest cancer risk, of 3 in-a-million, while DPM had a cancer risk more than 10 times higher than either arsenic or chromium-6. Using a combination of bivariate polar plots, source apportionment with positive matrix factorization (PMF), and other techniques, we found that arsenic was predominantly from reentrained dust that had been contaminated over previous decades from local arsenic emissions. Local sources were the main contributors to chromium and nickel concentrations. DPM concentrations were from a combination of emissions from the I-710 freeway and local arterial roads. These findings are being used by the community to develop an emission mitigation plan as part of the overall California AB 617 community air pollution reduction program. In addition to the scientific findings, we will present how results were shared and communicated with the community and how they are using the results to advance change.

16UA.3

Application of Machine Learning for Future Air Quality Predictions in Southern California.

KHANH DO, Arash Kashfi Yeganeh, Cesunica E. Ivey, *University of California, Riverside*

California's South Coast Air Basin (SoCAB) is well-known for extremely poor air quality due to its unique terrain and high levels of anthropogenic emissions. In this study, we use machine learning (ML) to recognize the natural pattern of ambient air pollutants in SoCAB and to explore the link between precursor emissions, meteorology, and $PM_{2.5}$/ozone. We investigated the historical changes of $PM_{2.5}$ and ozone using 25 years of air pollutant, emissions, and meteorological data. We tested the random forest regression (RFR) algorithm under multiple configurations to tune the prediction and provide the best air quality predictions. We first trained the RFR model with hourly meteorology and air pollutant data from 1994 to 2018. Meteorological data was retrieved from Ontario and Los Angeles International Airport monitoring stations, and air quality data were retrieved from the San Bernardino (CA) air monitoring station. The RFR training features were NO, NO_2, surface temperature, dew point temperature, visibility, surface pressure, relative humidity, wind speed, and wind direction. The RFR model was trained in five-year increments from 1994 to 2018. The R^2 ranged from 0.6 – 0.7 for historical hourly predictions. The model also enabled predictions of 2023 $PM_{2.5}$ and ozone using input data from a 2023 CMAQ simulation. The freedom of choosing input features enabled the investigation of $PM_{2.5}$ and ozone sensitivity to fluctuations in key variables, such as temperature and NO_x. These promising results indicate that ML can accelerate air quality research by augmenting traditional air quality modeling, reducing simulation time, and exploiting large datasets for historical simulations and future air quality predictions.

16UA.4

Estimating Dry Deposition of Atmospheric Aerosols by Rain Washoff from Urban Surfaces.

ALEXANDER JOHNSON, Cliff Davidson, *Syracuse University*

Building roofs comprise a major fraction of the overall horizontal surface area in urban environments and therefore are large receptors of dry deposited aerosols. After a long dry period, rainwater will wash the material from the surface and into stormwater runoff. Measuring the amount of suspended material in runoff from a building roof during a rainstorm could therefore potentially be used to estimate dry deposition to that surface during the antecedent dry period.

The objectives of this study were to experimentally estimate dry deposition to horizontal urban surfaces and to measure washoff of dry deposited material from the surfaces by rain. Two flat disks used previously to estimate dry deposition to horizontal surfaces were used along with two two bowl-shaped disks of similar size.

Experiments were conducted using the surrogate surfaces on the roof of Hinds Hall on the Syracuse University campus. For each experiment, the flat disks and bowl-shaped disks were exposed to collect dry deposition, and airborne concentrations were simultaneously be measured. Samples were then collected from the flat disks at the end of the exposure. In the subsequent rainstorm, fresh precipitation was collected, and runoff from the bowl-shaped disks was collected in sequential samples.

Samples were analyzed to estimate and compare the dry deposition fluxes and dry deposition velocities of fluoride, chloride, sulfate, and nitrate to the flat disks and bowl-shaped disks. The efficiencies of the washoff process for the same chemical species were also calculated using the samples from the bowl-shaped disks.

The results of this research are the first experimental data on rain washoff of dry deposited aerosols for carefully controlled surrogate surfaces. This information will be used to estimate dry deposition to actual building roofs and other flat urban surfaces.

16UA.5

Characterization and Variability of Urban Cooking Emissions Sources.

SUNHYE KIM, Jo Machesky, Drew Gentner, Albert A. Presto, *Carnegie Mellon University*

Cooking Organic Aerosol (COA) compounds form a significant proportion fraction of ambient $PM_{2.5}$ urban areas. COA is typically characterized by factor analysis of aerosol mass spectrometer data; there has been less focus on emissions from specific cooking sources. This study focuses on characterizing the variability of COA composition in urban areas to account for possible discrepancies between models and measured data.

This study measured emissions from 13 urban cooking sources in Pittsburgh and Baltimore using a mobile laboratory. We measured particle size and composition with the FMPS (fast mobility particle sizer), AMS, and aethalometer, as well as co-emitted gases (CO and CO_2). Emissions from most of the sampled restaurants were similar to both the COA mass spectra found in existing literature and to each other (R^2= 0.5-0.98). These high-resolution mass spectra had a high abundance of *m/z* 41 ($C_3H_5^+$) and 55 ($C_3H_3O^+$ and $C_4H_7^+$). We are currently working to compare size distributions of COA emissions across the restaurants.

One exception was the emissions from a commercial bakery, which showed distinctive CHN family peaks at *m/z* 58 ($C_3H_8N^+$), 86 ($C_5H_{12}N^+$), and 100 ($C_6H_{14}N^+$) that dominated the overall mass spectrum. These peaks were also present at smaller abundances at some of the restaurants where bread may have been baked on site.

Chemical transport models generally assume that all cooking sources emit particles of common composition and size. Therefore, the results of this study will directly inform any biases or errors inherent in this assumption. Understanding variability in cooking sources is especially important as models push to finer (~1 km) spatial resolution.

16UA.6

MAIA: A Satellite Investigation of PM Health Effects in Selected Global Cities. YANG LIU, David Diner, Howard Chang, Feng Xu, Jun Wang, Randall Martin, Christian L'Orange, Kristal Verhulst-Whitten, Sina Hasheminassab, *Emory University, Atlanta, GA*

Exposure to ambient particulate matter (PM) has been associated with various adverse health outcomes such as respiratory illness, cardiovascular diseases, adverse birth outcomes and premature death. PM is a complex mixture of chemical components with different sizes and shapes. Routine measurements of PM composition are costly and labor intensive, therefore are not readily available in most parts of the world. The sparse coverage of PM composition data presents a serious challenge to the assessment of population health effects due to PM exposure. To address this issue, NASA's Multi-Angle Imager for Aerosols (MAIA) investigation will generate daily estimates of PM composition estimates at 1 km spatial resolution in selected urban centers around the world. The MAIA satellite instrument is currently undergoing fabrication and testing, and is scheduled for launch in 2022 into sun-synchronous orbit aboard the General Atomics Orbital Test Bed-2 spacecraft. To provide sensitivity to aerosol properties such as optical depth, effective radius, and complex refractive index, MAIA's multispectral camera includes 14 bands in the ultraviolet (UV), VNIR, and shortwave infrared (SWIR), three of which are polarimetric, and is mounted on a gimbal to provide multiangular views of the target areas. Bayesian geostatistical regression models (GRMs) will be used to transform the retrieved aerosol optical and microphysical properties into near-surface mass concentrations of PM10, PM2.5, and speciated PM2.5 constituents (sulfate, nitrate, organic carbon, elemental carbon, and mineral dust). In addition to retrieved aerosol properties, the GRM predictors include geospatial data such as population and roadway densities along with meteorological parameters and estimated PM concentrations from the WRF-Chem chemical transport model. Filter-based PM speciation monitors within the Surface Particulate Matter Network (SPARTAN) plus a set of Aerosol Mass and Optical Depth (AMOD) samplers will be deployed to calibrate the coefficients of the GRMs. MAIA science team members, in collaboration with local researchers, will conduct epidemiological studies in different MAIA target areas to investigate the association of speciated particle mixtures with various health endpoints.

16UA.7

Firework Impacts on Air Quality in Metro Manila, Philippines during the 2019 New Year. GENEVIEVE ROSE LORENZO, Rachel Braun, Lin Ma, Eva-Lou Edwards, Connor Stahl, Mojtaba Azadi Aghdam, Andrea F Corral, Hossein Dadashazar, Paola Angela Banaga, Grace Betito, Gabrielle Leung, Shane Marie Visaga, Avelino Arellano, Maria Obiminda Cambaliza, Melliza Templonuevo Cruz, Alexander B. MacDonald, Ilya Razencov, Ed Eloranta, Robert Holz, James Bernard Simpas, Armin Sorooshian, *University of Arizona*

Fireworks affect air quality, visibility, atmospheric chemistry, and health. Yet, there have been no comprehensive physicochemical measurements of fireworks and their associated impacts in a megacity in Southeast Asia, where fireworks are customary. Novel 48-hour size-resolved particulate matter (PM) measurements were made before, during, and after New Year 2019 at the Manila Observatory in Quezon City, Philippines, as part of the Cloud, Aerosol, and Monsoon Processes Philippines Experiment (*CAMP^{2}Ex*). During the firework event, water-soluble ions and elements were mostly in the submicrometer diameter range. Total water-soluble bulk mass concentration was enriched 5.7 times, while the water-soluble mass fraction of $PM_{2.5}$ increased by 28.1% above background. Potassium and non-sea salt (nss) SO_4^{2-} contributed the most (70.9%) to the water-soluble mass, with their mass size distributions shifted to a larger submicrometer mode during the firework event, while NO_3^-, Cl^-, and Mg^{2+} (21.1% mass contribution) shifted from supermicrometer to submicrometer mode. Known firework components uninfluenced by secondary formation and with the highest enrichments (6.1 – 65.2) are identified as major firework tracers (Cu, Ba, Sr, K, Al, and Pb). They, excluding K, contributed only 2.1% to the total water-soluble bulk mass concentration. A K-rich cube and Cl^--rich crystal and capsule-shaped particles were detected via surface microscopy in the firework samples. Heavy surface aerosol loading observed with a High Spectral Resolution Lidar (HSRL) around the fireworks peak (22:00 – 03:00 local time) was associated with aerosol optical depth (AOD) values reaching 1.1, peak $PM_{2.5}$ concentrations, and reduced visibility. Enhanced particulate water-soluble mass fraction, enriched firework emission tracer concentrations, and shifts in mass size distributions during fireworks impact particles' respirability, hygroscopicity, and ability to form cloud condensation nuclei (CCN), while also altering uptake mechanisms for gases like SO_2 and influencing nearby waterbodies.

16UA.8

Performance and In-field Calibration for Low-Cost Sensors Measuring Ambient Particulate Matter in Kolkata, India.

V. FAYE MCNEILL, *Columbia University*

We present an in-field calibration of low-cost ambient particulate matter sensors (LCS) operating in greater Kolkata, India. Two datasets were examined: a network of 20 Clarity sensors operating from September 2018-April 2019 and a network of Purple Air sensors operating from August 2019-present. LCS were co-located with reference-grade PM monitors (RGM) operated by the West Bengal Pollution Control Board at Rabindra Bharati University (RBU), Victoria Memorial (VICTORIA), and Padmapukur (Howrah, PDM). Data from the co-locations were used to calibrate the LCS network using multiple linear regression and random forest approaches. Measured relative humidity and temperature were significant model features. Cross-calibration between co-located LCS-RGM pairs was tested. Calibrating PDM data using the model developed for the RBU co-located pair resulted in a 41.5% reduction of the RMSE. The cross-calibration yielded correct identification of days violating the 24h national ambient air quality standard for PM2.5 using the LCS network 85% of the time. The corrected data identifies days with an air quality index of “moderately poor” or worse 100% of the time, and “poor” or worse 97% of the time. This suggests that LCS can be a useful supplement to RGM networks for air quality management.

16UA.9

Discovery of Atmospheric Microplastics in Urban Emissions.

ANA MORALES, Jay Tomlin, Yoorae Noh, Andrew Whelton, Alexander Laskin, *Purdue University*

Micrometer and nanometer plastics (MNP) have become substantial environmental pollutants because of increased production and poor disposal management of various plastic products degrading in the environment. MNP particles were also recently deemed an emergent component of air pollution due to their ability to become airborne and undergo long-range atmospheric transport. Here, we reveal a substantial, yet unreported, source of atmospheric MNP in an urban area. The MNP were discovered in samples of steam water emitted at urban sewer repair sites, where the technique called plastic cured-in-place-pipes (CIPP) was employed. The CIPP installation procedure involves the chemical manufacture of a new plastic pipe inside an existing damaged pipe by blowing steam through the pipe, resulting in the release of MNP and other chemicals into the air. Optical imaging of MNP particles suspended in the steam water using a nano FlowCamTM showed a bimodal particle size distribution with the characteristic mean diameters of 300 nm and 3 µm, where particles of smaller mode exhibited high circularity and particles of larger mode showed substantial fractal dimensions. Electron microscopy analysis of the dry aerosol particles generated from the steam water showed abundant presence of even smaller MNP particles in the size range of 100-200 nm size, where smaller particles showed a higher degree of oxygenation. We investigated the chemical composition of MNP emitted during CIPP operations by employing multi-modal chemical imaging using SEM, Raman, and soft X-ray spectro-microscopy. This work provides a detailed description on the chemical composition of individual MNP particles related to CIPP manufacture, which is important in evaluating their contributions to urban environment.

16UA.10

Improved Prediction of Near Roadside Vehicle Emissions from PEMS and Laboratory Measurements.

AYLA MORETTI, David R. Cocker III, Matthew Barth, *University of California, Riverside*

Vehicle emissions are measured using dynamometers (coupled with test-cell emission instruments) 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-road particulate matter (PM) concentrations using these emission factors (EF) within emission models, such as the EPA's Motor Vehicle Emission Simulator (MOVES), are not in agreement with measured near-road PM concentrations. A majority of differences between the near-road ambient studies and MOVES could be due gas-particle partitioning that occurs immediately after the emissions rapidly dilute and cool in the ambient atmosphere. Gas-particle partitioning suggests that we need a better way to predict roadside emissions by extrapolating from PEMS and dynamometer-based measurements.

This research uses published volatility basis set (VBS) data coupled with new experimental data-using a variable residence and dilution tunnel connected to an engine. Using the VBS approach, the gas-particle partitioning of OA from a gasoline vehicle was modeled using Python to create a correction factor that can work with the outputted MOVES EF to correct for primary $PM_{2.5}$ from gasoline vehicles. This correction factor helps to bridge the gap between regulatory model estimations and what is measured near-roadways. Results indicate that, as suspected, the gas-particle partitioning plays a major role in final PM levels present in the atmosphere due to vehicle exhaust. This research explores sensitivity of dilution and temperature and shows that there is a bias in predicted roadside PM using the current transportation models.

16UA.11

Aerosol Acidity as a Driver of Aerosol Formation and Nutrient Deposition to Ecosystems.

ATHANASIOS NENES, Spyros Pandis, Maria Kanakidou, Armistead G. Russell, Shaojie Song, Petros Vasilakos, Rodney J. Weber, *LAPI/EPFL, Switzerland; ICE-HT/FORTH, Greece*

Nitrogen oxides (NO_x) and ammonia (NH_3) are central contributors to particulate matter (PM) concentrations worldwide. Ecosystem productivity can be modulated by the atmospheric deposition of this inorganic "reactive nitrogen". PM and nitrogen deposition responses to changes in the emissions of both compounds is complex and typically studied on a case-by-case basis.

