Plenary I: ASEEP Lecture

Tiny Critters, Huge Impacts: Ocean Microbes, Climate, and Health.

KIMBERLY PRATHER, *University of California San Diego*

In the 1990's, major advances enabled real-time measurements of the size and chemical composition of atmospheric aerosols. Since then, numerous field and lab studies have led to an increased understanding and appreciation for the impact of atmospheric aerosols on human health and climate. One of the largest remaining gaps in our understanding involves how biological processes in the ocean influence the composition of the marine atmosphere. Given their role in seeding clouds and affecting climate, it is critical to understand the factors controlling the size and composition of marine aerosols. This plenary lecture will provide an overview of studies in the NSF Center for Aerosol Impacts on Chemistry of the Environment (CAICE; https://caice.ucsd.edu). Over the past decade, CAICE scientists have successfully transferred the physical, chemical, and biological complexity of the ocean/atmosphere system into the laboratory at Scripps Institution of Oceanography. An overview will be provided of the key advances in CAICE studies and how this isolated ocean-in-the-lab approach has improved our understanding of the ocean on our atmosphere and climate. Finally, a discussion will be presented of recent studies investigating the factors controlling the ocean-to-atmosphere transfer of bacteria and viruses, including the SARS-CoV-2 virus that leads to COVID-19, and the implications for the health of residents living in and near coastal regions.

Plenary II: Friedlander Lecture

Electronic Cigarette: The Knowns, Known Unknowns, and Unknown Unknowns.

YIFANG ZHU, *University of California, Los Angeles*

Electronic cigarettes (E-cigs) are battery-operated devices gaining increasing popularity as an alternative to tobacco cigarettes. The global e-cig market is projected to reach $48.9 billion by 2025, with more than 70% of the market in North America and Europe. The number of e-cig users has also increased markedly, especially among adolescents. Yet, little is known regarding the physiochemical characteristics or health-related effects for the large array of aerosols that are inhaled and exhaled by e-cig users. With the rapid increase in e-cig users worldwide, secondhand exposure to e-cig aerosols has also become a serious public health concern. Through a series of studies, we have systematically characterized mainstream and secondhand e-cig aerosols in chambers, in laboratory indoor environments, and in vape shops. We found that e-cig device voltage, puff duration, puff volume, and e-liquid ingredients are important factors determining physiochemical properties of e-cig aerosols. We also summarize the evidence on the effects of e-cigs on indoor air quality, chemical compositions of mainstream and secondhand e-cig aerosols, and associated respiratory and cardiovascular effects. The use of e-cigs in indoor environments leads to high levels of fine and ultrafine particles similar to tobacco cigarettes. Concentrations of chemical compounds in e-cig aerosols are generally lower than those in tobacco smoke, but a substantial amount of vaporized propylene glycol, vegetable glycerin, nicotine, and toxic substances, such as aldehydes and heavy metals, have been reported. Exposures to mainstream e-cig aerosols have biologic effects, but only limited evidence showing adverse respiratory and cardiovascular effects in humans. Long-term studies are needed to better understand the dosimetry and health effects of exposures to secondhand e-cig aerosols. Future studies also need to focus on identifying vulnerable populations and monitor places that may contribute to high levels of secondhand exposures.

Plenary III
Aerosols in Chemistry and the Chemistry of Aerosols.
MURRAY JOHNSTON, *University of Delaware*

Aerosols provide a unique medium for studying chemical processes, while knowledge of chemical processes helps us understand and predict aerosol formation and growth in the atmosphere. In this presentation, the connection between aerosols and chemistry will be discussed, drawing from recent studies in our laboratory as well as the broader scientific community. From the “aerosols in chemistry” perspective, we will explore how chemical processes in aerosols may differ from those studied exclusively within a bulk phase or at an interface between two phases. Aerosols as media for performing chemical reactions provide the opportunity fine tune the interface-to-volume ratio and thereby control the relative reaction rates in the two regions. From the “chemistry of aerosols” perspective, we will explore how chemical processes contributing to growth of ultrafine particles, 100 nm in diameter and below, may change with particle diameter. The growth of smaller particles tends to be driven by interfacial processes while that of larger particles tends to be driven by volume processes, and the transition from one to the other occurs as particles grow. Finally, from both perspectives simultaneously, we will explore how aerosol processes can be exploited for chemical analysis – whether the motivation is molecular characterization of a bulk phase or airborne particulate matter.

Plenary IV
Mechanisms of Nanoparticle Formation and Their Health Effects.
ANGELA VIOLI, *University of Michigan*

An important step in predicting the growth of soot nanoparticles is understanding how gas phase variations affect the formation of their aromatic precursors. Once formed, these aromatic structures begin to assemble into nanoparticles and, regardless of the clustering process, the molecular properties of the aromatic precursors play an important role.

This presentation is divided in two parts: first we report on a detailed study of compounds formed in flames discussing formation mechanisms and their relative importance according to the environment. Using a unique computational model based on Monte Carlo techniques (named SNapS2), we are able to predict the structure and chemical evolution of various polycyclic aromatic compounds (PACs) and nanoparticle. PACs predicted in various conditions show diverse chemical properties, including aliphatic chains, five-membered, and heteroaromatic rings. Using graph theory and network analysis, we investigated the complex reaction network generated by SNapS2 and determined that the growth pathways of many PACs center around a few stable structures that also promote oxygen addition reactions due to their morphology and long lifetimes.

In the second part of the talk, we will address the health effects of PACs and nanoparticles. Indeed, one of the main issues related to the health effects of pollutants is their ability to cross biological cells, i.e. the transport through a physiological cellular membrane. The behavior of nanoparticles in a biological matrix is a very complex problem that depends not only on the type of nanoparticle but also on its size, shape, phase, surface charge, chemical composition, and agglomeration state. We present a theoretical model that predicts the average time of entry of nanoparticles in lipid membranes, using a combination of molecular dynamics simulations and statistical approaches. The model identifies four parameters that separate the contributions of molecules characteristics (i.e., size, shape, solubility) from the membrane properties (density distribution). The robustness of the model is supported by experimental data carried out in lipid vesicles encapsulating graphene quantum dots as nanoparticles. The new model, named LDA, is applied to the permeation of PAHs through various cellular membranes. Given the high level of interest across multiple areas of study in modulating intracellular targets, and the need to understand and improve the effects of nanoparticles and to assess their effect on human health (i.e., cytotoxicity, bioavailability), this work contributes to the understanding and prediction of interactions of nanoparticles and environmental media that affect fate, transport and risk.

Plenary V

Fine Particulate Matter: Interpreting Satellite Observations to Advance Understanding for Health Applications. RANDALL MARTIN, *Washington University in St. Louis*

Exposure to fine particulate matter (PM2.5) is the leading global environmental determinant of longevity. However, ground-level monitoring remains sparse in many regions of the world. Satellite remote sensing of aerosol optical depth offers global data to address this observational gap. Global modeling plays a critical role in relating satellite observations to ground-level concentrations. The resultant satellite-based PM2.5 estimates indicate pronounced variation around the world, with implications for global health and insight into the association of PM2.5 with health outcomes. Sensitivity simulations with the GEOS-Chem model provide information on the sources of ambient fine particulate matter contributions that affect human health. These capabilities offer information about the effects of COVID-19 lockdowns on air quality. The Surface Particulate Matter Network (SPARTAN) is designed to evaluate and enhance satellite-based PM2.5 estimates. Advanced high-performance modeling offers increasingly fine resolution to connect across scales. This talk will highlight recent advances in combining satellite remote sensing, global modeling, and ground-based measurements to improve understanding of PM2.5 for health applications from global toward urban scales.

1AC.1

Viscosity and Chemical Composition of Secondary Organic Aerosol from Real Healthy and Stressed Canary Island Pine Trees. NATALIE R. SMITH, Giuseppe Crescenzo, Anusha P.S. Hettiyadura, Kyla Siemens, Ying Li, Celia Faiola, Alexander Laskin, Manabu Shiraiwa, Allan Bertram, 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 secondary organic aerosols (SOA) with different properties when compared to SOA resulting from healthy plant emissions. The chemical composition of SOA determines particle viscosity, which in turn can impact photochemical aging of particles, their ability to act as cloud condensation and ice nuclei, and lifetimes of particulate pollutants in the atmosphere. In our previous study (in press), we showed that SOA from synthetic mixtures of VOCs simulating stressed plant emissions results in more viscous particles than SOA from mixtures representing healthy plant emissions. In this study, the molecular composition and viscosity were investigated for SOA generated from real healthy or aphid-stressed Canary Island pine (Pinus canariensis) trees, which are commonly used in landscaping. Aerosols were generated in a 5 m^3 environmental chamber at 50% relative humidity. Detailed information on particle molecular composition was gained through 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). At the time of writing the abstract, the actual viscosity of SOA particles has not been measured yet, but we hypothesize that stressed pine trees will produce more viscous aerosol particles. The predictions from the viscosity model will be compared to the experimental values measured via the poke-flow method. Comparison of viscosity and chemical composition for real healthy and stressed Canary Island pine SOA is novel, and it will advance our understanding of how tree stress influences physicochemical properties of SOA in an evolving environment.

1AC.2

Morphology and Viscosity Changes after Reactive Uptake of Isoprene Epoxydiols in Submicrometer Phase Separated Particles with Secondary Organic Aerosol Formed from Different Volatile Organic Compounds. ANDREW AULT, Ziying Lei, Nicole Olson, Yue Zhang, Yuzhi Chen, Andrew Lambe, Jing Zhang, Natalie White, Joanna Atkin, Mark Banaszak Holl, Zhenfa Zhang, Avram Gold, Jason Surratt, *University of Michigan*

Secondary organic aerosol (SOA), formed from the oxidation of volatile organic compounds (VOCs), is a large contributor to atmospheric fine particulate matter (PM2.5) and is commonly present in mixed inorganic-organic submicron particles. SOA formed from varying biogenic and anthropogenic VOCs results in unique aerosol physicochemical properties that modify climate impacts (i.e., water uptake). Understanding reactive uptake of VOC-derived semi-volatile oxidation products to inorganic-SOA mixed particles remains limited, particularly for particles at atmospherically-relevant sizes (~100 nm). These particles are particularly challenging to study as SOA can be quite viscous (i.e., solid or semi-solid), and mixed particles can have complex morphologies (e.g., core-shell). Herein, we show that the viscosity and morphology of initially core-shell (inorganic-organic) particles changed substantially after acid-catalyzed reactive uptake of isoprene epoxydiols (IEPOX), and that differences were highly dependent on VOC precursor (α-pinene, β-caryophyllene, isoprene, and toluene). SOA from two higher molecular weight precursors (α-pinene and β-caryophyllene) were less viscous after IEPOX uptake at 50% relative humidity (RH) based on atomic force microscopy (AFM) measurements, while SOA viscosities from lower molecular weight precursors (isoprene and toluene) did not change appreciably. The evolution of inorganic-SOA particle viscosity and morphology could alter the predicted impacts of SOA on air quality and climate.

1AC.3

Exploring Supramolecular Effects on the Viscosity and Phase State of Aqueous Organic-Inorganic Aerosols.