Here we present a simple but thermodynamically consistent approach that expresses the chemical domains of sensitivity of aerosol particulate matter to NH_3 and HNO_3 availability in terms of aerosol pH and liquid water content. From our analysis, four policy-relevant regimes emerge in terms of sensitivity: i) NH_3-sensitive, ii) HNO_3-sensitive, iii) combined NH_3 and HNO_3 sensitive, and, iv) a domain where neither NH_3 and HNO_3 are important for PM levels (but only nonvolatile precursors such as NVCs and sulfate). When this framework is applied to ambient measurements or predictions of PM and gaseous precursors, the “chemical regime” of PM sensitivity to NH_3 and HNO_3 availability is directly determined.

The same framework is then extended to consider the impact of gas-to-particle partitioning, on the deposition velocity of NH_3 and HNO_3 individually, and combined affects the dry deposition of inorganic reactive nitrogen. Four regimes of deposition velocity emerge: i) HNO_3-fast, NH_3-slow, ii) HNO_3-slow, NH_3-fast, iii) HNO_3-fast, NH_3-fast, and, iv) HNO_3-slow, NH_3-slow. Conditions that favor strong partitioning of species to the aerosol phase strongly delay the deposition of reactive nitrogen species and promotes their accumulation in the boundary layer and potential for long-range transport.

With this new understanding, aerosol pH and associated liquid water content can be understood as control parameters that drive PM formation and dry deposition flux and arguably can catalyze the accumulation of aerosol precursors that cause intense haze events throughout the globe.

16UA.12

How Spatially Correlated Are Ultrafine Particle Number and Fine Particle Mass at Urban Scales? PROVAT SAHA, Shayak Sengupta, Peter Adams, Allen Robinson, Albert A. Presto, *Carnegie Mellon University*

The epidemiological evidence for ultrafine particles (UFP; particles with a diameter less than 100 nm) causing chronic health effects independent of fine particulate matter (PM2.5) mass is inconclusive. A prevailing view is that UFP and PM2.5 mass have different spatial patterns in urban areas, which should allow epidemiological studies to distinguish their independent, chronic health effects. Here, we investigate the intra-urban spatial correlation of PM2.5 mass and UFP exposures in Pittsburgh, Pennsylvania. Measurements and predictions of a land-use regression model indicate a moderate spatial correlation between particle number concentrations (PNC; a proxy for UFP) and PM2.5 mass (R2 of 0.38 and 0.41, respectively). High-resolution (1-km) chemical transport model simulations predict a much stronger spatial correlation (R2 ~ 0.8). The true spatial correlation likely lays within this range, the width of which is due to the combined effects of measurement noise and incomplete representation of emissions and other processes in the model. The finding of moderate to strong spatial correlation was initially surprising because secondary aerosol contributes the vast majority of PM2.5 mass in cities like Pittsburgh. However, intra-urban spatial patterns are strongly influenced by local emissions. The spatial correlation of PNC and PM2.5 mass concentrations indicates that, in Pittsburgh, concentrations of these pollutants are driven by emissions from the same sources, especially traffic and cooking. Furthermore, both pollutants largely behave as passive tracers at time scales of one day or less required for transport across most urban environments. Although previous research has shown little temporal correlation between PNC and PM2.5 mass (which may allow epidemiological studies to differentiate acute health effects), our finding of moderate to strong spatial correlation may complicate the use of epidemiological analysis to separate the chronic health effects of PNC from PM2.5 mass.

16UA.14

Air Quality Impact During and After the COVID-19 Lockdown in Global Cities. Shaojun Zhang, Jiajun Gu, K. Max Zhang, BO YANG, Yuejie Wang, Yifan Wen, Ye Wu, Jiming Hao, *Cornell University*

The pandemic of coronavirus disease 2019 (COVID-19) resulted in the stringent lockdown worldwide to reduce the infection rate. We adopted a fixed-meteorology technique based on machine learning techniques to analyze the air quality impacts from the COVID-19 lockdown for 10 metropolitan areas globally. Compared with the without lockdown scenario, we estimated that the lockdown reduced ambient NO2 concentrations by 36% to 53% during the most restrictive periods with the Level-1 public health emergence response control actions in China. The traffic analysis during the same periods confirmed that traffic emission changes were a major factor in the substantial NO2 reduction but also associated with increased O3 concentrations. In China, the lockdown also reduced PM2.5 concentrations, though heavy pollution episodes occurred during certain days due to the enhanced formation of secondary aerosol. The analysis implies that the air pollution levels are likely to rebound quickly as the as the economy reopens.

16UA.15

Long-term Observations of Submicron Atmospheric Aerosol Concentrations - Effect of Legislative Regulations and Economic Transformations.

NADEžDA ZíKOVá, Petra Pokorná, Zdenek Wagner, Jakub Ondráček, Philip K. Hopke, *Institute of Chemical Process Fundamentals CAS*

Atmospheric pollutant concentrations have mostly been decreasing in the last decades in the developed parts of the world, for example in Central Europe, due to legislative mandates and subsequent regulations as well as economic transformations. For some pollutants, however, the decreases have slowed in the recent years. An example of such a pollutant is submicron atmospheric particles.

In the Czech Republic, long-term submicron measurements of the atmospheric aerosol were established in 11/2007 at Prague-Suchdol, an urban background station. Five-minute particle number size distributions from 10 to 500 nm were measured using a scanning mobility particle spectrometer (3034 TSI SMPS) that was later upgraded to ACTRIS project standards. Even earlier, in 2002, submicron measurements begun in Rochester, NY with a very similar system.

In the over 12-years long dataset (2007-2019), the temporal trends were analyzed and compared to the legislative, economic, and source structure changes both in Prague and Rochester. Mitigation strategies and economic factors affecting the atmospheric aerosol concentrations [1] differ at the two locations. Zhou et al [2] showed that a closure of a coal-fired power plant and promulgation of fuel quality policies reduced local mercury emissions in Rochester. In Prague, preliminary results show the total number concentrations increased from 2011 to 2016, in parallel with the industrial production index.

Substantial changes have been observed in the concentrations of the smallest diameter particles [3], with an expected influence of new particle formation events, such as midday peaks (apart from the two traffic-related ones) observed in Prague data.

Project LTAUSA19006 of the Ministry of Education, Youth and Sports of the Czech Republic is acknowledged for financial support.

[1] Squizzato et al., Atmos. Environ., 183, 209–224, 2018.
[2] Zhou et al., Sci. Total Environ.,. 650, 1327–1337, 2019.
[3] Masiol et al., Sci. Total Environ., 633, 59–70, 2018.

16UA.16

An Evaluation of Air Quality Impacts from Different Urban Greening Strategies in Los Angeles County.

SHAN GU, Celia Faiola, *University of California, Irvine*

Volatile organic compounds (VOC) in the atmosphere have significant impacts on the formation of secondary pollutants, such as ozone and secondary organic aerosol (SOA). In urban areas, anthropogenic VOC (AVOC) emissions are leading contributors to ozone and SOA formation, but the essential role of biogenic VOC (BVOC) emissions could become more important as AVOC emissions decrease and urban greening programs are more widely implemented. Recent studies have demonstrated that BVOC emissions in urban areas may be increasing because of the large increase in urban forest coverage. However, few studies have been carried out to assess the impact on air pollutants in urban areas. Therefore, this study investigated relative contribution of speciated VOC emissions from both anthropogenic and biogenic sources on ozone formation potential (OFP) and secondary organic aerosol formation potential (SOAP) in Los Angeles county. Speciated AVOC emissions were estimated using the 2014 National Emission Inventory (NEI), SPECIATE database, and the SMOKE processing system from US EPA. The local vegetation data from the county's records was utilized to estimate BVOC speciation and emissions. The analysis was repeated for a base case (based on the inventories) and a range of potential future scenarios to investigate the effect of planting isoprene emitters vs monoterpene emitters. The relative contribution of each emission sector to total VOC emissions and the corresponding OFP and SOAP for each scenario will be presented. These results can be used to help inform best practices for future urban greening programs.

16UA.17

Spatial Pattern of Trace Metal Concentrations in Southern California Associated With Brake and Tire Wear Emissions. FARZAN OROUMIYEH, Irish Del Rosario, Michael Jerrett, Jonah Lipsitt, Jonathan Liu, Suzanne E. Paulson, Beate Ritz, Jiaqi Shen, Yifang Zhu, *University of California Los Angeles*

With a reduction in exhaust emissions in response to technology advancements and rigorous regulations, the significance of non-exhaust emission sources is increasing. Non-exhaust emission sources including brake and tire wear are rich in metals and therefore they can cause oxidative stress and contribute to overall health effects of particulate matter (PM). The aim of the current work is to provide information on spatial pattern of metals associated with brake and tire wear in southern California.

Using gravimetric measurement, the abundance of 55 metals in fine and coarse PM was studied in 51 sampling sites across southern California. The samples were collected during two sampling periods in summer and winter. The average concentration of fine PM in summer and winter was shown to be at 9.0 and 9.8 µg/m^3 respectively while the average concentration of coarse PM was 8.9 µg/m^3 in both seasons. The average concentrations of trace metal elements in fine PM were Ba (17.4 ng/m^3), Cu (8.8 ng/m^3), Fe (188.8 ng/m^3), Sb (3.0 ng/m^3), Zn (10.2 ng/m^3) while the concentrations in coarse PM were Ba (18.6 ng/m^3), Cu (8.4 ng/m^3), Fe (302.5 ng/m^3), Sb (1.6 ng/m^3), Zn (6.9 ng/m^3).

Multi-criteria decision analysis (MCDA) model was implemented to categorize the sampling sites based on the braking frequency by incorporating spatial criteria such as the traffic intensity, slope variance and intersection density. Analysis of correlation matrix and enrichment factors of the trace elements allowed to verify the locations with higher brake and tire wear frequency. Primary tracers of brake wear particles showed relatively high correlation suggesting that these metals are potentially generated by abrasive vehicular emissions.

16UA.18

How Have Air Quality and Perceptions of Air Quality Changed in Medellin Due to the 2020 Covid-19 Pandemic? PABLO GARCIA, Polina Glovátina-Mora, Joshua D. Vande Hey, *University of Leicester*

With the beginning of the COVID-19 quarantine, significant changes in PM2.5 concentrations were observed in Medellin, Colombia. PM2.5 was reduced from an average of 40 µg m-3 for the 30 days before the start of the quarantine to 23.4 µg m-3 for the first 30 days of quarantine corresponding to a reduction of 6.4 µg m-3 in the 2020 concentration anomaly with the 2015-2019 period average with a peak anomaly of -26 µg m-3 during the second week of quarantine. In this context, we reproduced a survey and workshop undertaken earlier in 2019 to evaluate the level of reflexivity regarding changes in air quality caused by modifications in human activity patterns under quarantine restrictions. The Initial survey and workshop were aimed at exploring conceptualizations of air pollution and air quality in Medellin under the conditions of persistently severe air pollution. We explore the potential role of narratives in the formulation of environmental policy and in the development of effective communication strategies for policy changes and scientific results. Quantitative and qualitative analysis of changes in perceptions in the sample population are presented. Air quality data analysis along with the review of recent debates in critical environmental humanities contextualize the survey and workshop results.

16UA.19

Air Quality in Atlanta during the COVID-19 Pandemic.

JEAN RIVERA-RIOS, Taekyu Joo, Chris Peng, Jennifer Kaiser, Nga Lee Ng, *Georgia Institute of Technology*

The COVID-19 pandemic has led to unprecedented reductions in anthropogenic activities in the US and around the world. We conducted air quality measurements at the Georgia Institute of Technology campus starting the last week of April with the goal of understanding the effects of reduced activity on air quality. The sampling site is 840 m away from Interstate 75/85 and 30−40m above ground. Multiple studies have been performed at this site in previous years. The available instrumentation includes NO, NO_2 and O_3 measurements as well as speciated aerosol components measured using a High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS) and a Scanning Mobility Particle Sizer (SMPS). Volatile Organic Compounds were measured using a Proton-Transfer-Reaction Mass Spectrometer (PTR-MS). We compare these measurements with similar measurements performed in summer 2019 at the same site and with monitoring stations located throughout the city. Results indicate reductions in anthropogenic emissions of NO and NO_2. Aerosol mass loadings appear to be lowered as well, although it is difficult to attribute these reductions solely to the pandemic.

17AC.1

Organic Aerosol and Brown Carbon Evolution in Fresh Wildfire Plumes: Roles of Dilution-Driven Evaporation and Phenolic Chemistry. BRETT PALM, Qiaoyun Peng, Carley D. Fredrickson, Ben H. Lee, Lauren A. Garofalo, Matson A. Pothier, Sonia Kreidenweis, Delphine K. Farmer, Rudra Pokhrel, Yingjie Shen, Shane Murphy, Wade Permar, Lu Hu, Teresa Campos, Sam Hall, Kirk Ullmann, Xuan Zhang, Frank Flocke, Emily Fischer, Joel A. Thornton, *University of Washington*

The evolution of organic aerosol (OA) and brown carbon (BrC) in wildfire plumes, including the relative contributions of primary versus secondary sources, has been uncertain in part because of limited knowledge of the precursor emissions and the chemical environment of smoke plumes. We made airborne measurements of a suite of reactive trace gases, particle composition and optical properties in fresh western U.S. wildfire smoke in July through August 2018. We use these observations to quantify primary versus secondary sources of biomass burning OA (BBPOA vs. BBSOA) and BrC in wildfire plumes. When a daytime wildfire plume dilutes by a factor of 5 to 10, we estimate that up to one third of the primary OA has evaporated and subsequently reacted to form BBSOA with near unit yield. The reactions of measured BBSOA precursors contribute only 13±3% of the total BBSOA source, with evaporated BBPOA comprising the rest. We find that oxidation of phenolic compounds contributes the majority of BBSOA from emitted vapors. The corresponding particulate nitrophenolic compounds are estimated to explain 29±12% of average BrC light absorption at 405 nm (BrC Abs_{405}) measured in the first few hours of plume evolution, despite accounting for just 4±1% of average OA mass. These measurements provide quantitative constraints on the role of dilution-driven evaporation of OA and subsequent radical-driven oxidation on the fate of biomass burning OA and BrC in daytime wildfire plumes, and point to the need to understand how processing of nighttime emissions differs.

17AC.2

Atmospheric Evolution of Emissions from a Boreal Forest Fire: The Formation of Highly- Functionalized Oxygen-, Nitrogen-, and Sulfur-Containing Compounds. JENNA DITTO, Megan He, Tori Hass-Mitchell, Samar Moussa, Katherine Hayden, Shao-Meng Li, John Liggio, Amy Leithead, Patrick Lee, Michael Wheeler, Jeremy Wentzell, Drew Gentner, *Yale University*

Forest fires are major contributors of reactive gas- and particle-phase organic compounds to the atmosphere. We used high resolution tandem mass spectrometry to perform a molecular-level speciation of evolving gas- and particle-phase compounds sampled via aircraft from a boreal forest fire in Saskatchewan, Canada. We observed diverse multifunctional compounds containing oxygen, nitrogen, and sulfur (CHONS), whose structure, formation, and impacts are understudied. The abundance of particle-phase CHONS species increased with smoke plume age, from 19% to 40% of the relative abundance of observed functionalized organic aerosol (OA) over the first 4 hours of downwind transport. The relative contribution of particle-phase sulfide functional groups increased with age from 4% to 40% of observed OA abundance, and were present in up to 75% of CHONS compounds. The increases in sulfides were accompanied by increases in ring-bound nitrogen, and both rose together with CHONS prevalence. A complex mixture of intermediate- and semi-volatile gas-phase organic sulfur species was emitted from the fire and depleted downwind, representing potential precursors to particle-phase CHONS compounds. We discuss potential reactions that formed these CHONS species, and origins of the reduced sulfur-precursors. Together, these results demonstrate CHONS formation from nitrogen/oxygen-containing biomass burning emissions in the presence of reduced sulfur species, and highlight chemical pathways that may also be relevant in situations with elevated levels of nitrogen and sulfur emissions from residential biomass burning and fossil fuel use (e.g. coal), respectively.

17AC.3

FIREX 2018/2019 Particle- and Gas-Phase Measurements: Emissions, Factor Analysis and Aging From Mobile Mass Spectrometers. FRANCESCA MAJLUF, Jordan Krechmer, Edward Fortner, Conner Daube, Christoph Dyroff, Joseph Roscioli, Tara Yacovitch, Benjamin Sumlin, Andrew Lambe, Scott Herndon, Manjula Canagaratna, Rajan K. Chakrabarty, John Jayne, Douglas Worsnop, *Aerodyne Research, Inc.*

Better measurements and constraints of volatile organic compounds (VOCs) are critical to modeling the effects of increasingly frequent wildfires in the western USA on secondary organic aerosol formation and the oxidant budget. Using a Soot Particle Aerosol Mass Spectrometer (SP-AMS) and a Vocus Proton Transfer Reaction Mass Spectrometer (Vocus PTR) on board the Aerodyne Mobile Laboratory (AML) seven different fires over two years (FIREX 2018 and 2019) were sampled providing extensive chemical composition and aging information of both the gaseous (VOCs, oxidized VOCs) and particulate (black carbon, organic carbon) emissions from fires. Emission ratios calculated from SP-AMS and Vocus PTR measurements display statistically significant consistency with previous measurements of controlled fires in a laboratory setting. Within specific fires, chemically unique mass spectral signatures of smoldering and flaming are determined from factor analysis. Lastly, since our mobile platform sampled plumes across several distances, including directly adjacent from a fire, the effect of oxidative aging on gas phase species concentrations and on particle size and composition are characterized. Several photochemical aging markers and their reactivity with daytime and nighttime oxidants are investigated. These results are compared with in-situ aging experiments of fire plumes that are oxidized in an oxidation flow reactor.

17BA.1

Characterization of Pollen Fragments in Atmospheric Aerosol Using Chemical Tracers. CHAMARI MAMPAGE, Dagen Hughes, Lillian Jones, Nervana Metwali, Peter Thorne, Elizabeth Stone, *University of Iowa*

Pollen grains contain allergens that can trigger allergic responses. In the presence of water, pollen grains (10-100 µm) can osmotically rupture to produce pollen fragments (<3 µm). The current study examines pollen fragments, fungal spores, and bacteria in size-resolved atmospheric aerosols. During springtime in Iowa City, Iowa, fine particle ($PM_{2.5}$) concentrations of fructose (a chemical tracer of pollen) increased on rainy days, especially heavy thunderstorms, and peaked when a tornado struck nearby. PM samples size-separated across 5 impactor stages revealed mass distributions that ranged 0.25-2.5 µm, consistent with pollen fragments that were also detected in collocated measurements. Meanwhile, mannitol (a fungal spore tracer) in $PM_{2.5}$ peaked on a warm day following rain and was primarily in supermicron particles, in agreement with the intact diameters of fungal spores (1-30 µm). Bacterial endotoxins in $PM_{2.5}$ also peaked on rainy days, with their mass primarily distributed to coarse PM. While the $PM_{2.5}$ concentrations of fructose, mannitol, and endotoxin all increased on rainy days, the greatest relative increase in concentration and decrease in particle size was observed for the pollen tracer. Together, these observations suggest that pollen grains ruptured into pollen fragments in the atmosphere. Compared to intact pollen grains, pollen fragments have longer atmospheric lifetimes, greater deposition in the lower lung, undergo longer range transport, and have greater potential to impact cloud and ice formation and precipitation.

17BA.2

Characterization of Fluorescent Bioaerosols Under Extreme Weather Conditions.

DAGEN HUGHES, Chamari Mampage, Lillian Jones, Zehui Liu, Elizabeth Stone, *University of Iowa*

Although rainfall washes pollen grains from the atmosphere, rain can also osmotically rupture pollen to produce submicron pollen fragments that may carry allergens. Through a multi-platform field campaign based in Iowa City, IA in the spring of 2019, we combined single-particle fluorescence spectroscopy (WIBS-NEO) with offline measurements of chemical tracers and intact pollen grains to provide the first online characterization of pollen fragments in the atmosphere. Collocated measurements were compared with the WIBS-NEO to characterize the size-dependent fluorescence signal of pollen fragments. A convective thunderstorm during tree pollen season (May 18) increased the submicron fluorescent particle concentration from 0.1 cm^{-3} to a local maximum of 1.3 cm^{-3}. At their peak, 34% of submicron particles fluoresced compared to only 5% prior to the storm, indicating their enrichment relative to other particle types. These fluorescent particles were identified as pollen fragments using size-resolved mass concentrations of fructose, hourly pollen grain concentrations, and light microscopy. The increase in pollen fragments during the thunderstorm can be explained by the osmotic rupturing of pollen grains in the atmosphere and subsequent transfer to the Earth's surface by precipitation downdrafts. Though the thunderstorm was brief, the fluorescent signal from pollen fragments remained elevated for more than 11 hours. Pollen fragments were also observed in stratiform precipitation and other convective thunderstorms during the tree and weed pollen seasons. The pollen fragments observed by the WIBS-NEO ranged in optical diameter from 0.5–3.0 µm with the greatest concentrations observed at the lower size limit of the instrument suggesting a high concentration of pollen fragments in particles < 0.5 µm. Understanding the concentrations, properties, and occurrence of pollen fragments in the atmosphere is important because they represent an under-characterized aerosol source and their size affects their atmospheric lifetime, climate-relevant properties, and ability to penetrate into the human respiratory tract.

17BA.3

Bioaerosols and Dust Are the Dominant Sources of Organic P in Atmospheric Particles.

KALLIOPI VIOLAKI, Athanasios Nenes, Maria Tsagaraki, Marco Paglione, Stéphanie Jacquet, Richard Sempéré, Christos Panagiotopoulos, *EPFL, LAPI, Lausanne*

The Eastern Mediterranean Sea, as many regions throughout the world, is strongly P-limited, with atmospheric nutrients deposition affecting its primary productivity. Numerous previous studies highlighted the importance of atmospheric inorganic P in fertilizing oligotrophic areas, which been thought primarily originated from dust. The amount and origin of organic forms of P, however, is virtually unknown. A new methodology developed to characterize phospholipids in aerosol was applied to a year-long aerosol dataset collected in the Mediterranean. This information, together with other biomarkers were used to characterize the sources of organic P in aerosol using Positive Matrix Factorization (PMF). The results revealed that dominant sources of organic P compounds are the bioaerosols and the dust. The co-existing of those sources in the spring period increased the organic P up to 53% of total P with more than a half to originate from bioaerosols. The soluble P content from dust aerosols is the similar magnitude of potential bioavailable organic P emitted from bioaerosols (~4 Gg P y-1), especially during the stratification period, when surface water is mostly nutrient exhausted.

The atmospheric deposition of dissolved P contribute as much as 9% to new production, however, the role of the atmospheric deposition of P may be more important in the future since recent results based on observations and modeling predict a decrease in phytoplankton productivity in oceans due to an enhancement in stratification caused by the warming climate.

17HA.1

In Vitro Toxicity of Complex Aerosols from Woody Biomass Combustion. WILLIAM VIZUETE, Karsten Baumann, Jose Zavala, Prakash Doraiswamy, Jean Kim, Solomon Bililign, Marc Fiddler, Damon Smith, Robert Newman, Ryan Chartier, Hadley Hartwell, Laquaundra Hampton, Ese Ekhator, Jade Scales, Nalyn Siripanichgon, Erin Dowell, Rudra Pokhrel, Vikram Rao, Ninell Mortensen, Jackson Seymore, *University of North Carolina at Chapel Hill*

Airborne particulate matter (PM) is responsible for ~4.8 million premature deaths worldwide and 92% of those deaths occur in low and middle income countries (LMICs). In many LMICs exposure to woody biomass combustion emissions alone cause 2.8 million deaths. Emissions from woody biomass consist of PM, various volatile organic compounds, and other gases that are harmful to human health. Epidemiological and toxicological studies, however, have focused separately on the adverse health effects of exposures to gas-phase pollutants or PM. Much less is known about their combined effects or interaction with other pollutants. In addition, most studies use freshly generated particles that have not been photochemically aged. Because the components of PM constantly change due to photochemically-mediated transformations, the overall toxicity of the mixture is also likely to change. Due to the difficulty in producing these types of mixtures, the toxicity of dynamic and complex gas/PM exposures is currently understudied. We hypothesize that fresh and photochemically aged biomass emissions have different biological impacts. Through this work we have generated and chemically characterized fresh and photochemically aged emissions from a hardwood source in an indoor smog chamber and generated real time in vitro exposures of lung epithelial cells to emitted gas/PM mixtures at an air-liquid interface (ALI). This was accomplished using the CelTox Sampler; a novel instrument providing a more sensitive and realistic ALI in vitro exposure that enables studying biological and chemical impacts without the artifacts associated with conventional resuspension methods. The exposed cells were then analyzed for gene expression changes and cytotoxicity levels in an effort to correlate biological data with chemical characterization data. These analyses will provide new insights on the scientific drivers of the health impacts of woody biomass combustion, thereby informing future field studies, interventions, and policy changes.

17HA.2

Spatiotemporal Distribution and Source Apportionment of Macrophage Reactive Oxygen Species Activity of Ambient Fine Particulate Matter (PM2.5) in the Midwestern United States. YIXIANG WANG, Haoran Yu, Joseph V Puthussery, Sudheer Salana, Vishal Verma, *University of Illinois Urbana-Champaign*

Ambient fine particulate matter (PM2.5) causes millions of premature mortalities every year. To better monitor the air quality, the capability of the particles to generate reactive oxygen species (ROS), conveniently called the ROS activity is a promising air quality indicator that is linked to the PM2.5 toxicity. However, very limited studies had investigated the spatial and temporal distribution of ROS activity in a large geographical area. Moreover, most of those researches assessed the ROS activity using the chemical assays, which do not necessarily represent the cellular responses. To understand the spatial and seasonal distribution of the cellular ROS activity of ambient PM2.5 in the Midwestern United States, we collected a large number of ambient PM2.5 samples (N= 237) from five sites in and around Illinois: Bondville (IL), Chicago (IL), Champaign (IL), Indianapolis (IN), and St. Louis (MI) for one complete year. Cellular ROS activity was measured by exposing the rat macrophage cells to the PM2.5 water extract. Chemical compositions of the PM2.5 samples were also analyzed by measuring the concentration of elemental and organic carbon, water-soluble organic carbon, water-soluble metals, and inorganic ions. The correlation between cellular ROS and chemical composition indicates that transition metals (Cu, Fe, and Mn), and water-soluble organic carbon were highly correlated with the macrophage ROS activity. The spatial distribution of macrophage ROS shows a strong intercorrelation among all the sites. Despite being in a rural area impacted only by the agricultural emissions, the Bondville site showed the second-highest macrophage ROS activity. This highlights the importance of agricultural emissions on contributing to the health impacts associated with ambient PM2.5. The source apportionment analysis is currently underway, which will reveal the emission sources contributing to the PM2.5 oxidative stress in the Midwestern United States.

17HA.3

Biomass Burning Aerosol Components Impair Mitochondrial Functioning to Induce Toxicological Response in Lung Cell Lines. FARIA KHAN, Karina Kwapiszewska, Alicia M. Romero, Nasir Jalal, Krzysztof Rudzinski, Jason Surratt, Rafal Szmigielski, *ICHF, PAS, Warsaw, Poland*

Wildfires, biofuel combustion, and wood burning emit 10-15 Tg/yr of organic carbon (OC) into the atmosphere globally. The UV-light absorbing component of OC termed as “brow carbon” (BrC) contains a group of poorly characterized nitrated aromatic compounds (NACs). These NACs are important secondary products of urban biomass burning aerosol (BBA) involving nitrogen oxides (NOx) as key reactants. The present work assesses the inhalation toxicological effects of one primary marker of BB burning (levoglucosan) and six NACs including nitrated phenols (2-nitrophenol, 3-nitrophenol, and 4-nitrophenol), nitrocatechol, nitroguaiacol, and nitro-salicylic acid. Two in vitro lung cells models were used to assess the exposure effects of BBA: A549 (alveolar epithelial carcinoma cells) and BEAS-2B (bronchial epithelial normal cells). Acute toxicity effects occurred in both cell lines at 24- and 48-hours after exposure to solutions containing 100-200µg/mL of substances tested. The cellular and sub cellular organelle toxicity effects were more predominant in the BEAS-2B cell lines than in the A549 cell lines. A high number of apoptotic cells were observed after 24 hours, and late apoptotic cells at 48-hours as determined through flow cytometric analysis. The increase in cellular and mitochondrial reactive oxygen species (ROS) buildup was detected through confocal imaging and flow cytometry. The latter was the main reason for cellular death after exposure to BBA mixture. A decreased tetramethylrhodamine (TMRM) signal was also observed for the BBA treated cells, which indicates the impaired mitochondrial membrane potential as a major mechanism of induced toxicity in lung cells. The study highlights the potential inhalation effects of NACs in urban settings and raises the importance of controlling their emission rates for improved health conditions and decreased pulmonary diseases associated burden.

17IM.1

Simultaneous Optical Photothermal Infrared (O-PTIR) and Raman Spectroscopy of Submicrometer Atmospheric Particles. ANDREW AULT, Nicole Olson, Yao Xiao, Ziying Lei, *University of Michigan*

Physicochemical analysis of individual atmospheric aerosols at the most abundant sizes in the atmosphere (<1 µm) is analytically challenging, as hundreds to thousands of species are often present in femtoliter volumes. Vibrational spectroscopies, such as infrared (IR) and Raman, have great potential for probing functional groups in single particles at ambient pressure and temperature. However, the diffraction limit of IR radiation limits traditional IR microscopy to particles > ~10 µm, which have less relevance to aerosol health and climate impacts. Optical photothermal infrared (O-PTIR) spectroscopy is a contactless method that circumvents diffraction limitations by using changes in the scattering intensity of a continuous wave visible laser (532 nm) to detect the photothermal expansion when a vibrational mode is excited by a tunable IR laser (QCL: 800-1800 cm-1 or OPO: 2600-3600 cm-1). Herein, we simultaneously collect O-PTIR spectra with Raman spectra at a single point for individual particles with aerodynamic diameters <400 nm (prior to impaction and spreading) at ambient temperature and pressure, by also collecting the inelastically scattered visible photons for Raman spectra. O-PTIR and Raman spectra were collected for submicrometer particles with different substrates, particle chemical compositions, and morphologies (i.e., core-shell), as well as IR mapping with submicron spatial resolution. Initial O-PTIR analysis of ambient atmospheric particles identified both inorganic and organic modes in individual sub- and super-micrometer particles. The simultaneous IR and Raman microscopy with submicron spatial resolution described herein has considerable potential both in atmospheric chemistry and numerous others fields (e.g., materials and biological research).