RYAN DAVIS, Erik Huynh, Josefina Hajek-Herrera, *Trinity University*

The phase state of aqueous organic-inorganic aerosol particles is of interest for, e.g., understanding the aerosol impact on air quality and climate, the transmission of infectious disease through respiratory aerosols, and utilizing aerosols for micro-encapsulation processes. Despite this widespread interest, there remains significant uncertainty about the fundamental processes dictating the viscosity and phase state of aqueous organic-inorganic aerosols. Recently, it was demonstrated that supramolecular interactions between divalent inorganic ions and low-mass oxygenated organic molecules can lead to deviations from bulk expectations of viscosity, and enable humidity-dependent gel transitions in aerosol particles. It remains unclear whether this is a general effect occurring with all divalent ion-oxygenated organic combinations. Here, we discuss new experimental investigations that provides insight into aerosol supramolecular chemistry. Using Ca^{2+} as the divalent ion with a range of oxygenated organic molecules, we demonstrate that divalent ions can have different effects, dependent on the identity of the organic molecule. We identify three different Ca^{2+}-organic compositions with distinct humidity-dependent outcomes: Ca^{2+}-organic mixtures where gelation or vitrification is not observed, but have an increased viscosity (relative to predictions); mixtures where the viscosity is increased and a gel transition is observed; and mixtures where there is only a minor supramolecular effect (that is, mixtures behave similar to expectations based on bulk predictions). We discuss the underlying chemistry influencing supramolecular effects on aerosol viscosity and phase, and the potential impacts on atmospheric chemistry.

1AC.4

The Impacts of Aerosol Mixing State on N2O5 Uptake Coefficient.

YICEN LIU, Yu Yao, Jeffrey H. Curtis, Matthew West, Nicole Riemer, *University of Illinois at Urbana-Champaign*

Dinitrogen pentoxide (N_2O_5) is an important nighttime reservoir for NO_x. The heterogeneous hydrolysis on aerosol particles is considered as the main loss pathway for N_2O_5, removing NO_x from the atmosphere. Current models use the bulk composition of the particle population to calculate the N_2O_5 uptake coefficient (γ). While this is appropriate when the aerosol is internally mixed, it remains an open question how large the error is when the aerosol has a more complex mixing state, which is common in the real atmosphere. To better understand the role of mixing state in calculating γ, the stochastic particle-resolved model PartMC-MOSAIC was used to generate 100 scenarios with different input parameters, including primary gas and aerosol emissions, as well as meteorological parameters. Each scenario was simulated for 24 hours with hourly output, yielding a total of 2,500 populations with different aerosol compositions and mixing states. For each population, the uptake coefficient γ_{PR} was first calculated using the particle-resolved composition data and the parameterization of N_2O_5 hydrolysis from Riemer et al (2008), which is a function of the per-particle sulfate and nitrate content and the organic coating thickness. We then compared γ_{PR} for each population with the corresponding value γ_{mix} which we obtained by assuming that the population was internally mixed. Preliminary results show that for 25% of the populations the error in the uptake coefficient was larger than +/- 20%. We present a detailed process analysis that explains the reasons for this over or underestimation and shows the impacts on the predictions of ozone and aerosol nitrate concentrations.

1AC.5

Experimental Investigation of the Gas- and Particle-Phase Products and Mechanism of NO3 Radical Oxidation of Δ-3-Carene, α-Pinene, and Limonene.

MARLA DEVAULT, Paul Ziemann, *University of Colorado*

Oxidation products of monoterpenes have been shown to contribute to secondary organic aerosol (SOA) formation in the atmosphere. However, the nighttime oxidative processes, which are dominated by nitrate radical (NO_3) addition to alkenes, are not well understood. In order to address this gap, we have measured the SOA yields and identified gas- and particle-phase products of the nitrate radical-initiated oxidation of Δ-3-carene, α-pinene, and limonene. Based on these analyses, we have developed a chemical mechanism for each monoterpene that includes both gas- and particle-phase reactions, and quantified major SOA products. Experiments were conducted at ambient temperature and pressure, at 55% RH in a dark 8 m^3 Teflon chamber, and using N_2O_5 to generate NO_3 radicals via thermal decomposition. The initial monoterpene:N_2O_5 ratio was 3:1, deliquesced ammonium sulfate seed particles were used, and the aerosol was monitored online using an electron ionization thermal desorption particle beam mass spectrometer (EI-TDPBMS) and scanning mobility particle sizer. In addition, an iodide chemical ionization mass spectrometer measured gas-phase products. After reaction completion, SOA was collected onto Teflon filters and extracted for analysis. The bulk functional group composition was determined using a set of derivatization-spectrophotometric analysis techniques and attenuated total reflectance Fourier-transform infrared (ATR-FTIR) spectroscopy. Products containing nitrate groups, which includes most of the SOA, were separated and often quantified using high performance liquid chromatography with UV-Vis detection at 210 nm. Fractions collected based on this chromatogram were then analyzed using an electrospray ionization mass spectrometer, the EI-TDPBMS, ATR-FTIR, and derivatization-spectrophotometric techniques, leading to the identification of several acetal and hemiacetal dimer products. The mechanisms derived from the measured gas- and particle-phase products will inform regional and global models on the contribution of nighttime oxidation of monoterpenes to SOA.

1AC.6

Influence of Continuous NOX Injection on SOA Yield from Biogenic Precursors: Comprehensive Branching Ratio Study.

SAHAR GHADIMI, David Cocker, *University of California, Riverside*

α-Pinene plays an important role in atmospheric pollution due to its high SOA yield and it's global prevalence as the most abundant emitted monoterpene ($C_{10}H_{16}$) worldwide. α-Pinene undergoes photooxidation reactions to generate highly reactive $RO_2^{\cdot}$ species. Depending on atmospheric NO_x levels (and specifically NO levels), these $RO_2^{\cdot}$ species undergo further reaction via two competing mechanistic pathways ($HO_2^{\cdot}$ or NO), the extent of which reaction occurs is referred to as the "branching ratio (β)". Under low-NO_x conditions, $RO_2^{\cdot}$ radicals tend to react more with $HO_2^{\cdot}$ radicals to yield gas-phase products with lower volatility leading to higher SOA formation. Contrary, under high-NO_x conditions, $RO_2^{\cdot}$ radicals react with NO molecules resulting in the formation of the high volatile organic nitrates leading to lower SOA yields.

In this study, the correlation between SOA formation yield from α-Pinene precursor and β value was investigated in an atmospheric chamber. A series of experiments were designed using SAPRC modeling to oxidize α-pinene while maintaining constant β values throughout the experiment via continuous NO injection. The results will be compared to "classical" SOA yield experiments in which the NO and VOC was injected at the start of the experiment with β increasing throughout the experiment from near 1 to near 0. The outcomes of this novel study are critical for the development of more accurate atmospheric SOA models.

1AC.7

Hygroscopic Growth and Water Transport in Mixed Organic-Inorganic Aerosol Particles. JAMES F. DAVIES, Jack Choczynski, Ravleen Kaur Kohli, Craig Sheldon, Chelsea Price, *University of California, Riverside*

Recent measurements have revealed unique physical and chemical characteristics associated with mixtures of organic and inorganic molecules in aqueous aerosol particles [1,2]. Relative to their individual components, these mixtures may exhibit increased viscosity, slowed water transport, and phase transitions to liquid-liquid phase separated states and gels as a function of relative humidity (RH). Characterizing the RH response of these particles is important for exploring their role in atmospheric processes, such as cloud formation and heterogeneous reactions, and in disease transmission via respiratory aerosol.

In this work, we describe a new experimental approaching using a linear-quadrupole electrodynamic balance to levitate two aqueous particles [3]. Mie resonance spectroscopy is used to probe the size and refractive index of both particles, and to identify changes in phase state [4]. One particle acts as a fast-responding and accurate in-situ probe of the RH, while the response of the other particle is measured to elucidate its hygroscopic growth, condensed-phase diffusivity, and phase state as a function of RH. Through these measurements we will characterize the hygroscopic properties of mixtures of ammonium sulfate and organic molecules, such as citric acid, and directly measure both the rate of water diffusion and the aqueous concentration across the whole RH range. We will compare our results to predictions based on simple mixing rules and established thermodynamic models to validate their use in predicting the dynamics of mixed organic-inorganic particles.

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1AC.9

Aqueous Phase Photochemical Transformations of Phenolic SOA: Comparisons between OH Radical and Triplet Carbon Oxidation. CHRISTOPHER NIEDEK, Wenqing Jiang, Ryan Farley, Lan Ma, Stephanie Arciva, Cort Anastasio, Qi Zhang, *University of California, Davis*

Recent laboratory studies have shown aqueous-phase processing of phenolic compounds, often a large portion of wood combustion emissions, to be a significant source of aqueous SOA (aqSOA). Previous work into phenolic aqSOA relevant to biomass burning emissions has largely focused on relatively unsubstituted phenols (ex. phenol, guaiacol, and syringol). Less attention has been paid to highly substituted phenols which are more likely to partition into the aqueous phase due to their higher Henry's law constants.

This work is focused on characterizing the aqSOA formed via hydroxyl radical (OH) and triplet excited states of organic compounds ($^3C^*$) oxidation of a set of highly substituted phenols (guaiacyl acetone, vanillyl alcohol, syringyl acetone, syringic acid, tyrosol, and ferulic acid) using a soot particle high-resolution aerosol mass spectrometer (SP-AMS). The mass yields, bulk composition, and photochemical evolution of the aqSOA were studied. In addition, a thermodenuder was used upstream of the SP-AMS to gather the volatility profiles of the aqSOA for vanillyl alcohol and $^3C^*$. Some aspects of the bulk composition (ex. elemental ratios like O/C and H/C and signal intensities of $C_2H_3O^+$ (m/z 43) and CO_2^+ (m/z 44)) were similar between OH and 3C*-generated SOA. Notably, all aqSOA samples analyzed fall into a relatively small window in H/C-O/C space, implying a high degree of bulk chemical similarity and similar degrees of oxidation between OH and $^3C^*$-generated aqSOA. In contrast, OH-generated SOA had higher levels of acid-functionalization (as evidenced by CHO_2^+ signal intensity) while $^3C^*$-generated SOA had higher levels of oligomerization (as evidenced by dimer ion signal intensities). Volatility profile analysis demonstrates production of high molecular weight, low-volatility species in the aqSOA of vanillyl alcohol. The mass spectra of each phenolic aqSOA also reveal ions potentially useful as tracer species for ambient studies of biomass burning emissions.

1AC.11

Pressure Implication in Atmospheric Aerosols: Rate Constant and Product Formation. CLéMENT DUBOIS, Sebastien Perrier, Yinon Rudich, Sergey Nizkorodov, Frédéric Caupin, Thorsten Hoffmann, Chrisitan George, Matthieu Riva, *CNRS-IRCELYON*

Secondary organic aerosols are key players in the atmosphere formed, either by nucleation of low volatile compounds or by heterogeneous reactions occurring onto pre-existing aerosols. The formation and aging of atmospheric aerosols is the object of intense research. Therefore, we decided to focus on one physical aspect not considered in the atmospheric sciences hitherto: the pressure inside nanoparticles. Due to the Young-Laplace law's, the pressure inside nanometric aerosols can reach hundreds of bars. This pressure can affect chemical reactions, during which the molar volume of products differ from that of reactants. Thus, the pressure could allow the formation of compounds when the reaction mechanisms are favored under pressure. These reactions could aid in the formation and the growth of nanometric particles. To study the impact of the pressure on atmospheric aerosols, we placed aqueous samples containing glyoxal and ammonium sulfate under pressure using a high-reaction vessel. After different exposure times and pressures, the chemical composition of each sample was retrieved using high-resolution mass spectrometry and UV/Vis spectroscopy. The formation of reaction products was shown to be strongly (i.e., up to a factor of 2) slowed down under high pressures, typical of atmospheric nanoparticles. This may indicate that the reactional intermediate temporarily increases the total volume of the reaction, resulting in a decrease of the reaction products formation. To extend the analysis of the reactions under pressure, we developed an experimental system, allowing in-situ characterization of the absorbance of chemical compounds at various pressures. Chemical analyses were also performed using UHPLC-ESI-Orbitrap-MS to determine the chemical composition of the mixtures exposed to different pressures. Using this new system, we studied a large number of chemical mixtures to reveal the impact of pressure on atmospheric relevant systems. The chemical modification and/or a change in the rate constant can help predicting the formation of aerosols.