17IM.2

Evaluation and Applications of Methods for Quantification of Bulk Particle-phase Organic Nitrates Using Real-time Aerosol Mass Spectrometry. DOUGLAS DAY, Pedro Campuzano-Jost, Benjamin A. Nault, Brett Palm, Weiwei Hu, Paul Wooldridge, Ronald Cohen, Kenneth S. Docherty, J. Alex Huffman, Suzane de Sá, Scot T. Martin, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

Particle-phase organic nitrates ($pRONO_2$) in the atmosphere can contribute to secondary organic aerosol formation, represent a substantial loss of reactive nitrogen, and comprise substantial fractions of particle-phase nitrate (pNO_3). However, $pRONO_2$ is infrequently measured and thus poorly understood. There is increasing prevalence of aerosol mass spectrometers (AMS), which have shown promise for determining quantitative $pRONO_2$ contribution to aerosols. An approach that relies on relative intensities of NO^+ and NO_2^+ ions in the AMS spectrum, calibrated NO_x^+ ratio for NH_4NO_3, and inferred ratio for $pRONO_2$ has been proposed as a way to apportion pNO_3 signal to NH_4NO_3 and $pRONO_2$. This method is increasingly being applied to field and laboratory data. However, methods applied have been largely inconsistent and poorly characterized. We compiled an extensive survey of NO_x^+ ratios measured for various $pRONO_2$ compounds and mixtures from multiple AMS instruments, groups, and laboratory/field measurements. We show that the $pRONO_2$ NO_x^+ ratio can be estimated using a ratio referenced to the calibrated NH_4NO_3 ratio, a so-called "Ratio-of-Ratios" method (RoR=2.75±0.41). We systematically explore the basis for and uncertainties associated with quantifying $pRONO_2$ (and NH_4NO_3) with the RoR method using ground and aircraft field measurements conducted over a large range of conditions. The method is compared to another AMS method (PMF) and other $pRONO_2$ and related measurements, showing good agreement/correlation. PMF of thermal denuder measurements (applying RoR method) was conducted to construct thermograms and volatility basis sets of $pRONO_2$ for several campaigns, which were similar to those for less-oxidized oxidized organic aerosol PMF factors. A broad survey of ground/aircraft AMS measurements shows pervasive trends of higher contribution of $pRONO_2$ to pNO_3 with lower pNO_3 concentrations, which generally corresponds to shifts from urban-influenced to rural/remote regions.

17IM.3

Gas-phase Ion Structures of Molecules in Secondary Organic Aerosol: Infrared Photodissociation of Ions Across the Fingerprint Region. Corey Thrasher, Lemai Vo, Giel Berden, Jonathan Martens, Jos Oomens, RACHEL O'BRIEN, *William & Mary*

Secondary organic aerosol (SOA) is a large fraction of the organic particulate matter in the atmosphere with impacts on climate, air quality, and human health. This fraction presents a challenge for modelers and experimentalists, given the trace sample masses and the complexity of the organic mixtures, with thousands of different molecules found in an aerosol sample. Mass spectrometry can provide insights into the molecular composition of organic aerosols, however, information on the chemical structure and functional groups can be limited. By combining infrared multi-photon dissociation (IRMPD) from the FELIX free electron laser with mass spectral analysis using an ion trap mass spectrometer, we demonstrate a new way to characterize the gas-phase ion structure of organics in complex mixtures. We use this technique to generate IR action spectra (IRMPD yield vs. wavenumber) for major components of α-pinene SOA as well as standards used as tracers for SOA sources. In combination with computational analysis, this method can provide insights into the lowest energy gas-phase conformations of the ions. By using different ion adducts (Cs+, I-, H+) we can investigate the influence of the charging species on the ion conformation. This work demonstrates a new platform to study the structures of organic molecules formed in the atmosphere with utility for both analytical characterizations as well as fundamental physical chemistry studies of formation products and pathways.

17NM.1

Aerosol-assisted Production of Sodium Tungsten Bronze Particles for NIR Shielding. HAO TU, Wei-Ning Wang, Da-Ren Chen, *Virginia Commonwealth University*

Because of close-to-50% energy in solar radiation is in the infrared (IR) range, it is very desired to have transparent medium, e.g., window glasses, with NIR (near Infrared) shielding function in order to save the energy and cost on air conditioning of a building. Different kinds of NIR shielding transparent medium have been developed and applied, for examples, as automobile windshields and building windows. They are primarily composite membranes made by multilayers of polymer film, or metal (Ag/Au) sputter-coated on ceramics (ITO/ATO) (Padiyath et al., 2007). However, the polymer aging, high price of raw materials, and the requirement of complex coating equipment make limits the wide application of NIR shielding transparent medium. Rare-earth hexaboride particles were also proposed for the same applications (Takeda et al, 2008). Due to the high transmittance in visible range (VLT) and excellent absorption in NIR range, tungsten bronze oxides (MxWO3) are viewed as one of potential candidates for NIR shielding material which could be applied to transparent media. Liquid phase reactions are typically in making particles of tungsten bronze oxides. The majority of published MxWO3 research focus on CsxWO3 because of its the great performance in VLT and NIR shielding. Unfortunately, caesium (Cs) is expensive for large scale production.

In this study, we introduce a new aerosol-assisted method to produce crystalline NaxWO3 particles from low-cost precursors. The production process, evolved from that reported in our previous work (Tu, et al, 2020) is in one step, continuous and without any aftertreatment. The sizes of as-produced NaxWO3 particles could be controlled by adjusting the dilution and quenching of reaction agents. By investigating the size effect on VLT, we confirm that the smaller size of NaxWO3 particles have the higher VLT, consistent with what reported by Adachi, K. (2010) on the investigation of LaB6 for the same applications. The above finding offers an alternative and cheap way to improve the performance of MxWO3 particles on the VLT and NIR shielding. The detail of our production method and the findings will be presented in this talk.

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[3] Padiyath, R., Haak, C. and Gilbert, L. In Proceedings of the Annual Technical Conference-Society of Vacuum Coaters, 2007, p. 669.
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17NM.2

Microwave Plasma Technology for Conversion of Natural Gas to Value-Added Carbon Materials. RANDY VANDER WAL, Raju Kumal, Akshay Gharpure, Aayush Mantri, Kurt Zeller, Vignesh Viswanathan, George Skoptsov, *Penn State University*

Advanced microwave plasma technology practically and cost-effectively converts natural gas to value-added chemicals and premium carbon materials such as graphene and conductive carbon black analogues (CCBA) with no CO2 emissions and low capital and infrastructure expenditures. In this work a microwave driven plasma drives hydrocarbon decomposition – producing a variety of carbon nanostructures without the use of catalyst. With lower-energy requirements than conventional thermal plasmas, reactions in microwave plasmas are driven by electron kinetics rather than thermodynamics, and their non-equilibrium energy distribution opens reaction pathways that are unavailable with conventional chemical or thermal plasma processes. The form and purity of carbon material can be controlled by optimizing the several interrelated parameters that include methane to hydrogen ratio in the feed stream and reactor conditions such as input energy and formation temperature. Primary products include nanographene comprised of 2-6 sheets per stack with lateral dimensions between 100 and 500 nm, and graphitic carbon particles with structure analogous to conductive carbon blacks. Analytical techniques including high-resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), thermogravimetric analysis (TGA), Raman spectroscopy and electrical conductivity measurements are utilized to study the form and quality of these valued carbon materials. Optical spectra were collected and analyzed to determine the formation temperature of these carbons using blackbody radiation and C2* Swan band emission. The electrical conductivity of the as-produced CCBA material is higher than that of commercially available conductive carbon blacks. These results highlight the importance of advanced plasma technology for the economic utilization of natural gas by producing premium carbon materials.

17NM.3

Rapid and Selective Ammonia Sensing by Porous CuBr at Room Temperature Made by Flame-deposited and In-situ Annealed, Reduced and Brominated CuO Nanoparticles. ANDREAS GUENTNER, Nicolay Pineau, Markus Wied, Sotiris Pratsinis, *ETH Zurich, Switzerland*

Ammonia (NH_3), a major industrial commodity, is toxic as well as a tracer for food spoilage and putative breath marker for impaired kidney and liver function (e.g. cirrhosis, hepatic encephalopathy or injury). So there is strong interest in developing reliable sensors over a wide range of NH_3 concentrations: from 250 to 2900 ppb in mouth-exhaled breath down to few ppb in indoor air at high relative humidity (RH). Also, ammonia is present in gas mixtures containing a myriad of compounds demanding high selectivity.

So fast and selective detection of NH_3 at ppb concentrations with inexpensive and low-power sensors represents a long-standing challenge. Here, a room temperature, solid-state sensor is presented consisting of nanostructured porous (78%) CuBr films. These are prepared by flame-aerosol deposition and in-situ annealing of CuO onto sensor substrates followed by in-situ dry reduction and bromination that are continuously monitored in situ through the film resistance [1] affording excellent process control. Such porous CuBr films feature an order of magnitude higher NH_3 sensitivity and five times faster response times than conventional denser CuBr films. That way, rapid sensing of even the lowest (e.g. 5 ppb) ammonia concentrations at 90% RH is attained with outstanding selectivity (30 - 290) over typical confounders including ethanol, acetone, H_2, CH_4, isoprene, acetic acid, formaldehyde, methanol and CO, superior to state-of-the-art sensors [2]. This sensor is ideal for hand-held and battery-driven devices or integration into wearable electronics as it does not require heating.

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17UA.1

From Low-Cost Sensors to High-Quality Data: the Importance of Collocated Calibration Model Development for the AfriqAir Network. MICHAEL R. GIORDANO, Julien Bahino, Matthias Beekmann, Thomas Bigala, Paola Formenti, Mathieu Cazaunau, Corinne Galy-Lacaux, Jimmy Gasore, Theobald Habineza, Aliaksei Hauryliuk, Vincent Madadi, Carl Malings, Beatrice Marticorena, Stuart Piketh, Albert A. Presto, R. Subramanian, Daniel Westervelt, Veronique Yoboue, *OSU-EFLUVE, LISA/CNRS, UPEC, ENPC, UP*

AfriqAir is a hybrid network of low-cost sensors centered around reference monitors. About 50 Real-time Affordable Multi-Pollutant (RAMP), Clarity, and PurpleAir devices have been collaboratively deployed in Nairobi, Kigali, Accra, Abidjan, Niamey, Kinshasa, Zamdela (near Johannesburg), and other African cities. All devices use Plantower optical nephelometers for PM2.5. Generating high-quality data from low-cost sensors requires calibration models to accurately measure PM concentrations. One way to build such calibration models is by collocating reference-grade monitors with the sensors for a set amount of time before deploying the sensors to the target locations. One outstanding question that arises from this methodology is the applicability of the models developed in one location to another location as differences in ambient aerosol size distribution and chemical composition may greatly impact calibration models. Here we examine this question using data from low-cost sensors deployed in South Africa, Côte d'Ivoire (West Africa), and Uganda and Rwanda in East Africa. Calibration models for each location are developed and compared to calibration models developed in urban OECD locations (Pittsburgh, PA USA; the Greater Paris area, France; and Queens, NY, USA). Results show that the specific models for each location perform the best, but the urban OECD calibration models can do fairly well at reproducing measurements from reference-grade instruments collocated with the low-cost sensors deployed in some developing countries.

17UA.2

Impacts of Modifiable Factors on Ambient Air Pollution: A Case Study of COVID-19 Shutdowns. REBECCA TANZER GRUENER, Jiayu Li, Rose Eilenberg, Allen Robinson, Albert A. Presto, *Carnegie Mellon University*

Sources of air pollution that are known as modifiable factors such as traffic, cooking, and electricity emissions can be modulated either by changing activity levels or source intensity. Although air pollution regulations typically target reducing emission factors rather than altering activity, the COVID-19 related closures offered a novel opportunity to observe and quantify the impact of activity levels of modifiable factors on ambient air pollution in real-time.

We use data from a network of 27 low-cost Real-time Affordable Multi-Pollutant (RAMP) sensor packages deployed throughout Pittsburgh along with data from EPA regulatory monitors. The RAMP locations were divided into four site groups based on land use (Traffic, Urban, Suburban, and Industrial). Concentration measurements of $PM_{2.5}$, CO, and NO_2 following the COVID-related closures at each site group were compared to measurements from "business as usual" periods in March 2019 and 2020. Overall $PM_{2.5}$ concentrations decreased across the domain by 3μg/m^3. Intra-day variabilities of the pollutants were computed to attribute pollutant enhancements to specific emission sources (i.e. traffic and industrial emissions). The morning rush hour induced CO and NO_2 concentrations at the Traffic sites were reduced by 57% and 43%, respectively, which is consistent with the observed reduction in commuter traffic (~50%). There was no significant change in industrial related intra-day variability of $PM_{2.5}$ and CO at the Industrial sites following the COVID-related closures.

We observe that the morning rush hour enhancement from traffic emissions fell from 1.5μg/m^3 to ~0μg/m^3 across all site groups. This translates to a reduction of 0.125μg/m^3 in the daily average $PM_{2.5}$ concentration. If National Ambient Air Quality Standards (NAAQS) are tightened these calculations shed light on to what extent reductions in traffic related emissions are able to aid in meeting more stringent NAAQS.

17UA.3

Leveraging a PurpleAir Sensor Network to Inform Air Quality Action in Phoenix, Arizona. IAN VONWALD, Karoline Barkjohn, Samuel Frederick, Sue Kimbrough, Ben Davis, Nikki Peterson, Ira Domsky, Ron Pope, Andrea Clements, *U.S. EPA Office of Research and Development*

Affordable air sensors are revolutionizing how air quality is monitored. While many air sensor studies have focused on measurement accuracy and data correction, an important use of sensors is informing air quality action, since sensors can be deployed in dense networks that can capture local variations in pollution. For example, air quality in Phoenix, Arizona is adversely affected by seasonal woodburning, especially in the winter. The local agency mitigates this issue through control strategies including fireplace change-out programs and information campaigns on when or what not to burn. Programs such as these might benefit greatly from the neighborhood-level air quality measurements derived from a dense air sensor network.

Here, we use a distributed network of more than 30 PurpleAir particulate matter (PM) sensors deployed in Phoenix since November 2018 to identify local spatiotemporal air quality trends. We incorporate local meteorological data to focus on fine PM mass transport between areas where PM originates to areas that are most impacted, with three particular interests: (1) short-lived events that worsen air quality, such as fireworks from holiday celebrations, (2) seasonal events such as woodburning, and (3) unanticipated, unknown duration events such as the COVID-19 pandemic, in which travel restrictions and stay-at-home orders have been imposed. These results will demonstrate the potential of a distributed sensor network for tracking local air quality hotspots, improving understanding of how air quality is affected on shorter and longer time scales, and identifying areas that would benefit the most from control or mitigation actions.