1AC.12

State of Air Pollution and Its Health Effects on Human Health - A Case Study of Karachi, Pakistan. KAMRAN KHAN, Saiyada Masood, Sumayya Saied, Azhar Siddique, Mirza M. Hussain, Haider Khwaja, *University of Karachi, Pakistan*

Particulate matter pollution is the persistent interest with respect to environment and public health. Urban centers are mostly affected due to rapid industrialization and unplanned urbanization. The extensive assessment of $PM_{2.5}$ was performed in the current analysis to investigate $PM_{2.5}$ mass of the mega city, Karachi, along with the characterization and source apportionment. Three sites characterized by the typical urbanized environment of high vehicular emission and heavy population were selected. Two sites (AFOHS and Gulshan-e-Maymar, GM) were influenced by industrial emissions being situated in proximity while one site (Gulshan-e-Iqbal, GI) is categorized as residential area surrounded by commercial activities. Risk assessment of $PM_{2.5}$ was conducted whereas estimation of expected deaths was also quantified. During the study, $PM_{2.5}$ mass measured, were exceeding the WHO guidelines. High carbonaceous portion of $PM_{2.5}$ was also estimated at all three sites because of vehicular emission (BC_{IR}) and biomass burning (BC_{UV}). Source apportionment was performed by enrichment factor, mass reconstruction and factor analysis. It reveals the high contribution of natural and anthropogenic activities in elevated $PM_{2.5}$ mass concentration. Major components involved combustion of fossil fuels, soil re-suspension, and emissions from industries as well as vehicles. Backward-in-time trajectory was used to assess the long-range transportation of $PM_{2.5}$ at local and regional level. It shows significant impact on the concentration of atmospheric aerosols in which major portion comprises of anthropogenic sources paired with vehicular and industrial emissions and fossil fuel combustion. High morbidity rate was also endorsed by the results obtained from risk assessment carried out for daily $PM_{2.5}$ exposure level. Air Quality Index (AQI) was also measured at all three sites and found most of the air not suitable for health.

1AE.1

Laboratory Evaluation of Low-cost Optical Particle Counters for Environmental and Occupational Exposures.

SINAN SOUSAN, Swastika Regmi, Yoo Min Park, *East Carolina University*

Low-cost optical particle counters effectively measure particulate matter (PM) mass concentration and are easy to operate, portable, and compact. However, calibration differences between environmental and occupational settings have not been demonstrated. This study evaluated four commercially available PM low-cost sensors (OPC-N3 from Alphasense, SPS30 from Sensirion, AirBeam2 from HabitatMap, and PMS A003 from Plantower) in environmental and occupational settings. The mass concentrations (PM_1, $PM_{2.5}$, PM_4, and PM_{10}) of three aerosols (salt, Arizona road dust, and Poly-alpha-olefin-4 oil) were measured and compared with the GRIMM MiniWRAS as the reference instrument. For all aerosol types, the OPC-N3 and SPS30 were highly correlated (r=0.99) compared to the AirBeam2 (r=0.65-0.97) and PMS A003 (r=0.22-0.97), for environmental settings. In contrast, the OPC-N3 correlation varied (r=0.88-1.00), but the SPS30 and AirBeam2 exhibited high correlation (r=0.99), as did the PMS A003 (r=0.96-0.99), for occupational settings. Response significantly ($p <0.001$) varied between environmental and occupational settings for most particle sizes and aerosol types. Biases varied by particle size and aerosol type. For environmental settings, the SPS30 exhibited substantially low bias for salt aerosol for PM_1 (bias=-6.10) and $PM_{2.5}$ (bias=-0.82) measurements among all the low-cost sensors. In contrast, the OPC-N3 bias was low for dust (PM_1=-4.3 and $PM_{2.5}$=-10.63) and oil (PM_1=1.88 and $PM_{2.5}$=-8.92). AirBeam2 and PMS A003 biases were considerably high for all aerosol types and PM metrics. For occupational settings, all the low-cost sensors showed a high bias for all PM metrics. For intra-instrument precision, SPS30 exhibited high precision for salt within the recommended range (CV<10%) for environmental and occupational settings compared to other low-cost sensors and aerosol types. These findings suggest that SPS30 and OPC-N3 can provide a reasonable estimate of PM mass concentrations if calibrated differently for environmental and occupational settings using site-specific calibration factors.

1AE.2

Investigation into the Pulmonary Health Effects of Dust and Sea Spray Aerosol from the Salton Sea on Mice using Whole Body Exposure Chamber.

QI LI, Ryan Drover, Trevor Biddle, Mia Rose Maltz, David Lo, David R. Cocker III, *University of California, Riverside*

The Salton Sea is a 345mi^2 inland saline lake located in California imperial counties and fed by agricultural runoff. Due to a 2003 ordinance diverting water to San Diego county, the Salton Sea has been drying rapidly, exposing more lakebeds and causing the water to become hypersaline. This has caused significant ecology changes, resulting in algal blooms, fish and migratory bird die-offs, and an increase in dust production. As a result, serious concerns have been raised over the air quality in nearby areas. Surrounding communities suffer from one of the highest rates of childhood asthma in California at 20% - 22.4%, compared to an average of 14.5% for the rest of the state. While many types of particles may potentially contribute to the health effects, we focused on the dust particles and water spray aerosols. In this study, mice were exposed to either an aerosolized aqueous extract from dust surrounding the Salton Sea, filtered and aerosolized Salton Sea water, Alternaria aerosol, or filtered and aerosolized Pacific Ocean water separately for 7-day. Alternaria, a known effective fungal allergen, was used to set up a reference for an inflammatory lung response. Pacific Ocean sample served as a control to account for the potential inherent effects of saline water. Exposure experiments were conducted in the newly established dual animal whole body exposure chambers (540L per each). Particles were generated continuously with consistent size distribution and concentration of 1.5 $mg\ m^{-3}$ through experiments. Chemical component analysis was done by using a ToF-AMS. Seasonal component fraction change was found with organics varying from 5.9% to 19.7% in Salton Sea sprayed particles and from 12.1% to 19.9% in Pacific Ocean sprayed particles, as compared to high organic fraction of 82.3% in Alternaria particles and 29.7% in Salton Sea dust extraction. Flow cytometry, NanoString analysis and histology were used to characterize the immune response due to the exposure. Our results confirmed that Alternaria caused strong inflammatory response from mice. Conversely, Pacific Ocean aerosol failed to trigger an inflammatory response. The Salton Sea dust extract was able to trigger a strong inflammatory response distinct from Alternaria. Despite cellular infiltrates in the dust exposure, Salton Sea water failed to recruit key inflammatory cells. However, the Salton Sea water aerosol was capable of generating a small, but significant change in inflammatory gene expression distinct from the other exposures. Detailed discussion on gene expression change will be presented. Thus, the Salton Sea water spray may play a key role in the progression to asthma or other inflammatory diseases despite the inability to generate asthma alone in this study.

1AE.3

Openly Accessible Low-Cost Measurements for PM2.5 Exposure Modeling: Guidance for Monitor Deployment with a Similarity Metric. JIANZHAO BI, Nancy Carmona, Magali Blanco, Amanda Gassett, Edmund Seto, Adam Szpiro, Timothy Larson, Paul Sampson, Joel Kaufman, Lianne Sheppard, *University of Washington*

High-resolution, high-quality exposure modeling is critical for assessing the health effects of $PM_{2.5}$ in epidemiological cohorts. Sparse ground-level $PM_{2.5}$ measurements, as key model input, may result in two potential issues in high-resolution exposure prediction: (1) they may affect the models' accuracy in predicting the spatial distribution of $PM_{2.5}$; and (2) internal validation based on these measurements may not reliably reflect the model performance at the locations of interest (e.g., ambient $PM_{2.5}$ concentrations at cohort residential locations). This study aimed to use $PM_{2.5}$ measurements from an openly accessible low-cost $PM_{2.5}$ network, PurpleAir, with an external validation dataset at residential locations of a representative sample of participants from the Adult Changes in Thought - Air Pollution (ACT-AP) study to improve the accuracy of exposure prediction at the cohort locations, and propose a metric assessing the similarity between the monitor and cohort locations to guide future monitor deployment. We utilized a spatiotemporal modeling framework to incorporate $PM_{2.5}$ measurements from 51 "gold-standard" monitors and 58 PurpleAir monitors in the Puget Sound region of Washington into high-resolution exposure assessment at the two-week level from June 2017 to March 2019. We proposed a similarity metric based on principal component analysis (PCA) - the PCA distance - to assess the PurpleAir monitors' representativeness of the cohort locations. After including calibrated PurpleAir measurements as part of the dependent variable, the spatiotemporal validation (at the two-week level) R^2 and root-mean-square error, RMSE, improved from 0.84 and 2.22 $\mu g/m^3$ to 0.92 and 1.63 $\mu g/m^3$. The spatial validation R^2 and RMSE improved from 0.72 and 1.01 $\mu g/m^3$ to 0.79 and 0.88 $\mu g/m^3$. We found that the PurpleAir monitors with shorter PCA distances could improve the model's prediction accuracy more substantially than monitors with longer PCA distances, indicating the reasonability of this similarity metric. To our knowledge, this was the first attempt to evaluate the benefits of low-cost $PM_{2.5}$ measurements for long- and short-term exposure prediction at cohort residential locations and to provide practical guidance with a PCA-based similarity metric for future monitor deployment.

1AE.4

Emulating Chronic Near-Roadway Exposures for Studying Alzheimer's Disease. KEITH BEIN, Kelley Patten, Anthony Valenzuela, Christopher Wallis, Elizabeth Berg, Jill Silverman, Anthony S. Wexler, Pamela Lein, *University of California, Davis*

Epidemiological data link traffic-related air pollution (TRAP) to increased risk of Alzheimer's disease (AD). Preclinical data corroborating this association are largely from studies of male animals exposed acutely or subchronically to high levels of isolated fractions of TRAP. What remains unclear is whether chronic exposure to ambient TRAP modifies AD risk and the influence of sex on this interaction. Our study assesses the effects of chronic exposure to ambient TRAP on the time to onset and severity of AD phenotypes in a pre-clinical model and whether sex or genetic susceptibility influences outcomes. Male and female TgF344-AD rats that express human AD risk genes and wildtype littermates were housed in a vivarium adjacent to a heavily trafficked tunnel in Northern California and exposed for up to14 months to filtered air (FA) or TRAP drawn from the tunnel and delivered to animals unaltered in real-time. Refractive particles in the brain and AD phenotypes were quantified in 3-, 6-, 10-, and 15-month-old animals using hyperspectral imaging, behavioral testing, and neuropathologic measures. Particulate matter (PM) concentrations in TRAP exposure chambers fluctuated with traffic flow but remained well below 24-hr $PM_{2.5}$ National Ambient Air Quality Standards. Results show that *(1)* ultrafine PM was the predominant component of TRAP, *(2)* nano-sized refractive particles were detected in the hippocampus of TRAP animals., *(3)* TRAP-exposed animals had more amyloid plaque deposition, higher hyperphosphorylated tau levels, more neuronal cell loss, increased microglial cell activation, and greater cognitive deficits in an age-, genotype-, and sex- dependent manner. These data suggest that AD progression depends on complex interactions between environment and genetics and that current $PM_{2.5}$ regulations are insufficient to protect the aging brain. Results will be presented in combination with a comprehensive characterization of exposure dynamics at the tunnel facility.

1AE.5

Source-Resolved Variability of Fine Particulate Matter and Human Exposure in an Urban Area. BRIAN DINKELACKER, Pablo Garcia, Iannis Kioutsioukis, Peter Adams, Spyros Pandis, *Carnegie Mellon University*

Increasing the resolution of chemical transport model (CTM) predictions in urban areas is important to capture sharp spatial gradients in atmospheric pollutant concentrations and better inform air quality and emissions controls policies that protect public health. The chemical transport model PMCAMx was used to assess the impact of increasing model resolution on the ability to predict the population exposure to PM2.5 at 36 x 36, 12 x 12, 4 x 4, and 1 x 1 km resolutions over the city of Pittsburgh during typical winter and summer periods (February and July 2017). At the coarse resolution, county-level differences in predicted PM2.5 concentration can be observed, while increasing the resolution to 12 x 12 km resolves urban-rural gradients. Increasing resolution to 4 x 4 km resolves large stationary sources such as power plants and the 1 x 1 km resolution reveals intra-urban variations and individual roadways within the simulation domain. Despite improvements in the ability of the model to capture localized concentration gradients, the average population weighted PM2.5 concentration does not change significantly with resolution. This suggests that even medium resolution PM2.5 predictions may be sufficient to characterize average PM2.5 exposure. Individual source contributions to population exposure were assessed at the 1 x 1 km scale. During the winter simulation period, residential wood combustion had the largest contribution to total PM2.5. During the summer period, the contribution from residential wood combustion is negligible while power generation had the largest contribution to total PM2.5. The contributions of local sources such as on-road traffic, residential wood combustion, cooking, and miscellaneous area emissions to human exposure exceed their contributions to average PM2.5 in the area.

1AE.7

The Impact of Vegetated and Non-vegetated Roadway Barriers on Particle Concentrations and Toxicity. ROBY GREENWALD, Christina Fuller, Christa Wright, Haris Bejdic, *Georgia State University*

The Trees Reducing Environmental Exposures (TREE) simultaneously sampled particle concentrations in front of and behind roadway barriers along major interstate highways in the Atlanta metropolitan area. We measured PM2.5 and PM1 mass concentration, black carbon (BC) mass concentration, the particle number concentration (PNC), and the size distribution of ultrafine aerosols. In addition, we collected filtered samples of PM1 for use in in vitro toxicology experiments using human airway epithelial cells. Our sample sites include I-75/85 in Midtown Atlanta (with comparatively few tractor-trailer trucks) and numerous locations along the I-285 perimeter highway (with a higher fraction of tractor-trailer trucks). These sites encompass the range of roadway barrier options in the Atlanta area: simple chain-link fences, solid sound barriers, vegetated barriers, or both vegetated and solid sound barriers. Vegetated barriers exhibited the greatest reduction in particle concentrations in terms of PM or BC mass concentration as well as PNC. This effect was more pronounced for barriers comprised of species with larger canopy diameters and denser vegetation as assessed by leaf area index. The ultrafine size distribution was comprised of modestly smaller particles on the highway side of the barrier. In numerous cases, traffic sources from the non-highway side of the barriers reduced the difference in concentration from one side of the barrier to the other. In addition, when wind direction was from the barrier toward the highway, the difference in concentration was similarly reduced. Toxicological evaluation showed higher levels of cellular oxidative stress as assessed by the ratio of oxidized-to-reduced glutathione in exposed cells for particles collected on the highway side of the barriers. In addition, the production of reactive oxygen species (ROS) was higher in cells exposed to highway particles.

1AE.8

High-Resolution Social Cost Modeling Offers Insight into Efficiency-Equity Trade-Offs in Pollution Mitigation Strategies.

BRIAN GENTRY, Allen Robinson, Peter Adams, *Carnegie Mellon University*

Air pollution causes upwards of 100,000 premature mortalities per year in the United States, with fine particulate matter (PM2.5) causing a bulk of these mortalities. Measures to control air pollution are therefore a high-priority policy target that can yield large social benefits. Additionally, recent studies have demonstrated a significant difference in PM2.5 exposure between races, making air pollution control a key environmental justice issue. However, accurate modeling of health impacts of emissions requires extensive software experience and significant computational time.

Reduced complexity models (RCMs) seek to simplify this process by offering location-specific marginal social cost estimates for primary PM2.5 and major PM2.5 precursors, allowing for rapid screening of potential pollution mitigation policies. We extend the capabilities of one such model, EASIUR, to capture intra-urban area variabilities in social cost damages of primary PM2.5 emissions. This model combines the chemical transport model core of EASIUR to simulate the long-range transport of air pollutants with a Gaussian plume model for local transport. We find that social cost damages can vary by an order of magnitude within a single county, while spatially aggregated cost estimates are in good agreement with EASIUR and other RCMs. Social costs of primary PM2.5 may be previously underestimated due to spatial variation in marginal social cost estimates and emissions. Analysis of a source-receptor version of the model indicates that emissions in most urban areas also contribute to higher PM2.5 exposure among people of color than among white people. We demonstrate use of the tool by evaluating the distribution of benefits and costs of high electric vehicle adoption in the U.S. Combined with spatially resolved emissions inventories, this tool can be used to identify specific emissions sectors that yield great social benefits and reductions in exposure disparities across social groups.

1AE.9

Global Air Quality and Human Health Effects of Solid Biofuel Stove Emissions.

YAOXIAN HUANG, Debatosh Partha, Kandice Harper, Chris Heyes, *Wayne State University*

In this study, we employed the NCAR (National Center for Atmospheric Research) Community Earth System Model CAM5-Chem (Community Atmosphere Model coupled with Chemistry version 5.3) model to quantify the impacts of global solid biofuel stove emissions on ambient surface $PM_{2.5}$ (particulate matter with aerodynamic diameters equal to or less than 2.5 micrometers) and ozone (O_3) air quality and human health. Annual mean surface $PM_{2.5}$ and O_3 concentrations from global solid biofuel stove emissions averaged over 2006-2010 were up to 23.1 $\mu g\ m^{-3}$ and 5.7 ppbv, respectively, with large impacts found over China, India and sub-Saharan Africa for both $PM_{2.5}$ and O_3. The global annual total $PM_{2.5}$- and O_3-induced premature deaths associated with solid biofuel stove sector were 382,000 [95% confidence interval (95CI): 349,000-409,000], with the corresponding years of life lost as 8.10 million years (95CI: 7.38-8.70 million years). Our study highlights co-benefits of air quality and human health via promoting clean household energy programs over low-income and middle-income countries.

1AE.10

Investigation of Protection Efficiency for Masks Commonly Used for Ultrafine Particles and Their Effects on Aerosol Respiratory Deposition.

JINHO LEE, Wei-Chung Su, *University of Texas Health Science Center at Houston*

Exposure to ultrafine particles has been and continues to be an essential occupational and environmental health issue. To reduce the inhalation of ultrafine particles, wearing a mask is strongly recommended. This research investigated the protection efficiency of masks commonly used to prevent ultrafine particles from entering the human respiratory tract. Besides, the change of the regional aerosol respiratory deposition in the human upper airways due to the effect of mask-wearing was also studied in this research.

The experiments were conducted in a stainless-steel test chamber. A silicone mannequin face wearing the test mask covering the mouth and nose was placed side-by-side with an identical reference mannequin face. Surrogate aerosol (NaCl particles) in the size range of 10 to 200 nm were used as the challenge ultrafine particles. Two sets of particle sizers (SMPS) were employed to measure the aerosol size distribution entered the two mannequins. For the reference mannequin, measurements were taken only at the oral cavity throughout the experiments. For the test mannequin, measurements were recorded at the oral cavity with and without masks, as well as at the outlet of the TB airways with and without masks.

The N95 mask showed an overall high protection efficiency, and the protection efficiency was 84% on average for the particle sizes studied. In contrast, the cloth mask (20%) and the mask with a breathing valve (34%) showed generally low protection efficiencies. The N95 presented a relatively more decrease in deposition friction for all particle sizes studied. The cloth mask showed a general less decrease among all masks tested.

1AE.11

Morphometric Study of Varied Particle Size Fractions in Different Socio-Economic Urban Microenvironments of Northern India.

HIMANSHI ROHRA, Atar Singh Pipal, Ajay Taneja, Gursumeeran Satsangi, *Savitribai Phule Pune University, Pune, India*

Application of field emission scanning electron microscopy coupled with energy dispersive X-ray spectrometry (FESEM-EDX) was done to study the morphological characterization and elemental microanalysis of individual particles varied with distinct indoor micro-environments i.e., HIG, MIG and LIG. Particle dynamics investigation revealed a double modal pattern of distribution (0.25-0.5µm and 0.5-1.0 µm) in quasi-accumulation range. Tar balls (TB), soot particles and dust particles were extracted in observation from SEM images and surface elemental composition. Further study of shape descriptor parameters revealed particles to be non-uniform (circularity=0.6-0.7 and Aspect Ratio (AR): 1.5-1.9). Sphericity=1.0-2.9 inferred deviation of shape in microenvironments. Roundedness (RD)= 0.2-0.9 inferred variation of particle shape from perfect sphere to irregular. RD and AR varied in inverse and direct proportion with DAeq (Area equivalent diameter) suggesting elongation of particles with higher DAeq. Nevertheless, more spherical particles (soot and TB) were found in HIG than LIG and MIG. EDX spectra revealed Fe, K, Mg (crustal origin) were contained in PM0.5-0.25. Overall, findings imply that house type, fuel quality, kitchen type and social-economic conditions do strongly influence the morphology of particles in urban environments. Indoor air quality in LIG was significantly deteriorated with increased particle load (>25-40%) than MIG and HIG. The efforts paved in for better understanding of relationship between indoor microenvironments and human health will aid policy makers to design intervention policies for betterment of air quality in residential environments.

1CO.1

Ice Nucleation on Soot Particles: Measurements, Predictions and Implications. FABIAN MAHRT, Bernd Kärcher, Claudia Marcolli, *University of British Columbia*

Soot particles are emitted as a by-product of incomplete combustion processes. They play a critical role for air quality and human health. Soot particles also impact climate, directly by absorbing radiation and indirectly by acting as ice nucleating particles. Despite extensive previous work, the understanding of the climate impacts of soot remains incomplete, in large parts because a coherent understanding of the ice nucleation mechanism and ice activity of soot particles has not emerged. As a consequence, there remain large uncertainties associated with the soot-cloud interactions and associated feedbacks. A key example is aviation, where it has been hypothesized that the interaction of emitted soot particles with natural cirrus affects their microphysical properties and might lead to a large radiative forcing. However, such impacts are associated with large uncertainty due mainly to the lack of understanding the conditions in which aircraft-emitted soot particles nucleate ice.

Here, we integrate laboratory measurements, theory and cloud modelling to address the ice nucleation activity and mechanism of soot particles. Starting from soot ice nucleation laboratory measurements that evidenced a pore condensation and freezing (PCF) process, we developed a novel theoretical framework that incorporates the aggregate structure of soot particles in the description of ice nucleation by PCF. The soot-PCF framework treats the primary soot particles as spheres that aggregate together forming pores that are characterized by the primary particle size and overlap, as well as the contact angle between the particle surface and water. We used the soot-PCF framework to derive a new parameterization to describe the ice formation of aviation soot particles. The parameterization is well constrained by experimentally determined soot particle properties but is versatile and can easily be adjusted to soot particles with other characteristics, e.g. from different emission sources. Implementing the new parameterization into a high-resolution cirrus column model to study how aircraft-emitted soot particles, released from sublimating contrails, perturb natural cirrus clouds, we find that at most 1 % of the soot particles form ice crystals alongside homogeneous freezing. Our results have important implications for the climate impact of aviation.