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18AC.1

Chemical Transformation of Biomass Burning Organic Aerosol Due to Photolytic Aging. HONGMIN YU, Christopher Lim, Christopher Cappa, Jesse Kroll, Rachel O'Brien, *William & Mary*

Biomass burning organic aerosol (BBOA) is a major research focus because of its important role in atmospheric chemistry and radiative forcing. Due to its chemical complexity, there are gaps in our knowledge about the chemical aging processes of BBOA in the atmosphere. Since many photochemical aging experiments on BBOA are usually conducted for only a few hours, relatively little is known about the photo-aging pathways of the system over an extended timescale. Here we present the analyses of several BBOA filter samples derived from burning of various types of biomass fuels that were aged by photolysis over a timeframe of up to ~3.5 days. Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-FTIR), Offline-Aerosol Mass Spectrometry (Offline-AMS), and Ultraviolet–Visible Spectroscopy (UV/Vis) were used to measure the chemical changes in the aqueous sample extracts and evaluate how those changes can relate to the specific fuel type. This study finds an overall increase in oxidation state and decrease in the nitro group (-NO2) compounds in the samples with irradiation. The AMS signal of levoglucosan, a tracer organic species of BBOA, is also observed to decrease in the sample mixture possibly due to the photolytic formation of oxidants in the condensed phase. Several unique chemical characteristics were observed for some samples, which can possibly relate to their individual fuel type. Observed changes demonstrate the rates of photo-bleaching and oxidation that can occur in BBOA from different fuel types when photolyzed as dry particles over ~3.5 days.

18AC.2

Rethinking the Lifetime of Aged Biomass Burning Aerosol over the Southeast Atlantic Ocean. AMIE DOBRACKI, Steven Howell, Pablo Saide, Steffen Freitag, Allison Aiken, James Podolske, Arthur J. Sedlacek, Kenneth Thornhill, Jonathan Taylor, HuiHui Wu, Hugh Coe, Paquita Zuidema, *University of Miami*

Southern Africa produces approximately one-third of the world’s fire-emitted carbon, a relative contribution that is expected to increase with time. A westward outflow off the continent allows the aerosol to remain over the southeast Atlantic ocean (SEA) for one to two weeks, as large-scale subsidence prevents aerosol removal by deep convection and maintains a coherent vertical structure that is resistant to mixing with cleaner environmental air. These meteorological conditions along with chemical uniformity of the sources and the range of plume ages provided a unique natural laboratory for three field campaigns (NASA-ORACLES, DOE-LASIC, and UK Met Office-CLARIFY) (2016-2018) to study biomass burning aerosol aged beyond two days. *In situ* aerosol mass concentrations (organics, nitrates, sulfates, ammonium) derived from the ORACLES Aerosol Mass Spectrometer, combined with aerosol age (time since emission) estimates from the in-field aerosol forecasting model indicate biomass-burning aerosol ages typically exceed 4 days. Estimates of the organic nitrate, or the portion of the biomass-burning aerosol that is most susceptible to loss through photodegradation, indicate a decrease from 80% to <50% in the free troposphere over 4 days. During this time the relative percentage of black carbon increases from 5% to 13% as it is transported over the SEA. One important consequence is that the single-scattering-albedo decreases from 0.875 to 0.84 with age as organic aerosol, primarily nitrate and secondarily ammonium, is lost and black carbon is conserved, although changes in particle size, which may also be influential, have not yet been accounted for. We further assume that thermodynamic processes only affect the partitioning of the inorganic nitrate. Global aerosol models do not currently model the photodegradation of biomass-burning aerosol; it is hoped that these empirical results can provide a valuable model metric. The loss of organic aerosol after 2 days is predicted by chamber studies, however, *in situ* analysis of long range transport biomass burning aerosol, especially in the southern hemisphere, remains sparse.

18AC.3

Modeling of Furan Oxidation (via OH and NO3) within Biomass-Burning Regimes Based on New Results from Chamber Experiments. BENJAMIN BROWN-STEINER, Matthew Alvarado, Taekyu Joo, Nga Lee Ng, *AER*

We present the continuing development of a furan oxidation mechanism within the Aerosol Simulation Program (ASP) based on new and ongoing 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. The importance of furan and furan-derived species found within biomass burning plumes, including furfural and methylfurans, for SOA formation are well-established, but constrains on chemical production regimes are lacking. The GTEC chamber experiments, which use a Filter Inlet for Gases and AEROsols coupled with time-of-flight chemical ionization mass spectrometer (FIGAERO-HR-ToF-CIMS) 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. New experimental constraints under both dry (RH < 5%) and humid (RH ~ 50-60%) conditions inform the development of a furan oxidation mechanism. We present this mechanism, along with initial experimental results, and discuss remaining uncertainties.

18BA.1

Biodegradation of Phenol and Catechol in Cloud Water: Comparison to Chemical Oxidation in the Atmospheric Multiphase System. Saly Jaber, Audrey Lallement, Martine Sancelme, Martin Leremboure, Gilles Mailhot, Brabara Ervens, ANNE-MARIE DELORT, *ICCF, CNRS, Université Clermont Auvergne*

Among monocyclic aromatics in the atmosphere, phenol is of particular interest for air quality as it is considered one of the main pollutants listed by the US Environmental Protection Agency (US EPA list) since it represents a risk for humans and the environmental biota. Using GCxGC-HRMS, we detected and quantified phenol among 100 semi-volatile compounds in cloud samples collected at the puy de Dôme station (France)[1]. We investigated the potential biodegradation of phenol and catechol in clouds using two strategies [2]: 1) a metatranscriptomic analysis showed in-cloud activity of microorganisms. We detected transcripts of genes coding for phenol monooxygenases (and phenol hydroxylases) and catechol 1,2-dioxygenases. 2) 145 bacterial strains isolated from cloud water were screened for their phenol degradation capabilities, 93% of them (mainly *Pseudomonas* and *Rhodococcus strain*s) were positive. These findings highlighted the possibility of phenol degradation by microorganisms in cloud water.

In our recent study [3], we measured the biodegradation rates of phenol and catechol, by one of the most active strains selected during our previous screening in clouds (*Rhodococcus enclensis*). For catechol, biodegradation is about 10 times faster than for phenol. The experimentally-derived biodegradation rates are included in a multiphase box model to compare the chemical loss rates of phenol and catechol in the atmospheric gas and cloud aqueous phases to their biodegradation rate in the aqueous phase only. Degradation rates in the aqueous phase by chemical and biological processes for both compounds are predicted to be similar to each other. During day-time, catechol biodegradation rates even exceed the chemical aqueous phase loss and contribute to ~20% to the total catechol transformation rate in the atmospheric multiphase system. Our results suggest that atmospheric multiphase models may be incomplete for soluble organics as biodegradation may represent an unrecognized efficient loss of such organics in cloud water.

Financial support.
Research has been supported by a school grant to the first author from the Walid Joumblatt Foundation for University Studies (WJF), Beirut, Lebanon, and the French National Research Agency (ANR) (grant nos. ANR-17-MPGA-0013and ANR-13-BS06-004-01).

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18BA.2

Application of DNA-Stable Isotope Probing to Study Airborne Methanotrophs. KEVIN DILLON, Valdis Krumins, Aishwarya Deshpande, Lee Kerkhof, Gediminas Mainelis, Donna Fennell, *Rutgers, The State University of New Jersey*

The growth and activity of bacteria have been heavily studied in nearly every environment on Earth, but there have been limited studies focusing on the air. Bacteria can be suspended in the air for a long enough time such that substrate metabolism and growth could occur. Previous studies have noted the presence of active bacteria in the air. This activity suggests the potential for microbes to grow in the air outside of water droplets on volatile compounds such as CH_4. To examine airborne microbial communities, we aerosolized enrichment cultures of methane-oxidizing bacteria (methanotrophs) into 320 L rotating gas-phase bioreactors and assessed the half-lives and distributions of the particles. We investigated the ability of airborne methanotrophs to grow on CH_4 using DNA-stable isotope probing (DNA-SIP). The cultures were aerosolized into gas-phase bioreactors and amended with 1500 ppmv $^{13}CH_4$ or $^{12}CH_4$. The cells were suspended in the air for five days, harvested, and analyzed for ^{13}C incorporation into DNA by gradient fractionation/qPCR methods. Based on our data, low biomass is the main limitation for utilizing the DNA-SIP method for detecting activity of airborne methanotrophs. However, some results demonstrated ^{13}C incorporation into DNA, indicating growth in air, while other experimental replicates did not. Specifically, one replicate demonstrated that members of the family Methylococcaceae metabolized and grew on CH_4 while in the airborne state. We conclude that methanotrophs outside of water droplets in the air can potentially grow under certain conditions. Future work will further investigate the metabolic potential of bacteria outside of water droplets in the air.

18BA.3

Assessment of a Low-Power Active Bioaerosol Sampler Performance. SYDONIA MANIBUSAN, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Bioaerosol samplers are increasingly important for understanding the biological component of our air, given their potential to cause negative health effects such as disease transmission or exacerbation of respiratory diseases. REPS-Active is an active sampler which collects bioaerosols using overlapping ferroelectric polymer film to capture particles onto the film by electrostatic forces. This is based on the technology established by the Rutgers Electrostatic Passive Sampler (REPS).

Physical collection efficiency for REPS-Active was determined in three environments (e.g., residence, laboratory, and outdoors) using an optical particle counter and condensation particle counter by comparing concentrations with and without REPS-Active in the sampling stream at different operational flow rates (0.1, 0.5, and 1.0 L/min). The flow rate of 1.0 L/min had the most efficient capture of particles per sample time and efficiencies of 22.0 ± 4.2% by particle number concentration and 35.8 ± 8.5% by mass concentration for particles 0.02 – 20 µm in diameter. This particle diameter range includes fungal spore, bacteria, and viral sizes. This confirms that REPS-Active captures particles within our target size ranges.

Demonstration of bioaerosol collection of REPS-Active was conducted in 24-hour tests in two environments (e.g., residence and outdoor). REPS-Active was collocated with active reference samplers for comparison: the SAS Super 180 Air Sampler and IOM Sampler. Initial findings show that REPS-Active captured 134.6 ± 97.7% of culturable bacteria compared to the IOM sampler indoors.

Given the current pandemic caused by the COVID-19 virus, it is essential to have versatile and low-cost sampling tools capable of collecting representative bioaerosol samples over long sampling times. These results demonstrate the REPS-Active sampler's potential as a novel tool for bioaerosol investigation. The open flow design of REPS-Active operates at low flow rates with little to no pressure drop, which allows for portable, extended sampling with battery-powered air movers.

18HA.1

Ordinal Logistic Regression Analysis between Household Energy (Agricultural Residues, Wood and Dung) Consumption and Women's Health in Rural Punjab. NABEELA FARAH, *University of Agriculture, Faisalabad, Pakistan*

Energy is a basic essential of human life. Around the world all domestic tasks and energy related activities in household are women centric. Since, naturally women get involved in household responsibilities with fuel collection and cooking, in this way the energy utilization has certain effects on women's health. Due to socially determined measures, women accept a better extent of the burden of low quality fuel utilize. This study examined the ill-health effects of household energy consumption in three districts of Punjab (Pakistan). The exposure of smoke and health outcomes were self-reported. Data collected from 480 women was analyzed by using ordinal logistic regression model. The odd ratios for agricultural waste, wood and dung showed significant relationship for various diseases. It was concluded that the use of inferior biomass fuels was significantly positively associated with chest pain, coughing, asthma, breathing problems, headache and eye allergy. Increasing the share of households relying on inferior biomass had implications for human health particularly for women health. Less expensive fuels were more inflammatory for a longer time and emission for more smoke so the result of chronic or acute diseases. It was studied an unfortunate crucial point for women's health. So the study recommends management and prevention of such drastic health hazards to avoid vicious circle of rural women's health.

18HA.2

Assessing the Impacts of Residential Mechanical Ventilation Systems on Indoor/Outdoor Particulate Matter and Adult Asthma Outcomes in Chicago, IL.

INSUNG KANG, Kari Abromitis, Yicheng Zeng, Parham Azimi, Anne Evens, Anna McCreery, Rachel Scheu, Amanda Gramigna, Timothy Crowder, Griselda Baca, Brent Stephens, *Illinois Institute of Technology*

The Breathe Easy Project is a three-year longitudinal, randomized, crossover study of installing residential mechanical ventilation systems to improve indoor air quality (IAQ) and asthma-related health outcomes in 40 existing homes with at least one adult asthmatic in Chicago, IL USA. This work presents preliminary results on the impacts of mechanical ventilation systems on indoor and outdoor pollutant concentrations, including particulate matter (i.e., PM2.5: 0.3-2.5 µm and PM10: 0.3-10 µm in aerodynamic diameter, estimated using optical particle counters), and adult asthma outcomes. The homes were divided into three groups receiving one of three types of ventilation systems: 1) continuous exhaust-only ventilation systems (13 homes); 2) intermittent central-fan-integrated-supply (CFIS) ventilation systems (15 homes); and 3) continuous balanced supply and exhaust ventilation systems with energy recovery ventilators (ERV) (12 homes). Field measurements included four weeklong periods of IAQ and indoor environmental data collection for approximately one year during the pre-intervention period, followed by another four visits after the intervention (resulting in 8 total visits per home, except for 20 homes that did not receive their final visit due to COVID-19 stay-at-home orders). Baseline health and demographic surveys and monthly asthma control surveys were completed by 51 participants. Preliminary results indicate that the average indoor concentration of PM2.5 and PM10 (not calibrated) decreased by 64% and 58%, respectively, after the introduction of the ventilation systems, while the average outdoor concentration of PM2.5 and PM10 decreased by 45% and 47%, respectively. Homes with continuous balanced ventilation systems had the largest average indoor reductions (PM2.5: 78%, PM10: 76%), followed by intermittent CFIS ventilation systems (PM2.5: 60%, PM10: 54%) and then by continuous exhaust-only ventilation systems (PM2.5: 57%, PM10: 44%). Further analysis related to health effects and calibration is still ongoing.

18HA.3

Estimating the Evolving Public Health Impacts of Wildfires in California over the Past Two Decades.

ANIKENDER KUMAR, Melissa Venecek, Xin Yu, Yiting Li, Michael Kleeman, *University of California, Davis*

Wildfire activity has increased in many parts of the world over the past two decades due to changes in temperature and precipitation patterns associated with global change. Wildfire activity has also increased in California, especially during recent summer months. Wildfires emissions increase concentrations of airborne particulate matter (PM) mass in the region immediately adjacent to the fire and over long transport distances, leading to regionally elevated aerosol loadings. These high PM concentrations from wildfires can have a significant impact on air quality leading to public health impacts including mortality and/or increased severity of COVID-19 illness. As anthropogenic emissions decline in California, increasing wildfire emissions play a larger role in determining the public health impact from air pollution.