1CO.2

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

Biofuel combustion is an important source of light absorbing organic carbon (OC), also known as brown carbon (BrC). In this work, we applied spectrophotometry to characterize methanol-extracted BrC from filters collected during ‘real-world’ biofuel combustion emissions tests in India and Malawi, including various wood stoves (‘traditional’, ‘improved’ and ‘chimney’) and artisanal ‘charcoal’ kilns. Extracts’ average mass absorption coefficient ($MAC_{bulk,\lambda}$) at near-ultraviolet to blue wavelengths was the highest for ‘traditional’, followed by ‘improved’, ‘chimney’, and ‘charcoal’; Absorption Angstrom Exponent (AAE) showed the opposite trend. $MAC_{bulk,\lambda}$ in UV wavelengths were positively correlated with elemental carbon to organic aerosol ratio (EC/OA), although less so than in lab cookstove studies. Unlike EC/OA, modified combustion efficiency (MCE) exhibited a weak positive correlation with $MAC_{bulk, \lambda}$, indicating that EC/OA was a better indicator of combustion conditions associated with BrC production. Imaginary refractive indices of BrC at 551 nm (k_{551}) were anti-correlated with wavelength dependence (w), suggesting that less wavelength dependent BrC has higher light absorptivity. $MAC_{bulk,\lambda}$ correlated with the fraction of OC evolving at 615°C (OC3/OC) and anti-correlated with OC evolving at 310°C (OC1/OC). This association is consistent with a link between BrC absorptivity and OC volatility, and suggests that BrC absorption may be parameterized using existing OC data. EC/OA is strongly negatively correlated BrC contribution to total aerosol light absorption. BrC showed high absorption contribution ranging from 48% to 80%, on average, at 365 nm depending on mixing state assumptions. We are now estimating the direct radiative effect (DRE) of BrC from biofuel combustion over India using the BrC light-absorption properties obtained from our experiments in conjunction with MERRA reanalysis dataset.

1CO.3

Design and Evaluation of a New Source Sampler for on-Field Emission Measurement from Combustion Sources.

JYOTI KUMARI, Kashish Jain, Kumail Zaidi, Gazala Habib, *Indian Institute of Technology Delhi*

Previous inventories have identified biomass fuel combustion in cooking stoves as one of the major source of aerosol emissions in India. The emission factors reported in numerous recent studies are based on controlled tests conducted in the simulated kitchens in the lab using single fuel type. Few field experiments have reported higher emission factors compared to lab-based measurement however, still, the database needs representative enrichment to refine emission estimates. A new source sampler has been designed for the on-field collection of PM2.5, near real-time quantification of its microphysical and optical characteristics (i.e. Number concentration, Absorption, and scattering coefficients) and gaseous pollutant's emissions from combustion sources. The sampler consists of a portable dilution tunnel, ejector dilutor, zero-air generator, and power supply unit. The dilution tunnel has been evaluated for the particle losses and homogenous mixing along the length of the tunnel. The results showed insignificant particle losses inside the tunnel at different dilution ratios (20:1 to 40:1). A pilot study was conducted in Haryana, India showed that the PM2.5 emission factors were 2.5-4.5 times higher from the use of mixed fuel (i.e. fuelwood and dung cake) compared to use of fuelwood and cow dung alone separately. The paper will discuss the evaluation of the source sampler and on-field emission factors of PM2.5, OC, EC, BC, and gaseous pollutants for residential biofuel cookstove.

1CO.4

The Role of Oxidizer Concentration, Fuel Consumption Rate, and Dilution Conditions on Near-source Aerosol Emissions from Lignocellulosic Biomass and Constituent Burning.

LUKE MCLAUGHLIN, Erica Belmont, *University of Wyoming*

The majority of global primary organic aerosol (POA) emissions are produced from biomass burning (BB), and POA are understood to have negative impacts on humans and the environment. POA emissions have a broad range of physical properties, such as particle size, quantity, and volatility, and these properties are closely related to near-source burning conditions. The properties of POA are difficult to predict due to the natural complexities of BB, including variability in near-source burning conditions such as oxygen availability, fuel consumption rate, and dilution gas temperature. In this work, aerosol emissions were measured in a controlled laboratory setting from burning of lignocellulosic biomass and major lignocellulosic biomass constituents in inert and oxidative environments to better understand the influence of fuel composition, dilution conditions, and oxygen availability on the number and size of aerosols formed during BB. Fuel mass and fuel consumption rate were also investigated for their influence on aerosol emissions, and an aerosol volatility assessment was performed. A summative model for aerosol emissions prediction from BB was developed and tested, and results were compared to experimental measurements from woody and herbaceous biomass samples. Results showed significant influences of fuel type, oxygen availability during burning, and dilution conditions on the number and size of aerosols formed, and nucleation mode particles dominated the emissions in all of the conditions investigated here. Absolute fuel consumption rate increased with increased reaction environment oxygen level and fuel mass, and aerosol size positively correlated with fuel consumption rate. The summative model predicted number emissions for biomass pyrolysis and combustion and mass emission factors for biomass combustion well. However, the model less successfully captured the measured mass emission factors for biomass pyrolysis. The applicability of the proposed model and reasons for the discrepancies between the model and experiments were investigated in this work.

1CO.5

Carbon Black and Hydrogen Production: An Optimized Reaction Mechanism for Methane Pyrolysis. AMBUJ PUNIA, James Tatum, Larry Kostiuk, Jason S. Olfert, Marc Secanell, *University of Alberta*

Methane pyrolysis (anaerobically decomposing methane at high temperatures) can be used to transform methane into carbon black and hydrogen without any greenhouse gas emissions. The carbon black can be used in many commercial products and the hydrogen can be used in many energy applications. This process depends on the temperature and pressure and during the process, other intermediate species, such as acetylene (C_2H_2), ethylene (C_2H_4) and ethane (C_2H_6), are also observed. Accurate prediction of these species requires an understanding of the formation and consumption kinetics and the development of a reaction mechanism consisting of the different elementary reactions occurring inside the reactor. However, a mechanism that accurately predicts this process in the temperature range of 1000-1400 K and 0.1-4 atm does not exist.

In this contribution, a previously proposed reaction mechanism by Dean was modified, and the best fit values of the pre-exponential factors were obtained using sensitivity analysis and optimization. A significant improvement in the model predictions was observed once the optimal pre-exponential factor values were implemented in the reaction mechanism. The numerical results obtained in the temperature and pressure range of 1000-1400 K and 0.1-4 atm, respectively, were validated against the gas-phase species profiles obtained from the literature. Additionally, an in-house batch reactor experimental facility was created, and the decomposition products were analyzed at 4 atm and in the temperature range of 873-1273 K, and the model was compared to the new experimental data. The model can be used to design new reactors which optimize carbon black and hydrogen production.

1CO.6

Solid-Phase Excitation-Emission Matrix Spectroscopy for Chemical Analysis of Combustion Aerosols. Gaurav Mahamuni, Jiayang He, Jay Rutherford, Byron Ockerman, Arka Majumdar, Gregory Korshin, Edmund Seto, IGOR NOVOSSELOV, *Univertsity of Washington*

Exposure to ultrafine combustion aerosols such as particulate matter (PM) from residential woodburning, forest fires, cigarette smoke, and traffic emission have been linked to adverse health outcomes. Excitation-emission matrix (EEM) spectroscopy presents a sensitive and cost-effective alternative for analysis of PM organic fraction. However, as with other analytical chemistry methods, the miniaturization is hindered by a solvent extraction step and a need for benchtop instrumentation. We present a methodology for collecting and in-situ analysis of airborne nanoparticles that eliminates labor-intensive sample preparation and miniaturizes the detection platform. Nanoparticles are electrostatically collected onto a transparent substrate coated with solid-phase (SP) solvent - polydimethylsiloxane (PDMS). The PM organic fraction is extracted into PDMS and analyzed in-situ, thus avoiding liquid-phase extraction. In the SP-EEM analysis, we evaluated external and internal excitation schemes. Internal excitation shows the lowest scattering interference but leads to signal masking from PDMS fluorescence for $\lambda < 250$nm. The external excitation EEM spectra are dependent on the excitation light incident angle; ranges of 30-40° and 55-65° show the best results. SP-EEM spectra of woodsmoke and cigarette smoke samples are in good agreement with the EEM spectra of liquid-phase extracts. The SP-EEM technique can be used to develop wearable sensors for exposure assessments and environmental monitoring.

1CO.7

Effects of Polyoxymethylene Dimethyl Ether (PODE) Blended Fuel on Diesel Engine Emission. MUTIAN MA, Laura-Helena Rivellini, Nethmi Kasthuriarachchi, Qiren Zhu, Yichen Zong, Wenbin Yu, Wenming Yang, Markus Kraft, Alex Lee, *National University of Singapore*

Diesel engine emission is one of the major sources of particulate matter (PM) that are associated with negative climate and health impacts. Studies have shown that Polyoxymethylene Dimethyl Ether (PODE) blended diesel can reduce total PM emission, yet few have studied its impact on PM chemical characteristics. This work investigates the effects of different PODE volume blends on diesel engine exhaust. Emissions were generated by a single-cylinder diesel engine test bed operated at low, medium, and high loading conditions (30%, 50%, and 60%, respectively). Black carbon (BC) and organic aerosol (OA) were characterized by a soot-particle aerosol mass spectrometer (SPAMS, Aerodyne Research) and a 7-wavelength aethalometer (AE33, Magee Scientific). The results show that OA was the dominant component contributing 45-75% of total PM mass. PODE reduced both BC and OA emissions in general with more prominent effect at low and high engine loadings (e.g. >70% reduction). While the OA-to-BC ratio decreased as the engine loading increased, this ratio increased with PODE vol%. In addition, positive matrix factorization (PMF) identified three hydrocarbon-like OA (HOA) components that were mixed with different mass fraction of BC. The mass fraction contribution of the factor with the lowest BC fraction increased as PODE vol% increased. This is likely due to PODE can reduce the fuel pyrolysis process and subsequently enhance the particle oxidation process which increased OA fraction. Brown carbon (BrC) absorption was observed across all PODE blends with the highest contribution to the total aerosol absorption under the low loading conditions (14%). Recent studies have found similar PMF factors (i.e., BC and HOA mixed in different degree) and BrC absorption contributions from on-road engine emissions. This work provides insights toward the changes in diesel engine emissions and its environmental implication caused by PODE blended fuel.

1CO.8

Repeatable Emission Studies of Controlled Biomass Pyrolysis and Combustion Using a Cone Calorimeter Set-Up. VILHELM B. MALMBORG, François-Guillaume Ide, Dan Madsen, Ioannis Sadiktsis, Michaël Toublanc, Patrick van Hees, Andrew Grieshop, Joakim Pagels, *Lund University, Sweden*

Recent work highlights the influence of combustion phase on properties of particles emitted during diverse biomass combustion types. However, systematic study is limited by the highly variable combustion conditions within and across burns. Flow reactor experiments with simple fuels (e.g., benzene) can reduce variability to probe different conditions, but this approach does not directly represent biomass combustion emissions.

In this study, we bridged this gap by using birch wood samples in a cone calorimeter according to ISO 5660-5 to control total heat flux (HF) and gas (air/N2) flow rates to simulate distinct conditions (pyrolysis, well- and under-ventilated combustion). We conducted over 40 experiments with widely ranging HF and flow conditions while monitoring fuel mass loss to quantify emission yields. An Aerosol Mass Spectrometer (AMS), a multi-wavelength aethalometer and a particle size spectrometer (DMS5000) measured time-resolved evolution in particle properties during burns. We also collected filters for offline analysis of OC/EC, PAHs/oxy-PAHs and UV-Vis absorption by methanol extracts.

Pyrolysis conditions (in N2) generated high primary OA emission factors (0.03-0.5 g/g). The Absorption Ångström Exponent (AAE) was 2-3 for pyrolysis conditions, with marginally increased AAEs with higher HF values. For high-flow combustion, we observe increasing eBC emissions (0.005 to 0.01 g/g) and decreasing AAE to values in the range 1.7-1.2 for higher HF, and OA emissions reduced by two orders of magnitude compared to pyrolysis conditions. Low-flow and oxygen-starved combustion was associated with extreme PAH emission factors, up to 0.1 g/g (~100 times higher than under well-ventilated conditions).

Further analysis of the data set will parameterize emissions based on conditions underlying diverse biomass combustion modes and aim to unify observations collected at different scales (e.g., cook stoves, wild fires, heating stoves).

1CO.9

Global Emissions of Hydrogen Chloride and Fine Particulate Chloride from Anthropogenic Sources and Biomass Open Burning. BINGQING ZHANG, Huizhong Shen, Xiao Yun, Qirui Zhong, Barron Henderson, Shu Tao, Armistead G. Russell, Pengfei Liu, *Georgia Institute of Technology*

Gaseous and particulate chlorine species play an important role in tropospheric chemistry, visibility reduction, and human health. The current global chlorine emission inventory was developed in the 1990s with coarse resolution and no later update, which has limited our chemical transport modeling studies of the role of chlorine in the atmosphere. Here, we develop a global emission inventory of HCl and particulate Cl (pCl) including 6 sectors (i.e., energy, industrial, residential, waste open burning, biomass open burning, and agricultural sectors), 14 subsectors, and 34 types of fuel based on published up-to-date data. These emissions are gridded at 0.1° × 0.1° spatial resolution for the period 1960-2014. The estimated emissions of HCl and pCl in 2014 are 2192 Gg (with uncertainty range -50% ~ 51%) and 2289 Gg (with uncertainty range -60% ~ 43%). Emissions of HCl are from multiple major sources, including coal combustion processes in power plants (17%), waste open burning (23%), and biomass open burning (21%). Emissions of pCl are mostly from biomass burning, including indoor biofuel burning (28%), biomass open burning (44%), and crop residue burning (17%). The global emissions in early years such as 1960 are similar to the present level, due to the emissions from anthropogenic processes increased in the early years and decreased after, and emissions from biomass remain relatively constant in the study period. Our results are lower than previous global emissions estimated for 1990 but within the uncertainty range. Our results are also comparable with other regional emission estimations in China, India, and the US. Our study highlights the importance of non-SSA (sea salt aerosol) continental sources of chlorine, and the results can be used to simulate chlorine chemistry in chemical transportation models as well as provide a baseline for estimating more detailed regional emissions.

1RA.1

The 3rd Atmospheric Radiation Measurement (ARM) Mobile Facility Deployment to the Southeastern United States (SEUS): Updates on Siting, Instrumentation, and Opportunities for Inter-agency Coordination. CHONGAI KUANG, Scott Giangrande, Shawn Serbin, Gregory Elsaesser, Pierre Gentine, Thijs Heus, John Peters, Mariko Oue, James Smith, Allison Steiner, *Brookhaven National Laboratory*

The DOE 3rd ARM Mobile Facility (AMF3) will be relocating to the Southeastern United States (SEUS) with a planned operational start in Spring 2023. The SEUS region is characterized by: high vegetative emissions of volatile organic compounds (e.g., isoprene and monoterpenes); a wide range in anthropogenic emissions (e.g., NOx) from proximity to rural areas and dense urban cores; biomass burning from periodic prescribed and unplanned burning; and large amounts of secondary organic aerosol. This AMF3 deployment is a unique opportunity to improve understanding and model representation of coupled aerosol, cloud, and land-surface processes in an environment where such processes are strongly driven by local forcings. A defining aspect of this AMF3 deployment is an expectation for long-term (~5 year) observations to account for seasonal to annual variability that may limit appropriate attribution of local to larger-scale phenomena. Understanding this role of spatiotemporal variability (e.g., atmospheric thermodynamic variability, variation in land-surface properties and seasonality) across aspects of the climate system is a key motivator for AMF3 SEUS studies. This is especially true for characterizing the relationships between aerosol and land-surface processes over a diverse patchwork of natural, managed, and urban landscapes found across the SEUS. The Site Science Team (SST) is tasked to help identify the most impactful SEUS science drivers, locations, key instruments and measurement strategies to address wider climate-process study needs. Building on previous siting criteria, instrument justifications, updates and interactive feedback sessions provided to the broader community, the SST will present its latest planning updates, including recent site short-list feedback to map relevant SEUS science themes to a narrower subset of potential AMF3 locations. These efforts steer towards a comprehensive accounting (e.g., science plan) for eventual scientific opportunities as more deployment specifics become available.

1RA.2

Temporal Trends in the Emissions and Impacts of Monoterpenes in the Southeastern U.S. Demonstrate the Dominant Influence of Low-Concentration, Highly Reactive Compounds. DEBORAH MCGLYNN, Graham Frazier, Laura E. R. Barry, Koong Yi, Xi Yang, Manuel Lerdau, Sally Pusede, Gabriel Isaacman-VanWertz, *Virginia Tech*

More than 10,000 hours of chemically speciated biogenic volatile organic compound (BVOC) data have been collected at the Virginia Forest Research Lab, in Fluvanna County, Virginia. Data were collected using gas chromatography – flame ionization detection that was automated to take hourly air samples from within the forest canopy. With these data, changes in the diurnal profiles of individually resolved monoterpene species are identified over the course of the year. While all monoterpene species exhibit peak concentrations in the nighttime and early morning hours in the fall, winter, and spring, a small number of low-concentration species shift to a daytime and early evening peak in the summer months. Some of the species that exhibit this shift are highly reactive, so, while this shift does not substantially impact the temporal trends in total monoterpenes, it has significant implications for atmospheric reactivity in the summer months. In this presentation, we use co-located ecological measurements of sap flow, leaf area index (LAI), and PhenoCam data alongside positive matrix factorization to understand the importance of daytime peaks in low-concentration monoterpenes on regional reactivity and aerosol formation.

1RA.3

Seasonal Contribution of Isoprene-Derived Organosulfates to Total Water-Soluble Fine Particulate Organic Sulfur in the United States. YUZHI CHEN, Tracy Dombek, Jenny Hand, Zhenfa Zhang, Avram Gold, Andrew Ault, Keith Levine, Jason Surratt, *University of North Carolina at Chapel Hill*

Organosulfates (OSs) are the most abundant class of organosulfur compounds (OrgS) in atmospheric fine particulate matter ($PM_{2.5}$). Globally, isoprene-derived OSs (iOSs) are the most abundantly reported OSs. The methyltetrol sulfates (MTSs), formed from multiphase chemical reactions of isoprene-derived epoxidiols (IEPOX) with acidic sulfate aerosols, are the predominant iOSs. A recent study revealed that the heterogeneous hydroxyl radical (•OH) oxidation of fine particulate MTSs yields several highly oxygenated and functionalized OSs previously attributed to non-IEPOX pathways. By using hydrophilic interaction liquid chromatography interfaced to electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (HILIC/ESI-HR-QTOFMS), iOSs were quantitatively characterized in $PM_{2.5}$ collected from 20 ground sites within the Interagency Monitoring of Protected Visual Environments (IMPROVE) network during the 2016 summer and winter seasons. Total water-soluble sulfur (TWS-S) and sulfur in the form of inorganic sulfate (Sinorg) were determined by inductively coupled plasma-optical emission spectroscopy (ICP-OES) and ion chromatography (IC), respectively. The difference between TWS-S and Sinorg was used as an upper bound estimate of water-soluble OrgS concentration. Significantly higher OrgS concentrations, coincident with elevated iOS concentrations, were observed only in summer. On average, iOSs (130 ± 60, up to 240 ng m-3) explained 29% (± 7%) of OrgS and 5% (± 2%) of organic matter (OM = 1.8*OC) in summertime PM2.5 collected from the eastern U.S. For the western U.S., iOSs (11 ± 6 ng m-3) account for 6% (± 5%) of OrgS and 0.7% (± 0.4%) of OM. This study provides critical insights into the abundance, prevalence, spatial variability of iOSs across the U.S.

1RA.4

Atmospheric Transport of Pesticides and PFAS through Dry and Wet Deposition. Eve Painter, JENNIFER FAUST, *College of Wooster*

Pesticides are a unique class of chemical contaminants that humans deliberately introduce to the environment in large quantities. Once applied to crops, pesticides enter the atmosphere through spray drift, volatilization, and wind erosion of soil. Many pesticides favorably partition to aerosol particles and undergo atmospheric transport. Pesticides can then return to Earth's surface through dry and wet deposition. Our objective is to identify and quantify pesticides in particulate matter, rainwater, and snow samples collected in the central United States in order to explore spatial and temporal trends in pesticide deposition fluxes. A three-stage impactor is used to collect particles down to a size cutoff of 0.05 µm. Samples are extracted and then analyzed by liquid chromatography quadrupole time-of-flight mass spectrometry (LC-QTOF-MS) to identify unknown pesticides through suspect screening and non-targeted analysis. Precipitation samples are also collected at the same sites, extracted and concentrated by solid-phase extraction (SPE), and analyzed by high-resolution mass spectrometry. Preliminary results have shown that the insecticide diethyltoluamide (DEET) and the herbicides atrazine and simazine are present in rainwater collected in Ohio between 2018-2021. Future work will use air mass back trajectories and statistical testing to assess whether local or regional sources dominate pesticide deposition fluxes.

1RA.5

Gas and Particle-phase Measurements in a Rural Oil and Gas Production Region with a Vocus PTR-ToF-MS. LEIF JAHN, Daniel C. Blomdahl, Nirvan Bhattacharyya, Catherine Masoud, Kristi McPherson, Pearl Abue, Kanan Patel, Lea Hildebrandt Ruiz, Pawel K. Misztal, *University of Texas at Austin*

We deployed a Vocus proton transfer reaction time-of-flight mass spectrometer during spring 2021 to Karnes City, Texas, a rural region located in the Eagle Ford Shale that is impacted by emissions from nearby natural gas and oil extraction and processing facilities. The Vocus is sensitive to a wide range of volatile organic compounds (VOCs) and we were able to identify a variety of VOCs associated with ambient background emissions as well as periodic pollution events. Pollution events typically lasted for several hours and were characterized by heightened concentrations of specific VOCs and were associated with several types of activities. These include pesticide spraying for agriculture, the emission of saturated and aromatic hydrocarbons that are likely from natural gas flaring or other upstream fossil fuel processes, and the emission of styrene and other compounds from nearby industrial sources. Likely oxidation products from these emissions were also observed during some pollution events. Ambient particle composition was also analyzed with a Vocus Inlet for Aerosols (VIA) that was deployed during part of the field campaign, which utilizes an activated carbon scrubber and heated particle inlet to analyze condensed-phase molecules. Measurements with the VIA suggest the presence of oxidized aromatics and other OVOCs in the particle phase. These measurements provide important insight into VOC emissions and the potential for SOA formation and health impacts in this and similar regions that are impacted by upstream fossil fuel and industrial processes.

1RA.6

Characterization of Aerosol Vertical Profiles over the Western North Atlantic Ocean during the North Atlantic Aerosols and Marine Ecosystems Study (NAAMES).

FRANCESCA GALLO, Kevin Sanchez, Bruce Anderson, Matthew Brown, Ewan Crosbie, Carolyn Jordan, Claire Robinson, Taylor Shingler, Michael Shook, Kenneth Thornhill, Elizabeth Wiggins, Edward Winstead, Luke Ziemba, Richard Moore, *NASA Langley*

Marine regions dominated by pristine atmospheric conditions and low-lying clouds, are the most susceptible to perturbations in aerosol properties and represent the highest source of uncertainty in global climate models. One major contribution to this uncertainty stems from the poor understanding of aerosol-cloud interactions under natural conditions and during periods when the marine boundary layer aerosol is impacted by particles of continental origins. With the objective of improving the understanding of marine aerosol-cloud-climate interactions in marine environment, between 2015 and 2018, NASA conducted the North Atlantic Aerosols and Marine Ecosystems Study (NAAMES) field campaigns in the Western North Atlantic. The NAAMES C-130 research aircraft flew during three NAAMES field campaigns (NAAMES-1 November 2015, NAAMES-2 May 2016, and NAAMES-3 September 2017) providing in-situ samplings of aerosol, trace gases, clouds and meteorological parameters under different seasonal regimes. The standard flight pattern included vertical spirals where the C-130 descended from high altitude to low-latitude (and vice versa) and collected aerosol and clouds measurements as a function of altitude. In this study, we examine the datasets collected from 38 spirals during the three NAAMES field campaigns under varying conditions, and we present a comprehensive characterization of the vertical profiles of aerosol properties. Summary statistics of the remote marine atmosphere prevalence of new particle formation and the competing influences of long-range transport versus local boundary layer aerosols will be discussed.