In this study, the source-oriented UCD/CIT chemical transport model was used to simulate wildfire PM contributions to PM0.1 and PM2.5 in California for a 17-year period (2000–2016). Gridded anthropogenic emissions were prepared using the raw emissions inventory provided by the California Air Resources Board (CARB). Wildfire emissions were obtained from the Global Fire Emissions Database (GFED). Wildfire contributions to PM0.1 and PM2.5 were compared to contributions from anthropogenic sources using the source-apportionment routines in the UCD/CIT model. Further, the Benefits Mapping and Analysis Program (BenMAP) was used to estimate the number of mortalities from wildfire in California during the study period. Results carried out with 4 km horizontal spatial resolution suggest that wildfires contribute ~10% to total population weighted annual average PM2.5 concentrations, and up to 45% of the acute monthly average PM2.5 concentrations in the recent years over California. The public health impact of past wildfire events and the likely impact of a severe wildfire on the incidence and severity of COVID-19 will be estimated based on the latest epidemiological evidence. The results from this study help to put wildfire emissions in context as an emerging public health threat.

18IM.1

A Dual-Droplet Approach to Characterizing Hygroscopic Growth using a Linear Quadrupole Electrodynamic Balance.

JACK CHOCZYNSKI, James F. Davies, *University of California, Riverside*

Aerosols in the atmosphere scatter and absorb atmospheric radiation, serve as cloud condensation nuclei (CCN), act as substrates for chemical processes, and impact air quality and human health. The physiochemical properties of atmospheric aerosols must be well characterized to understand their impact and predict their behavior in the atmosphere. Their optical and hygroscopic properties are of particular interest because they impact the radiative balance of the earth through direct and indirect aerosol effects.

In this work we use a linear quadrupole electrodynamic balance (LQ-EDB) for the contactless analysis of single aerosol droplets by levitation with electric fields. Droplets are exposed to controlled relative humidity (RH) and Mie resonance spectroscopy is used to determine their size and refractive index in response to changes in RH. Measurements of RH-dependent processes such as hygroscopic growth, deliquescence, efflorescence, and phase separations, require accurate in-situ RH determination, which is achieved through the use of a probe droplet. We simultaneously trap two droplets of different composition (a probe NaCl or LiCl droplet, and a sample droplet) and use the size and/or refractive index response of the probe to determine the RH.

The hygroscopic growth properties of model chemical systems using atmospherically relevant compounds will be explored. We are particularly interested in the hygroscopic response of systems containing mixtures of inorganic salts (e.g. NaCl, (NH4)2SO4, and CaCl2) and oxygenated organic compounds, such as carboxylic acids and sugar-alcohols. The chemical systems and methods discussed here will form the basis for the interpretation of more complex mixtures that better represent real aerosol.

18IM.2

Measurements of Aerosol Hygroscopic Growth as a Function of RH Using a Humidity-controlled Fast Integrated Mobility Spectrometer.

JIAOSHI ZHANG, Steven Spielman, Yang Wang, Susanne Hering, Jian Wang, *Washington University in St. Louis*

A humidity-controlled fast integrated mobility spectrometer (HFIMS) was previously developed for fast measurements of aerosol hygroscopic growth (Pinterich et al., 2017). Compared to traditional Humidified Tandem Differential Mobility Analyzers (HTDMA), the HFIMS significantly accelerates hygroscopicity measurements by taking advantage of the capability of the FIMS to rapidly characterize the size spectrum of humidified particles. However, the fast hygroscopicity measurements are limited to a single RH. In this study, we extend the fast measurements to a wide range of RH, therefore allowing comprehensive characterization of aerosol hygroscopic growth over atmospheric relevant RH range, particle phase transitions (e.g., deliquescence), and the variation of aerosol hygroscopic parameter (kappa) with RH.

A dual-channel humidifier with two humidity conditioners in parallel is implemented to achieve quick stepping of aerosol RH. By alternating between the two aerosol conditioners, the HFIMS provides aerosol hygroscopic growth of 6 particle diameters under 6 RH levels ranging from 30% to 90% every 30 min. A humidigraph of size classified particles from 25% to 85% RH can also be obtained by scanning the RH in 10 min, allowing fast characterizations of the deliquescence and efflorescence of aerosol particles. The performance of this improved HFIMS was characterized and validated using laboratory-generated ammonium sulfate aerosol standards. Ambient aerosols in an St. Louis urban area are characterized using the HFIMS and the results will be presented.

18IM.3

Exploring the Physicochemical Properties of Aerosol Using a Linear Quadrupole Electrodynamic Balance.

JAMES F. DAVIES, Jack Choczynski, Chelsea Price, Brandon Wallace, Thomas Preston, Ryan Davis, *University of California, Riverside*

From seeding clouds to scattering and absorbing light, aerosol play a significant role in the atmosphere and have profound effects on the global environment. To fully anticipate the changing impacts of aerosol over their lifetime, we must understand how key physicochemical properties develop as evaporation/condensation, oxidative aging and other chemical mechanisms evolve the composition of the particle phase.

We have developed a suite of methods based around single particle levitation using a linear quadrupole electrodynamic balance. The radius and refractive index of micron-sized aerosol particles is measured using Mie resonance spectroscopy and compositional information is determined by coupling to paper spray mass spectrometry. With these methods we explore the hygroscopicity, optical properties, phase morphology and mass transport in droplet samples in a contactless manner, allowing us to effectively simulate environmental conditions.

In this work, we report a newly developed dual-droplet approach that allows us to accurately quantify in-situ relative humidity and report hygroscopic growth for a range of model aerosol particle systems. Additionally, we explore the use of aerodynamic forces to characterize the density of levitated samples. We will focus discussion on mixed organic and inorganic particles (calcium chloride and sugars; citric acid and ammonium sulfate) that have recently been shown to exhibit interesting phase morphologies, such as gel formation, and water transport characteristics.

18NM.1

Controlled Synthesis of Alumina in a Spray Flame Aerosol Reactor.

ONOCHIE OKONKWO, Sukrant Dhawan, Sanmathi Chavalmane, Pratim Biswas, *Washington University in St. Louis*

Alumina has gained importance as a catalyst and catalyst support for industrial processes such as Claus, reforming, methanol synthesis processes and others. Conventionally, alumina supported catalysts are synthesised by wet synthesis methods such as precipitation, co-precipitation, and impregnation. These methods are multi-step, batch processes with significant waste treatment requirement. Flame synthesis, unlike conventional wet synthesis methods, is an easily scalable, continuous one step synthesis method for catalyst manufacture [1]. Studies have shown that the structure of alumina used as catalyst support are not altered by highly dispersed deposited metal active centres[2]. The effectiveness of alumina supported catalyst depends on the phases of alumina present in the catalyst, pore structure and surface area [3, 4]. Unlike alumina synthesised typically by the calcination of aluminium hydroxides and oxyhydroxides, there is a dearth of studies focused on the characterisation of alumina made by flame synthesis technique. Consequently, this presentation will focus on the characterisation of the crystallinity, pore structure and morphology of alumina synthesised by the spray flame aerosol reactor using x-ray diffraction, N2 – physisorption, and transmission electron microscopy. The precursor, dispersion oxygen and sheath oxygen flow rates are varied to investigate their effects on the properties of flame made alumina. The results will be discussed to demonstrate the controlled synthesis of alumina using the flame aerosol reactor.

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18NM.3

Implementing On-line Laser Diagnostics to Monitor the Reactive Spray Deposition Technology (RSDT) for Catalyst Manufacturing. EVANGELOS K. STEFANIDIS, Thomas A Ebaugh, Stoyan Bliznakov, Leonard Bonville, Francesco Carbone, Radenka Maric, *University of Connecticut*

The Reactive Spray Deposition Technology (RSDT) has been developed to synthesize nanoparticles in a flow reactor and deposit them directly on a target substrate. This flame-based method is proved to be effective for the manufacturing of highly active catalysts in a single step process but requires an optimization of the operative parameters to tailor the properties of the final products. The characterization of the produced nanoparticles necessary to achieve the process optimization is routinely performed off-line on samples of the final products, manufactured while keeping constant the process parameters. It appears that the implementation of laser diagnostics able to provide on-line information about the size, number concentration, crystallinity, and other characteristics of the synthesized nanoparticles, would substantially accelerate the process optimization due to on-line feedback about the sensitivity of the product properties to the process parameters. It would also offer the capability of monitoring slowly transient deposition processes of multilayered products with not-uniform characteristics such as size and crystallinity. In this study, we tackle the technical difficulties of implementing spectroscopic laser diagnostics in the complex RSDT flame reactor. A millimeter-sized measurement volume in the RSDT is illuminated by pulsed laser light with a wavelength of 532 nm while the induced light emission is collected at an angle by a train of optical components redirecting it into a spectrograph equipped with a fast gated and intensified CCD camera. Appropriate camera gating and light filtering allowed us to distinguish between the signals emitted by static light scattering, Stokes Raman scattering, and particle incandescence. The three signals are related to the number concentration, composition, and size of the light emitters in the measurement volume but the deconvolution of these properties is not trivial. Preliminary testing of a propane jet flame synthesizing Platinum nanoparticles gave promising results and the challenges of the quantitative result interpretation are currently being addressed.

18UA.1

Contributions of Cooking and Biomass Burning to Primary Organic Aerosol in Delhi. SAHIL BHANDARI, Gazala Habib, Joshua Apte, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Delhi, India experiences extremely high concentrations of primary organic aerosol (POA). No prior source apportionment study has captured the influence of biomass burning (BBOA) and cooking (COA) on POA. Here, we quantify the contributions of BBOA, COA, and hydrocarbon-like organic aerosol (HOA) by applying positive matrix factorization (PMF) on mass spectrometer data resolved by the time of day (six 4-hour segments) over two seasonal periods. We utilized the Multilinear Engine (ME-2) based EPA PMF tool and conducted detailed uncertainty analysis for statistical validation of our results. In addition to HOA, COA is found to be a major constituent of POA in monsoon and BBOA is found to be a major constituent of POA in the winter. Neither COA nor BBOA was resolved in the seasonal (not time-resolved) analysis. The COA mass spectral profiles (MS) are consistent with reference profiles from around the world, particularly resembling MS of heated cooking oils with a high m/z 41. The BBOA MS have a very prominent m/z 29 in addition to the characteristic peak at m/z 60, consistent with previous MS observed from wood burning. In addition to separating the POA, our technique also captures changes in MS profiles with the time of day, a unique feature among source apportionment tools available. In addition to the primary factors, we separate 2–3 OOA components. When all factors are recombined to total POA and OOA, our results are consistent with seasonal PMF analysis conducted using IGOR PET and EPA PMF. Results from this work can be used to better design policies that target primary sources of organic aerosols in Delhi.

18UA.2

Characterization of the Complex Mixture of Urban and Biomass Burning Aerosols Under the Influence of Transboundary Smoke Haze in Southeast Asia. LAURA-HELENA RIVELLINI, Nethmi Kasthuriarachchi, Mutian Ma, Alex Lee, *National University of Singapore*

Biomass burning (BB) emissions, including agricultural burning, peat fires and tropical forest wildfires, in Southeast Asia (SEA) can impact air quality and climate at local and regional scales. The mixture of BB and urban emissions together with active photochemistry encountered in SEA outflow lead to complex transboundary haze. In this study, a soot-particle aerosol mass spectrometer (SP-AMS) was deployed in Singapore, a highly urbanised city in SEA, to investigate BB and typical urban emissions over the northeast and southwest monsoons in 2019. The SP-AMS was operated with the dual vaporization scheme so that non-refractory particulate matter, refractory black carbon (rBC), and trace metals could be characterized simultaneously with a single instrument.

The inclusion of rBC and trace metal in positive matrix factorization (PMF) allows better identification of distinctive types of BB organic aerosol (BBOA) for each monsoon period compared to conventional PMF approach. BBOA components were clearly identified during both periods but they exhibited different chemical characteristics. In particular, the southwest monsoon was strongly impacted by transboundary smoke haze caused by Indonesian wildfires. Our results show that BBOA from transboundary smoke was highly oxygenated and associated different trace metals (e.g., K^+, Rb^+, Tl^+ and Mn^+). In contrast, the BBOA component identified during the northeast monsoon gave intense signals at $C_2H_4O_2^+$ (i.e., BBOA tracer), suggesting relatively fresh emissions, and higher N:C ratio. Although its associations with refractory materials were weak, it was correlated with a hydrocarbon-like OA with low refractory carbon association. Concurrent optical measurements further indicate that the transboundary smoke haze was less light absorptive compared to the one identified during northeast monsoon. This provides first field evidence that the types of BB and/or atmospheric processing can have substantial impacts on the chemical characteristics and light absorption properties of BBOA in Southeast Asia.

18UA.3

Nighttime Chemistry of Biomass Burning Plumes in Urban Areas: A Dual Mobile Chamber Study. SPIRO JORGA, Kalliopi Florou, Christos Kaltsonoudis, Jack Kodros, Christina Vasilakopoulou, Spyros Pandis, *Carnegie Mellon University, University of Patras*

Wildfires and human-induced biomass burning are sources of gaseous and particulate pollutants in the atmosphere. Although, important changes in the size distributions and the chemical composition of the biomass burning aerosol during daytime chemistry have been observed, the corresponding changes at nighttime or in winter where photochemistry is slow, have received relatively little attention. In this study, we tested the hypothesis that nightime chemistry in biomass burning plumes can be rapid in urban areas using a dual smog chamber system.

Ambient air during cold nightime periods with high concentrations of biomass burning organic aerosol (OA) was introduced in both chambers. Ozone was added in one of them (perturbed chamber) and upon reaction with the existing NO_x formed NO_3 radicals. The other chamber was used as a reference to monitor the natural evolution of the system. Following the injection of ozone (approx. 150 ppb), rapid secondary organic aerosol formation was observed in all experiments. NO_3 radicals were measured in the perturbed chamber. The OA mass concentration increased by 20-70% in just one hour, while an average increase of 50% in the O:C ratio of OA was observed. Nitrate formation was detected with most of it (on average 70%) being organic nitrate. The AMS mass spectrum of the formed OA showed similarities with oxidized OA mass spectra during winter in urban areas and with spectra from biomass burning plumes oxidized under dark conditions with nitrate radicals.

19AC.1

Exploring the Properties of Brown Carbon Aerosol in Levitated Droplets. CHELSEA PRICE, Alison Bain, Thomas Preston, James F. Davies, *University of California, Riverside*

Aerosol in the atmosphere undergo a myriad of physical and chemical transformations and impact their surrounding environment in various ways. Aerosol particles containing brown carbon chromophores absorb solar radiation, leading to warming of their surroundings that may impact their role as cloud condensation nuclei. It is important to determine the physical and optical properties of brown carbon aerosol in order to more fully understand their role in the atmosphere.

In this work, a linear quadrupole electrodynamic balance with a broadband light source is used to illuminate suspended brown carbon droplets for Mie resonance spectroscopy. The back-scattered light is measured, and morphology dependent resonances are used to ascertain the size, refractive index, and dispersion properties. Brown carbon is strongly absorbing at shorter wavelengths (<450 nm) but less so at long wavelengths (>600nm), allowing resonance spectra to be measured in both absorbing and non-absorbing regions using a broadband illumination. From these data, we explore the hygroscopic growth and light scattering behavior of three soluble brown carbon components suspended in aqueous droplets: 4-nitrocatechol, 4-nitrobenzoic acid, and 4-nitrophenol.