1RA.7

Scattering-Constrained Coarse Mode Retrieval (SCMR) of Sea Spray Aerosol Concentration using a Submicron Particle Sizer and 3-Wavelength Integrating Nephelometer.

Jeramy Dedrick, LYNN RUSSELL, Georges Saliba, Dan Lubin, *Scripps Institution of Oceanography*

Improved quantification of sea spray aerosol concentration and size is important for assessing natural aerosol effects on clouds and climate. We present a new method to retrieve size-resolved coarse mode aerosol, namely sea spray, by combining measurements from a submicron particle sizer and 3-wavelength integrating nephelometer: Scattering-Constrained Coarse Mode Retrieval (SCMR). SCMR is based on the correlated relationship of supermicron scattering to sea spray mass during clean marine conditions. Three-wavelength scattering error derived from comparisons of nephelometer measurements to Mie theory-simulations provides a family of coarse mode size distributions that can be used to identify a unique solution of lowest residual to the large accumulation mode measured by the submicron mass size distribution. Applying SCMR to measurements from the Department of Energy Atmospheric Radiation Measurement (ARM) Layered Atlantic Smoke Interactions with Clouds (LASIC) campaign at Ascension Island demonstrates successful retrieval for approximately 65% of clean marine periods. Minimal fit residuals occur most frequently when total particle concentrations are low and the supermicron scattering fraction is high. Retrieval performance was reduced in seasons with small supermicron scattering fractions and high wind speeds that may impact the sample inlet 50% cutoff diameter. Comparison of SCMR to a previously developed primary marine aerosol fitting algorithm applied to LASIC size distributions yielded similar mode fitting parameters (size and width) at a comparable success rate. SCMR provides the opportunity for investigators to make effective estimates of sea spray aerosol concentrations across sub- and supermicron size regimes during clean marine conditions.

1RA.8

Analysis of Wintertime Alaskan Sea Spray Aerosol Using Single-Particle Mass Spectrometry. JUDY WU, Jun Liu, Jamy Lee, Lucia Upchurch, Patricia Quinn, Son Nghiem, Kerri Pratt, *University of Michigan*

The Arctic has warmed more rapidly than the global average, and as a result, reduced summertime sea ice is delaying fall sea ice freeze-up in the Arctic and altering the region during the fall-winter transition. Atmospheric aerosol particles can affect climate because 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. Due to logistical challenges in the remote Arctic wilderness, few aerosol measurements have been made during the cold and dark winter, limiting our understanding of aerosol-climate interactions in this season. To better understand Arctic atmospheric processes and to bridge the current seasonal aerosol observation gap, an aerosol time-of-flight mass spectrometer (ATOFMS) was deployed in the November – December 2018 Aerosols during the Polar Utqiaġvik Night (APUN) field campaign near Utqiaġvik, AK to provide real-time size-resolved individual particle chemical composition. Collected during the APUN campaign, the ATOFMS single-particle mass spectra serve as chemical fingerprints to reveal information about particle sources and atmospheric chemical processes. Based on the presence of specific marker ions, sea spray aerosol (SSA) was found to account for a significant fraction of the ~800,000 individual particles chemically analyzed in the study. Both fresh (nascent), non-chloride-depleted SSA particles and partially aged (chloride-depleted and nitrate- and sulfate-enriched) SSA particles were observed. Offline ion chromatography shows agreement with the ATOFMS SSA mass concentrations. We examine the abundance of the nascent SSA in the context of the local open water using satellite-based data. The abundance of fresh SSA particles in this study shows that SSA production continues to be an important local source even during the sea ice freeze up period, which is important to consider as the Arctic is transitioning to larger areas of open ocean in a changing climate.

1RA.9

Sea Spray Aerosol Generation Experiments in the Summertime High Arctic Pack Ice. JESSICA MIRRIELEES, Rachel Kirpes, Carlton Rauschenberg, Allison Remenapp, Yao Xiao, Nurun Nahar Lata, Vanessa Boschi, Swarup China, Andrew Ault, Amanda Grannas, Patricia Matrai, Kerri Pratt, *University of Michigan*

Aerosols are generated through several mechanisms in the summertime High Arctic, including the production of sea spray aerosol from sea ice leads under elevated wind speed conditions. To study the connections between seawater and sea spray aerosol, seawater was collected from nine locations (including open sea ice leads, a marginal ice zone, and a location near the North Pole) on board the icebreaker Oden during August – September 2018 as part of the Arctic Ocean 2018 Expedition (AO18) – Microbiology-Ocean-Cloud Coupling in the High Arctic (MOCCHA). The seawater collected from these sources was used to carry out a set of nine experiments using a 210 L marine aerosol reference tank (MART) with a plunging jet aerosol generation system. The number concentration and size distribution of the generated sea spray aerosol particles were measured during each MART experiment. Aerosol particles were also collected for subsequent offline analysis by Raman microspectroscopy, providing individual particle functional group analysis, including identification of marine organic compounds, and computer-controlled scanning electron microscopy with energy-dispersive x-ray analysis (CCSEM-EDX), providing individual particle morphology and elemental composition. Additionally, the salinity, carbon content, nitrogen content, and chlorophyll concentration of the seawater, as well as the concentration of single-celled organisms in the seawater, were measured for each experiment. The connections we observed between seawater and sea spray aerosol composition will be discussed in this presentation.

1RA.10

Wintertime Chemistry of Ionic and Carbonaceous Species of Fine Aerosol Particles at an Arid Desert Region in North-Western India. SAYANTEE ROY, Rishabh Dev, Gazala Habib, Ramya Sunder Raman, *Indian Institute of Technology Delhi*

The arid desert region to North-western India, also known as the Great Indian Thar desert is characterized by a unique topography, climatic conditions, and vegetation cover from the rest of India. However, due to the lack of measurement and characterization of aerosols at such locations, the factual information of the aerosol chemistry and properties are unknown. Moreover, owing to the number of sprawling towns in the region and the probable influx of transboundary pollutants, the question regarding source contribution which actually determines the aerosol chemistry, locally, is also unanswered. Therefore, herein, we report the wintertime chemistry, microphysical and optical properties of fine particulate matter investigated from mid-October 2020 to end of January 2021 in Bikaner, Rajasthan, India. Additionally, the contribution of firework displays during one of the major festivals in India i.e., Diwali has also been addressed. The site selection has been done following IMPROVE protocol to identify a regionally representative location. A 5-channel Speciation Air Sampling System (SASS) was used to collect $PM_{2.5}$ particles (every alternate day for 24-hour duration) onto multiple filter substrates to identify the characteristics of the water-soluble inorganic ion (WSII) and carbonaceous species (CS) using ion chromatography and OC-EC analyzer. Real-time PM mass, Black Carbon (BC), and particle scattering were also measured using Quartz Crystal Microbalance, AE-33 aethalometer, and IN102 nephelometer. Despite being an area dominated by desert dust, the atmospheric chemistry is significantly governed by anthropogenic activities rather than dust sources agreeing with the fact of increased biomass burning and absence of dust events during the winter. The fine particle concentration (< 4.0 µm) was found to be dominant, most significantly during Diwali and winter haze periods. Probable source contribution and causality will be discussed along with the relationship between regional meteorology and aerosol species.

1RA.11

Submicron Aerosol Composition and Source Contributions across the Kathmandu Valley, Nepal. Benjamin Werden, Michael R. Giordano, Khadak Mahata, Md. Robiul Islam, Siva Praveen Puppala, Arnico Panday, Robert J. Yokelson, Elizabeth Stone, PETER F. DECARLO, *Johns Hopkins University*

High levels of air pollution are observed throughout the Kathmandu valley of Nepal, with an average wintertime PM1 of 102 µg/m^3 and daily peaks over 200 µg/m^3. Differences in concentration and and source contributions measured across 3 separate sites within the Kathmandu Valley indicate the importance of multi-site measurements for understanding air quality across an air-shed. Using a mini-Aerosol Mass Spectrometer (mAMS) non-refractory PM_1 (NR-PM_1) was measured at 3 sites in the valley interior: Dhulikhel on the valley edge, Ratnapark in the city center, and suburban Lalitpur. Organic aerosol (OA) was the largest contributor to NR-PM_1 mass, and BC the second largest component. OA is on average 49% of PM_1 and BC 21%. The average background PM1 outside the valley was 48 µg/m^3, with an average urban enhancement of 58 µg/m3. SO_4 is 3.6 µg/m^3 outside the valley, 7.5 µg/m^3 in the urban center, and 12.0 µg/m^3 in the suburban brick kiln region. Chl has an average concentration of 1.9 µg/m^3 at background, 6.2 µg/m^3 at Ratnapark, and 4.8 µg/m^3 at Lalitpur, an increase of 3.3 and 2.5 times respectively. PMF identified seven OA factors: Four primary sources, and three secondary organic aerosol sources (SOA). Hydrocarbon-like OA (HOA), biomass burning OA (BBOA), trash burning OA (TBOA), and a local sulfate containing OA (sLOA) are the primary sources. OOA is over 50% of all mass outside the valley, and 36% within, making it the largest OA component. HOA is the largest primary OA source, contributing up to 21% of all OA, and 44% of BC. TBOA comprises 12% of OA, and 20% of BC, and BBOA is 15% of OA, and only 4% of all BC.

1RA.12

Using Observational Constraints to Improve Aerosol Pollution Attribution over India. SIDHANT J. PAI, Colette L. Heald, Hugh Coe, James Brooks, Mark W. Shephard, Enrico Dammers, Joshua S. Apte, Gan Luo, Fangqun Yu, Christopher D. Holmes, Chandra Venkataraman, Pankaj Sadavarte, Kushal Tibrewal, *Massachusetts Institute of Technology*

The Indian subcontinent is subject to some of the highest levels of ambient air pollution in the world, with over 99% of the population living in areas that exceed the World Health Organization guidelines for fine particulate matter. Recent research has demonstrated that a significant fraction of the total aerosol burden is secondary in nature, making air pollution management a regional problem. Despite this, regional $PM_{2.5}$ pollution models and associated health assessments in India are largely based on simulations that have not been evaluated rigorously against in situ measurements, primarily due to the historical dearth of such observations. Here, we demonstrate that, while bulk $PM_{2.5}$ observations are somewhat well-simulated by the model, a comparison with airborne measurements highlights large biases in the ammonium and nitrate aerosol simulations. A comparison of five different emissions inventories over the region illustrates large spreads in emissions estimates, particularly for ammonia. We use satellite retrievals from the CrIS and TROPOMI instruments to constrain model emissions of NH_3 and NO_x and incorporate process-level changes to improve the model. The resulting simulation demonstrates significantly lower bias when validated against speciated airborne aerosol measurements, particularly for nitrate and ammonium aerosol. Using the observationally validated simulation, we estimate that fine aerosol pollution accounts for approximately 1.4 million annual premature deaths in India. While no single emissions sector is paramount, the RCO (residential, commercial and other) and energy sectors contribute the most (24% and 21% respectively) to populated-weighted $PM_{2.5}$ exposure across India, with important regional heterogeneity. Significant differences in source attributions between the Base and Modified simulations highlight the urgent need for speciated aerosol observational constraints at the surface and in the free troposphere to provide more accurate aerosol compositional information, improve the regional modelling of fine particulate, and enable informed air-quality management decisions.