19AC.2

Quantifying the Contributions of Functional Groups to Light Absorptivity of Brown Carbon by a Two-layer Mapping Algorithm. KUNPENG CHEN, Jin Chen, King-Fai Li, Manuel Valdivia, Roya Bahreini, Ying-Hsuan Lin, *University of California, Riverside*

Brown carbon (BrC), defined as organic compounds with significant light absorption in ultraviolet (UV) and near-UV region, has been identified as an important warming source in the troposphere. Laboratory and field studies have provided extensive information about BrC composition (e.g., chemical formula), but the climate forcing by individual BrC constituents is not fully understood. To bridge the chemical variability with optical response, evaluation of light absorptivity for BrC at molecular level is required. Since the authentic chemical standards of most detected BrC compounds are not commercially available, recent research has used time-dependent density functional theory (TD-DFT) to simulate the ultraviolet-visible (UV-Vis) spectra. However, the simulated spectra may be subject to various degree of bias, depending on different computational models and assumptions within TD-DFT. Here, we developed a two-layer vector decomposition structure to map the bias between experimental and theoretical spectra into chemical information, including molecular structures and functional groups. We used the experimental spectra of conjugated compounds from the MPI-Mainz UV/VIS Spectra Atlas of Gaseous Molecules of Atmospheric Interest and calibrated the simulated spectra against experimental data in an attempt to reduce the bias. A supervised learning was carried out to fit the weight coefficients in our algorithm, which obtains a semiempirical operator to parameterize the bias. For new detected BrC compounds, its UV-Vis spectrum can be evaluated by the TD-DFT simulated spectrum plus the bias estimated by the operator. With bias-corrected UV-Vis spectra, we can attribute the alternation of light-absorbing properties in different ranges of wavelength to specific functional groups and estimate the imaginary refractive index corresponding to BrC molecules. Further, the assembled patterns of conjugated functional groups which are known to induce light absorption in the troposphere will also be presented.

19AC.3

Molecular Characterization of Atmospheric Brown Carbon Chromophores Formed in Irradiated Proxies of Aqueous Secondary Organic Aerosol. MARIA MISOVICH, Anusha P.S. Hettiyadura, Wenqing Jiang, Qi Zhang, Alexander Laskin, *Purdue University*

Guaiacyl acetone (GA), a prominent product found in biomass burning emissions, partitions rapidly into atmospheric aqueous phase systems such as fogs. In the aqueous phase, GA undergoes rapid oxidation reactions to form aqueous secondary organic aerosol (aqSOA). The photooxidation of GA in aqueous solution was examined in this study as a proxy of aqSOA formation related to atmospheric ageing of biomass burning emissions. An aqueous solution containing GA was oxidized by the triplet excited state of an aromatic carbonyl (3C*), produced from dimethoxybenzaldehyde in an irradiation experiment. Samples of the resulting reaction mixtures were collected at different reaction times, and chemical components of the aqSOA mixtures were analyzed using reversed phase liquid chromatography (LC) interfaced with a photodiode array detector (PDA) and a high resolution Orbitrap mass analyzer (HRMS) operated with an electrospray ionization (ESI) source. Recorded UV-Vis and HRMS spectra of the LC separated aqSOA components showed that less polar products, eluting at late retention times (>50 min), dominate light absorbing brown carbon (BrC) properties of aged aqSOA formed at longer irradiation times, while chromophores composed of relatively small polar species, eluting at <30 min, dominate BrC absorption at shorter irradiation times. Normalized top down UV-visible absorbance plots indicate that total BrC absorbance initially increases with irradiation, but decreases as irradiation continues. Overall, LC-PDA-HRMS chromatograms indicate three classes of products with strong light-absorbing characteristics. Elemental formulas were assigned to each class of products using HRMS data. The first class of products includes the monomeric products of GA functionalized with different groups. The second class includes various GA dimers and other oxygenated compounds with two aromatic rings. The third class of products contains nonpolar aromatic compounds formed as a result of non-pyrogenic charring processes.

19BA.1

Correlations of Fluorescent Aerosol Cytometry with Genomics and Mycometry Distinguish Significant Reductions in Airborne Fungal Loads Following Large School Renovations. MARINA NIETO-CABALLERO, Odessa M. Gomez, Richard Shaughnessy, Mark T. Hernandez, *University of Colorado Boulder*

Real-time fluorescent aerosol cytometry (InstaScope, DetectionTek, CO) was compared to concurrent recovery of airborne β-N-acetylhexosaminidase (Mycometer air, Mycometer Inc., FL) to assess the respective ability of these methods to detect significant changes in airborne loads of fungal biomass in response to building renovations. Condensation growth tube collection, or CGTC, (Spot Sampler, Aerosol Devices, CO) was used to concurrently collect aerosol from the renovated schools in order to characterize airborne genetic material with two different approaches: (i) quantitative polymerase chain reaction (qPCR), and (ii) high throughput sequencing (HTS). These simultaneous collocated aerosol measurements, targeting airborne fungal concentrations, were acquired from more than 60 occupied classrooms in 26 different public schools. Composite, site-randomized observations were acquired prior to, and immediately following, major building renovations. As judged by ANOVA and Spearman’s ranking, a statistically significant association was observed between direct fluorescent aerosol cytometry counts and biochemical (β-N-acetylhexosaminidase) measurements, which detected significant reductions in airborne fungal loads following building renovations. Gene copy numbers estimated by quantitative polymerase chain reaction (qPCR) of the DNA extracted from the CGTC air sampling, suggested that some of the airborne fungi recovered possessed a wide range of gene copies, corresponding to a universal 18S rRNA gene as an amplification target. High throughput “shotgun” sequencing was also performed on the DNA extracted from CGTC air samples. With aerosol sample times under 30 minutes, these results show that the CGTC sampling can recover and preserve enough airborne microbial DNA for high-fidelity metagenomic analyses in sampling durations less than an air change rates typically observed in K-12 classrooms.

19BA.2

Effect of Dust and Ammonia Reduction Strategies on Air Quality and Bioaerosols in Alternative Housing for Laying Hens. MAGALI-WEN ST-GERMAIN, Valérie Létourneau, Araceli Dalila Larios Martínez, Stéphane Godbout, Caroline Duchaine, *IUCPQ-U.Laval, Canada*

The new Code of Practice for the Care and Handling of Pullets and Laying Hens (2017) mandates the transition from conventional cages to alternative housing systems. Among them, non-cage systems provide space for improved freedom of movement for each animal. Non-cage systems also contain litter, so hens can perform natural behaviors such as foraging and dustbathing. Although beneficial for animal quality of life, non-cage housing systems may have a negative impact on air quality and respiratory health of workers and animals. Thus, the Research and Development Institute for the Agri-Environment (IRDA) studied three strategies to mitigate dust and ammonia, both common air contaminants in hen housing: 1) reduction of litter surface area, 2) oil aspersion and adding a moisture absorbent in the litter, and 3) oil aspersion and a heating floor for the litter. The experience was carried out in an experimental farm. The farm included twelve identical rooms of 1.2 x 2.5 x 2.4 m. Each room was conditioned to lay twelve Lohmann LSL-Lite hens (19 weeks of age). Concentration of air contaminants (dust, ammonia, endotoxins and microorganisms) per cubic meter were studied in treated experimental non-cage housing systems and compared to those of non-treated systems. Reduction efficiencies (%) of air contaminants concentrations were used to evaluate the impact of the strategies on air quality and bioaerosols. Oil-based strategies reduced from 87 to 98% of dust particles of all size fractions. However, no effect on ammonia, cultivable and total bacteria and mold concentrations was observed, along with human pathogenic agents. Reduction efficiencies of the strategies against total endotoxins still need to be confirmed by upcoming analysis.

19BA.3

The Effects of Relative Humidity on Fungal Growth in Dust Collected from the International Space Station. NICHOLAS NASTASI, Ashleigh Bope, Marit Meyer, John Horack, Karen C. Dannemiller, *The Ohio State University*

Inhalation of dust and bioaerosols is a major source of human exposure to microbes in the indoor environment, including on the International Space Station (ISS). Microbial communities are associated several health effects and can degrade spacecraft materials. Growth is limited by water availability, and elevated relative humidity (RH) levels are sufficient to facilitate growth in house dust. However, it is not known how RH interacts with dust and microbial communities from the ISS. The goal of this study is to simulate suboptimal RH conditions and quantify microbial growth in ISS dust. Dust was collected from HEPA filters on the ISS ventilation system. On Earth, dust was incubated at constant RH conditions (50, 60, 70, 80, 85, 90, and 100%) for two weeks at 25°C. In addition, the time-of-wetness (TOW) framework to model this growth was evaluated by varying 85% and 100% RH for 6, 12, and 18 hours per day. Total fungal quantity was measured by quantitative polymerase chain reaction (qPCR). ISS dust had a starting concentration (pre-incubation) ranging $2.17\text{x}10^4$–$1.36\text{x}10^7$ fungal spore equivalents (eq.) per mg dust. Constant (24 hours/day) equilibrium RH (ERH) incubations showed a significant trend between fungal growth and ERH (Spearman R2=0.77, P<0.0001). After two-week, constant (24 hours/day) ERH incubations, fungal growth activation occurred starting at 80% ERH ($2.86\text{x}10^5$–$9.26\text{x}10^7$ fungal spore eq. per mg dust) and more growth occurring as ERH increases to 100% ($8.20\text{x}10^8$-$3.32\text{x}10^{10}$ fungal spore eq. per mg dust). TOW models matched most closely to an activation limited growth model at 85% ERH, while at 100% a deactivation limited model was observed. These results highlight the need to continue monitoring relative humidity and microbial communities on human occupied spacecraft to ensure the astronauts health, spacecraft integrity, and planetary protection.

19CM.1

Aerosol Emissions Control from Water-lean Solvents for Post-combustion CO2 Capture. Vijay Gupta, Paul Mobley, JONATHAN THORNBURG, Lucas Cody, David Barbee, Jacob Lee, Roger Pope, Ryan Chartier, Marty Lail, Jak Tanthana, *RTI International*

Water-lean solvents (WLS) for CO_2 capture gained interest because of their reduced parasitic penalty from energy needed for solvent regeneration. Commercial implementation, however, hinges on successful control of amine emissions. Previous research studied aerosol emissions from aqueous solvents, similar information is not available for emissions from use of these novel water-lean solvents.

We conducted studies from fundamental and operational aspects to reduce the overall amine emissions from RTI's non-aqueous solvent eCO2Sol™. We used our 4-6 kW equivalent bench-scale gas absorption system (BsGAS). It consists of a CO_2 absorber column with intercoolers and water wash section, and a solvent regenerator column with a thermosiphon reboiler and interstage heaters. A simulated flue gas with 15% CO_2, 2.3-4.2% H_2O was used. SO_3 particulates were generated by reacting SO_2 with O_2 in air over a silica supported V_2O_5 catalyst at 450°C. The SO_3 particulates mimic the presence of SO_X and fly ash in the flue gas that provide nucleation sites for growth of aerosols. SMPS and APS instruments monitored the aerosol particle size distribution. A FTIR spectrometer monitored total amine emissions at the absorber and wash outlets. Process variables were liquid/gas ratio (L/G, mass basis), intercooling profile, absorber lean solvent temperature, water wash L/G, water wash return temperature, and flue gas inlet saturation temperature. The CO_2 capture rate was maintained close to 90% capture rate.

Results from parametric testing suggested that the presence of the aerosols in the flue gas could increase the overall emissions by 10X compared to the baseline emissions from NAS's vapor pressure. The temperature bulge in the absorber column drove aerosol growth. The PCA and PLS techniques applied to the parametric data derived a multivariate statistical model. The final model predicated aerosol emissions with ±15% accuracy.

19CM.2

Quantifying the Air Quality Benefit of a Novel Dust Suppression Technique. JASON MIECH, Matthew Fraser, Pierre Herckes, *Arizona State University*

Fugitive dust generated by wind passing over disturbed soils, such as those located at construction sites and landfills is a common problem found in arid environments like the Southwestern United States. In Maricopa County specifically, this fugitive dust contributes so much to the particulate matter in the air that the EPA has labeled the county as an air quality non-attainment zone. Current mitigation techniques include frequent spraying of the soil with water or a magnesium chloride solution. These techniques carry several disadvantages such as using large volumes of water, environmental issues due to frequent truck use and resulting emissions, and their limited effectiveness. Researchers at the Center for Bio-mediated and Bio-inspired Geotechnics at ASU have developed a novel soil stabilization technique called Enzyme Induced Carbonate Precipitation (EICP). This solution offers a one-and-done, cost-effective, and sustainable application that forms a calcium carbonate crust on top of the at-risk soil to prevent erosion and dust entrainment.

This presentation will cover the air quality impacts from field applications of the EICP solution over a month-long period at the Apache Junction Landfill and preliminary results from a long-term monitoring period at the Salt River Landfill. Plots of land were observed at the landfills to test the effectiveness of the EICP solution against controls. The air quality, specifically PM_{10}, was monitored at both sites with Clarity Air Sensors. In the short-term study there was no statistical difference detected between the treated and untreated plots during high wind periods. This led to the conclusion that the soil at this landfill was not being liberated by wind and contributing to the PM_{10} concentration. For the long-term study, a wind sensor and air samplers will be deployed, while chemical analysis of the soil and collected PM_{10} will be performed to determine the environmental impact of the EICP solution.

19CM.3

High-temperature Resistant Nanofiber and Its Filtration Application. QISHENG OU, David Y. H. Pui, *University of Minnesota*

Nanofiber materials has wide application in both air and liquid filtrations. A thin layer of nano-scaled fibers can significantly enhance filtration efficiency of a base filter media, especially for submicron contaminants. The slip flow around nanofibers helps to reduce flow resistance and filtration efficiency, leading to improved filter quality factor (Figure of Merit). Most current available nanofiber materials are polymer based, which limits their application at high temperature environments. In this study, a generation method of producing high-temperature resistant nanofibers will be presented. The produced short fibers have diameters in a few hundred nanometers and can sustain temperature at 1000 oC or higher. These nanofibers were first deposited onto several conventional air filtration substrates, and examples will be given in terms of the enhancement of filtration performance. The preliminary results show not only improved filtration efficiency and quality factor at submicron size at clean stage, but also extended filter lifetime under contaminant loading scenarios. Demonstrations will then be given in modifying conventional hot gas filtration media with these nanofibers, including both metallic fiber media (in super-micron size) and ceramic powder-based membranes. Their filtration performance will be evaluated with laboratory-generated soot particles as a surrogate to mimic engine emission application, as an example of the potential applications of this novel nanofiber materials. Detailed results and discussion will be given in the presentation.

19HA.1

Air Quality and Human Health Effects of Global Gasoline and Diesel Sectors. YAOXIAN HUANG, Nadine Unger, Kandice Harper, Chris Heyes, *Wayne State University*

Transportation emissions from the global gasoline and diesel fuel vehicle fleets play an essential role in affecting the air quality and human health. In this study, we quantify the impacts of the global on-road gasoline and diesel emissions on air quality and human health using the NCAR CESM global chemistry-climate model for year 2015 emissions from the IIASA GAINS inventory. We focus on $PM_{2.5}$ and ozone (O_3) impacts for both air quality and human health associated with the gasoline and diesel sectors. Annual mean surface $PM_{2.5}$ concentrations for the global gasoline and diesel emissions were up to 6.0 and 3.0 $\mu g\ m^{-3}$ respectively. For the gasoline sector, we found that there were large increases in surface $PM_{2.5}$ concentrations over China, Southeast Asia, and North America. For the diesel sector, substantial increases in surface $PM_{2.5}$ concentrations were found over India, China, and the Middle East. In terms of surface O_3, increases in annual mean surface O_3 concentrations attributable to gasoline and diesel sectors were up to 8.5 ppbv and 6.7 ppbv, respectively. Global annual total $PM_{2.5}$- and O_3-induced premature deaths for gasoline and diesel sectors for the year 2015 were 115,000 [95% confidence interval (CI): 69,000-153,600] and 122,100 (95% CI: 78,500-157,500), with corresponding years of life lost of 2.10 (95% CI: 1.23-2.66) and 2.21 (95% CI: 1.47-2.85) million years. We developed a metric of regional premature death rates, defined as regional annual total premature deaths normalized by regional annual total vehicle distance traveled for each fuel type. Regional premature death rates varied by a factor of eight and two orders of magnitude for the gasoline and diesel sectors, respectively, with India showing the highest for both gasoline and diesel sectors.

19HA.2

Interpretation of Satellite Remote Sensing Data for Application to Air Quality and Health. RANDALL MARTIN, Melanie Hammer, Aaron van Donkelaar, Erin McDuffie, Crystal Weagle, Brenna Walsh, Matthew Cooper, *Washington University, St, Louis, MO*

Fine particulate matter (PM2.5) is a leading mortality risk factor. However, ground-level monitoring remains sparse in many regions of the world. Satellite remote sensing from multiple instruments and algorithms offers a global data source to address this issue. Chemical transport modeling (e.g. GEOS-Chem) plays a critical role in relating these satellite columnar aerosol optical depth observations at ambient relative humidity to ground-level PM2.5 mass concentrations at controlled relative humidity. The resultant satellite-based estimates of PM2.5 indicate dramatic variation around the world, with implications for global public health. A recent Surface Particulate Matter Network (SPARTAN) offers valuable measurements to evaluate and improve satellite-based PM2.5 estimates. Sensitivity simulations with the GEOS-Chem model provide information on the sources of ambient PM2.5 contributions that affect human health. Algorithmic advances applied to the TROPOMI instrument yield new insight into the air pollution mixture. This talk will highlight recent advances in combining satellite remote sensing, chemical transport modeling, and ground-based measurements of atmospheric aerosols to improve understanding of air quality and health.

19HA.3

Sensitivity of Inorganic PM2.5 to Present and Future Emission Changes and Implications for Reduced Complexity Models. CARLOS HERNANDEZ, Sonal Nayak, Spyros Pandis, Peter Adams, *Carnegie Mellon University*

Reduced complexity models (RCMs) generally produce $PM_{2.5}$ health damages by marginally perturbing precursor emissions, and then quantifying the downwind impacts on human mortality. However, marginal health damages may be used for impact analyses where policies result in non-marginal emission changes, or for future policy scenarios where emission baselines differ from those used to develop RCMs. In both cases, present-day marginal health damages may not capture potential changes to $PM_{2.5}$ sensitivity. In this work, we explore changes in the sensitivity of inorganic $PM_{2.5}$ resulting from large perturbations and future changes to the emission baseline. Simulations from the PM-CAMx chemical transport model are used to develop health damages resulting from a 25% emission reduction from present and future case baselines in the continental U.S. Present case emissions are derived from the 2008 National Emissions Inventory. Future case emissions are estimated by scaling present case emissions uniformly to correspond with 2057 emission totals under the RCP 4.5 scenario. Month-long simulations for January and July are used to account for seasonal differences in emissions and chemistry. Simulations outputs are used to estimate seasonal and annual nationwide health damages for inorganic $PM_{2.5}$. Emissions for NH_3, NO_x, and SO_2 change by +25%, -66% and -83%, respectively, between the present and future cases. Health damages for NH_3 decrease by 83% across both months, while changes for NO_x and SO_2 are modest. Health damages for NO_x increase by 100% and decrease by 30% for January and July, respectively, due to the seasonally varying role NO_x plays in regulating the oxidant pool. We find that RCM health damages are largely robust, however analysts should practice caution when evaluating scenarios with changes to NH_3, or where seasonal differences are of concern. Future work will consider the role of changing demographics and wealth on health damages.

19IM.1

Analysis of the Unresolved Complex Mixture of Intermediate Volatile Organic Compounds in Gas Chromatograph-Mass Spectrum Data using Positive Matrix Factorization. Quanyang Lu, Christopher Hennigan, Albert Presto, Yunliang Zhao, Neil Donahue, ALLEN ROBINSON, *Carnegie Mellon University*

We present a new approach based on Positive Matrix Factorization (PMF) to better characterize the unresolved complex mixture (UCMs) in gas-chromatograph–mass-spectrometer (GC-MS) data. The goal of this work is to recover information on the chemical composition of the intermediate volatility organic compounds (IVOC) UCM for use in source apportionment and for simulation of secondary organic aerosol formation. We identified the chemical character of the PMF factors by comparison with reference compounds in the NIST mass spectral database. This technique can recover more detailed compositional information than traditional UCM assignments. PMF analysis of mobile source samples (gasoline, diesel and aircraft) show the effects of emissions control technologies, fuel composition and engine load on IVOC composition. For example, gasoline vehicle sources show increasing fraction of alkanes and oxygenates and decreasing fraction of single-ring aromatics (SRAs) from small off-road engine (SORE) to newer on-road vehicles. IVOC emissions from biomass burning show very different composition than mobile sources, with a large fraction (>50%) of IVOC oxygenates. Combing PMF technique with chemical mass balance model (CMB) on samples collected in a highway tunnel, we show that even though diesel vehicles represented only 20% of fuel consumption, they contributed around 70% of mobile source IVOCs. PMF analysis on ambient samples in Pasadena, CA show very high fractions (>70%) of oxygenates, where minor hydrocarbon IVOC peaks in early afternoon suggest contributions from local evaporative emissions. SOA modelling on mobile source emissions under low- and high-NOx conditions highlighting the importance of IVOC chemical information in chemical transport models. This technique can be applied to both archival and future GC-MS data analysis.

19IM.2

Consideration of Dynamic Gas-Particle Partitioning in National-Scale Emission Inventories. BENJAMIN MURPHY, Aditya Sinha, Quanyang Lu, Claudia Toro, Amara Holder, Ying Hsu, Madeleine Strum, Hugo Denier van der Gon, Justine Geidosch, Ingrid George, Andrew Grieshop, Michael Hays, Darrell Sonntag, George Pouliot, Havala Pye, David Simpson, Allen Robinson, *United States Environmental Protection Agency*

Conventional particle emission measurement and inventory methods (i.e. the EPA National Emission Inventory) characterize total particle mass and composition as the mass of material collected on a filter (e.g. Teflon, glass fiber or quartz) or with an online technique (e.g. aerosol mass spectrometer) during typical operation. Standard protocols for measuring PM emission factors exist for important sources like wood combustion, vehicle exhaust, or energy generation, and some of these protocols account for ambient processes such as particle enhancement from vapor condensation during cooling. However, this accounting is variable across source categories and among countries. For condensable organic matter, additional shifts in gas-particle partitioning are possible as plumes dilute to ambient concentrations and temperatures. Chemical transport model studies have clearly demonstrated the importance of these processes when predicting ambient particle concentrations, both in the U.S. and elsewhere.

Our goal is to improve existing EPA emissions estimation techniques with up-to-date knowledge of organic aerosol volatility. We demonstrate methods for applying speciation profiles to PM emission factors that distribute the organic emissions into lumped groups consistent with the Volatility Basis Set framework and consider complications from several issues including potential missing semivolatile organic compounds. We also discuss potential inconsistencies between speciation profile datasets and emission factor databases and make the case for greater harmonization and detailed emissions reporting, particularly for sources with high organic contribution. We focus on efforts involving engine-exhaust sources with profiles now available in the SPECIATEv5.0 database (https://www.epa.gov/air-emissions-modeling/speciate) and profiles recently developed for open and controlled combustion of biomass measured in lab and field studies. These efforts involve offline measurements that can be readily applied to other sources and source classes as well.

19IM.3

Multidimensional Chromatogram Binning – Positive Matrix Factorization Analysis for Gas Chromatography – High Resolution Mass Spectrometry Datasets. MICHAEL WALKER, Raul Martinez, David Hagan, Haofei Zhang, Lindsay Yee, Allen Goldstein, Brent Williams, *Washington University in St. Louis*

Techniques that couple thermal desorption with gas chromatography – mass spectrometry (GC-MS) provide insight into the chemical composition of organic compounds in the atmosphere, which can aid in the identification of the sources of organic aerosol (OA). Recent advances in instrumentation, such as the high time resolution afforded by Thermal Desorption Aerosol Gas Chromatograph (TAG) instruments, or the use of high-resolution (HR) mass spectrometers can offer further information on OA composition. However, these techniques also generate large, complex sets of data that challenge traditional data processing techniques, necessitating novel analysis methods. Previous studies have successfully leveraged a chromatogram binning approach in combination with positive matrix factorization (PMF) to identify covarying compounds across multiple TAG samples, but so far these methods have not been applied to HR datasets.

Proper data alignment, along with the removal of signal related to the analytical technique, are critical aspects of the chromatogram binning process. While HR-MS data can aid in more precise removal of unwanted data features, it also presents additional challenges in the data alignment process. To demonstrate, two datasets related to the Southern Oxidant and Aerosol Study (SOAS) are considered. Despite differences in the two analytical techniques, the first a TAG-style, in-situ characterization of organic aerosol with a one-dimension separation, and the second an offline analysis of filters using a two-dimensional gas chromatography (GCxGC) separation, a generalized workflow can be applied. Dynamic mass-to-charge (m/z) calibration, retention time shift corrections, and multidimensional binning aligns the chromatograms. Measurement artifacts and internal standards are removed through a combination of peak fitting and iterative factor analysis approaches, yielding chromatograms that can be successfully analyzed by PMF to reduce the dimensionality of these complex datasets.

19UA.1

Aerosol Composition in Pasadena, CA during the COVID-19 Pandemic. BENJAMIN SCHULZE, Christopher Kenseth, Yuanlong Huang, Harrison Parker, John Crounse, Paul Wennberg, John Seinfeld, *California Institute of Technology*

The COVID-19 pandemic offers an unprecedented opportunity to evaluate the response of ambient aerosol in the Los Angeles Basin to dramatic reductions in NO_x and VOC emissions associated with transportation and economic activity. Here, we present results of ongoing measurements of sub-micrometer aerosol at Caltech (Pasadena, CA) using an Aerodyne HR-ToF-AMS, SMPS, and 12-h filter samples analyzed offline with LC/ESI-MS. The extended deployment (April 8th–present) provides comparison of aerosol composition and concentration across a gradient of meteorological conditions and traffic levels. Decadal trends in aerosol abundance and speciation are also examined via comparison to measurements from the CalNex 2010 campaign. Established metrics are used to assess the efficiency of urban SOA formation (e.g., OA/ΔCO vs. photochemical age) and extent of atmospheric evolution (e.g., van Krevelen diagram), while positive matrix factorization (PMF) is applied to AMS data to differentiate OA subtypes and possible sources based on their mass spectra, time series, diurnal/weekly cycles, and correlations with molecular tracers identified via LC/ESI-MS. This “unnatural” experiment affords a glimpse into a potential future of urban air quality in which vehicular emissions are significantly reduced due to the ongoing electrification of cars and trucks across North America, suggests new scientific challenges that complicate air-quality management, and will allow for more accurate prediction of the trajectory of air quality in the decades to come.

19UA.2

Identifying the Transport and Evolution of Oxidized Organic Aerosol across the Urban Core of San Antonio. FANGZHOU GUO, Alexander Bui, Edward Fortner, Sujan Shrestha, Subin Yoon, Rebecca J. Sheesley, Sascha Usenko, Tara Yacovitch, Scott Herndon, James Flynn, Robert Griffin, *Rice University*

San Antonio is the seventh most populous city in the United States and the second-most populous city in Texas. Over the past decade, San Antonio has been one of the most rapidly growing large cities in the country, contributing to the city’s deteriorating air quality. To understand the sources of particulate matter (PM) that contribute to the degradation of San Antonio’s air quality, two mobile air quality laboratories were deployed and operated to the southeast (Traveler’s World (TW) Recreational Vehicle Park, upwind) and northwest (University of Texas at San Antonio (UTSA) campus, downwind) of downtown San Antonio in May 2017. Chemical characterization of non-refractory submicron PM (NR-PM_1) at high time resolution was conducted at TW using an Aerodyne high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) and at UTSA using an Aerodyne soot-particle aerosol mass spectrometer (SP-AMS) in laser-off mode from May 12 to 16. Additional measurements included meteorological parameters and trace gas mixing ratios (of ozone, total nitrogen oxides, total reactive nitrogen, carbon monoxide, and volatile organic compounds). Results from both AMS instruments indicate large sulfate and organic aerosol (OA) plumes. Positive Matrix Factorization (PMF) analysis of the high-resolution spectra identified hydrocarbon-like OA (HOA), a less oxygenated OA (LO-OOA), and a more oxygenated OA (MO-OOA) at both sites. Based on the location and meteorological data of the two sites, a model is constructed to characterize the formation rates of LO-OOA and MO-OOA across the city of San Antonio. Given the uniform 3-factor solutions from the PMF, the modeling analysis allows us to investigate the evolution of secondary organic aerosol species from upwind to downwind on an urban scale.

19UA.3

Secondary Organic Aerosol Formation and Product Distributions of α-pinene Oxidation in Ambient Perturbation Experiments. JEAN RIVERA-RIOS, Adam Wright, Zijing Zhang, Jennifer Kaiser, Nga Lee Ng, *Georgia Institute of Technology*

Volatile organic compounds (VOC) are oxidized in the atmosphere leading to the formation of secondary organic aerosols (SOA) and ozone, known pollutants. Usually, VOC oxidation is studied in laboratory chamber experiments with carefully controlled reaction conditions. In this study, we oxidized α-pinene in an outdoor chamber, using ambient air from downtown Atlanta, GA. The experiments began by introducing and sampling ambient air within an outdoor chamber. This was followed by a small α-pinene perturbation. The injected α-pinene was then oxidized under ambient conditions, leading to SOA formation and a variety of oxidation products. Gas-phase products were measured using a Proton Transfer Reaction Mass Spectrometer (PTR-MS) and Iodide adduct Chemical Ionization Mass Spectrometer (I^--CIMS). The CIMS was equipped with a Filter Inlet for Gases and Aerosols (FIGAERO) enabling particle-phase measurements along with an Aerosol Mass Spectrometer (AMS) and Scanning Mobility Particle Sizer (SMPS). Our results show a variety of SOA yields and product distributions that depend on ambient conditions. Important variables include but were not limited to NO_X and O_3 concentrations as well as other variables such as temperature and light intensity. Analysis of experimental and ambient SOA data using positive-matrix-factorization (PMF) showed that distinct environmental conditions influence the formation of LO-OOA and MO-OOA, PMF factors that have been previously observed during ambient measurements. The results of this work highlight the ability of ambient perturbation experiments to shed light on PMF factor identities and origins.