1SI.1

Measuring the Performance of Masks as Source Control Devices for Respiratory Aerosols. WILLIAM LINDSLEY, Francoise Blachere, Brandon Law, Raymond Derk, Justin Hettick, Karen Woodfork, William Goldsmith, James Harris, Matthew Duling, Brenda Boutin, Theresa Boots, Jamye Coyle, Timothy Nurkiewicz, Donald Beezhold, John Noti, *National Institute for Occupational Safety and Health*

Universal mask wearing is recommended to help control the spread of SARS-CoV-2, the virus that causes COVID-19. Masks reduce the expulsion of respiratory aerosols into the environment (called source control) and can offer some protection to the wearer. However, masks vary greatly in design and construction material, and testing is required to determine their effectiveness. Masks are often characterized using filtration efficiency, airflow resistance, and fit factors, which are standard metrics used to test masks and respirators as personal protective devices. However, none of these standard metrics are direct measurements of the ability of a mask to block aerosols during coughing and exhalation. We measured the source control performance of 15 cloth masks (which included face masks, neck gaiters, and bandanas), two medical face masks, and two NIOSH-approved N95 filtering facepiece respirators by determining their collection efficiency for aerosols ≤ 7 µm expelled during simulated coughing and exhalation. These measurements were compared with filtration efficiencies, airflow resistances, and fit factors on manikin headforms and humans. Source control collection efficiencies for the cloth masks ranged from 17% to 71% for coughing and 35% to 66% for exhalation. Filtration efficiencies of the cloth masks ranged from 1.4% to 98%, while the fit factors were 1.3 to 7.4 on the headform and 1.0 to 4.0 on human subjects. The correlations between the source control collection efficiencies and the standard metrics were statistically significant in all but two cases, but none of the correlations were strong. Our results suggest that a better understanding of the relationships between source control collection efficiency and metrics like filtration efficiency, airflow resistance, and fit factor are needed to develop simple quantitative methods to estimate the effectiveness of masks as source control devices for respiratory aerosols.

1SI.2

Particle Size Distributions of Infectious Aerosols: Implications for Preventing Transmission.

KEVIN FENNELLY, *NIH/NHLBI*

The current pandemic of coronavirus disease 2019 (COVID-19) has intensified interest once again in the transmission of respiratory pathogens. Such interest has vacillated since the outbreaks of multidrug resistant tuberculosis (MDR-TB) in the 1980s and 1990s, the Severe Acute Respiratory Syndrome coronavirus (SARS-CoV-1) pandemic of 2003, the H1N1 influenza pandemic of 2009, and the Middle East Respiratory Syndrome coronavirus (MERS-CoV) epidemic since 2012. I reviewed the research literature from the past twenty years on direct patient sampling of respiratory pathogens from cough aerosols and exhaled breath. Aerosols from both exhaled breath and cough aerosols are log normally distributed, suggesting that those producing the most infectious aerosol may be ‘super-spreaders.’ All pathogens were found predominately in small particle aerosols (< 5 microns mass median aerodynamic) diameter, and less so in larger aerosol particles. No pathogens were found only in large particle aerosols (> 5 microns). Over the past twenty years, infection control guidelines have used transmission within close proximity as a marker of exposure to large particle aerosols. This logic is fallacious, as humans expel polydisperse aerosols containing a mixture of both small and large particles. These data suggest that health care workers and others in close contact to persons with respiratory infectious diseases that are novel or potentially lethal should be protected by the use of N95 respirators at a minimum, as well as by engineering and administrative control measures currently used for airborne transmission. (These data have been published in Lancet Respiratory Medicine 2020.)

1SI.3

On the Intricate Relationship between Ventilation, Deposition and Airborne Virus Transmission in Indoor Environments.

K. MAX ZHANG, Bo Yang, Khaled Hashad, Alfredo Rodriguez, *Cornell University*

We have developed a detailed computational fluid dynamics (CFD)-based aerosol dynamics model and conducted extensive model evaluations against experimental datasets that characterized indoor turbulence, evaporation and deposition. Applying this model in realistic indoor environments in hospitals and schools enabled us to elucidate the intricate relationship between ventilation, deposition and droplet/aerosol transmission. Higher ventilation rate leads to shorter particle resident time and higher surface deposition, but also results in longer particle travel distance. Capturing surface deposition is critical to quantify particle number balance, even though fomite transmission may not be important. Our results support the argument that 5-micron size cut between aerosol and droplets is arbitrary and we showed the more reasonable size cut to be between 85 and 115 microns, which is consistent with the proposed 100 microns size cut. For examples, droplets of initial size of 80 microns can travel much further than 6 feet under realistic indoor environments.

1SI.4

In-Vitro Investigation of Exhaled Particle Deposition and Ventilation in Office Settings. STEPHANIE EILTS, Linhao Li, Zachary Pope, Christopher J. Hogan, *University of Minnesota*

Exhalation of infectious micrometer-sized particles has been strongly implicated in the spread of respiratory infections. An important fundamental question is then the fate of infectious exhaled particles in indoor environments, i.e., whether particles will deposit, and if so, on what surfaces, or whether they will remain suspended in an aerosol until ventilation leads to clearance. We investigated the interplay between particle deposition and ventilation using model experiments with a breathing simulator manikin in a model office environment. The breathing simulator utilized anatomically correct exhalation and inhalation breathing waveforms as well as an anatomically correct manikin to simulate human breathing. The breathing simulator output a fluorescein tagged particles with a mass distribution spanning the 1-3 um range. The test office module was a 19.2 m x 6.9m x 2.6 m room that consisted of three rows of desks with nine manikin occupants (including the simulator). Particle dispersion throughout the office space was tracked by measuring the deposition flux on passive substrates placed in several locations throughout the room, both on horizontal and vertical surfaces. Aerosol mass concentrations were determined using impingers, and surface-specific deposition velocity was then calculated for each passive substrate using deposition flux mass concentration measurements. Four different test conditions were created by changing the simulator location with respect to the return grilles and diffusers in the room as well as through the use of different air change rates and MERV ratings of filters. Deposition measurements under all test conditions revealed enhanced deposition onto horizontal upward faces surfaces, surfaces within 2 m of the breathing simulator, and on non-passive surfaces near return grilles. However, with the exception of surfaces close to the simulator and non-passive return grille exteriors, we found that particles are more likely to remain suspended in the air until removal by ventilation, as opposed to depositing within the office space.

1SI.5

Ventilation Systems and COVID-19. Sunil Kumar, David Klassen, Tatiana Baig, MARIA KING, *Texas A&M University*

To objective of this study is to help processing facilities with optimized ventilation parameters to mitigate COVID-19 transmission among workers as well as spoilage organism and pathogen spread with the air flow. Meat processing plants are uniquely susceptible to the effects of the virus due to the cold temperature, and high aerosol particle (fat and protein) concentration at the facilities.

Our research on the chemistry of the viral proteins using biolayer interferometry shows that the COVID-19 virus binds to fat particles that become aerosolized during meat processing and stay suspended in air, enabling rapid virus transfer in the facility and a greater potential of transmission between workers. To reduce the spread of virus aerosols, many fabrication rooms implemented mitigation measures including the installation of plastic dividers between employees. Based on facility layouts, we developed computer models of air flow using the Computational Fluid Dynamics (CFD) program ANSYS Fluent, that confirm that these partitions help prevent the exposure of employees to air that may contain the virus. Air properties including temperature, relative humidity, air velocity and pressure were measured at every step of the process. We evaluated the air flow models using computer generated streamlines which show the path of air moving in the facility. In addition, on-site bioaerosol collection was conducted with the wetted wall cyclone (WWC) high air volume samplers at different locations in facility, where the air flow model indicated turbulent vortices. Our research shows that simple modifications, such as adding a roof on top of the partitions, could optimize their effect in reducing the transmission of airborne particles. However, consideration of individual plant circumstances is required for effective mitigation measures. This presentation is also outlining a process for a universal air flow model to examine the spread of infectious viral or bacterial aerosol particles at other plants.

1SI.6

Dynamic Behavior and Fate of Model Respiratory Fluids Aerosol in Indoor Environments. LUCY NANDY, Emma Tackman, Miriam Freedman, *The Pennsylvania State University*

Recent research suggests respiratory **aerosol transmission** in COVID-19, influenza, and other infectious diseases in indoor environments. To better understand the role aerosols play in the transmission, there is a requirement to quantify the emission rate, air exchange rate, deposition onto surfaces and size distribution of particles of respiratory fluids for estimating aerosol exposure in the indoor environment. The fate of indoor aerosol is governed by the physical principles of transport – dispersion and deposition on surfaces, depending on the droplet size and phase state.

Our goal is to develop a chemical and physical understanding of transmission mechanics of aerosol particles including their advection and deposition properties. We investigate deposition and bounce factor of aerosol particles that involve Brownian diffusion for fine dry particles less than 200 nm in an experimental plexiglass chamber with peak number concentrations occurring at particle sizes of < 50 nm. At high concentrations, coagulation and deposition dominate aerosol transmission for such small particles; we, therefore, estimate size-resolved decay rates and overall wall loss for different aerosol compositions. We also utilize transmission electron microscopy to characterize particles deposited and collected on substrates to determine their two-dimensional size, as well as viscometer and tensiometer measurements to characterize sticking efficiency on surfaces. In addition, we measure particle bounce to quantify the phase state (solid, semi-solid, viscous liquid, liquid) of aerosol particles, and hypothesize that aerosol viscosity and surface morphology play an important role in particle concentrations and consequences. For the study, we use aerosol particles generated from aqueous solution of physiological concentrations of salt, surfactant, and mucin. This research effort will support future approaches for quantifying aerosol transmission, exposure, and risk management from the source to transport through model indoor environments.

1SI.7

Airborne Murine Coronavirus Persistence Circumscribing Efflorescence Humidity Thresholds in Saliva Microaerosols. MARINA NIETO-CABALLERO, Eddie Fuques, Odessa M. Gomez, Shuichi Ushijima, Margaret Tolbert, Alina Handorean, Mark T. Hernandez, *University of Colorado Boulder*

An accepted murine analogue for the environmental behavior of human SARS coronaviruses, was aerosolized in cell culture media and in artificial saliva microdroplets to observe its airborne infectious potential while juxtaposed to values reported for relative humidity-dependent efflorescence.

Contained in a dark c.a. 10 m^3 chamber maintained at 22^oC, Murine Hepatitis Virus (MHV) was aerosolized with a 6-jet Collison Nebulizer with and without artificial saliva entrainment, in particle size distributions corresponding to those hosting SARS-CoV-2 virus expelled from infected humans' respiration. As judged by quantitative PCR from samples collected with condensation growth tube technology after 20 minutes of aerosolization, more than 85% of the airborne MHV was recovered from microdroplets, with mean aerodynamic diameters between 0.56 µm and 3.2 µm at low (25%) and high (60%) relative humidity levels.

As judged by its half-life, obtained from time-series observations of up to two hours and calculated from the median tissue culture infectious dose ($TCID_{50}$), saliva was found to be protective of airborne murine coronavirus at low, medium, and high RHs as compared to cell culture media entrainment. Through a relative humidity range germane to conditioned indoor air in the U.S. (60% < RH < 40%), saliva was mildly protective, with an average half-life of 60 minutes. However, when MHV was sustained in an airborne state below reported efflorescence thresholds (*i.e.*, approximately 40% RH), its average half-life doubled to 120 minutes at 25% RH under otherwise identical conditions.

These results suggest that the phase change behavior of saliva components can affect the patterns of infectious potential that β-coronaviruses exhibit while airborne, significantly extending their persistence under the drier humidity conditions encountered indoors. These results are particularly relevant, as many airborne viral infectivity studies are exclusively performed with cell culture media.

1SI.8

Aerosol Phase Changes Relevant to the Airborne Survival of Pathogens. ERIK HUYNH, Anna Olinger, David Wooley, Josefina Hajek-Herrera, Ryan Davis, *Trinity University*

The phase state of respiratory aerosol particles and droplets has been linked to the humidity-dependent airborne and surface survival of pathogens. Thus, to understand and inform strategies to mitigate the spread of infectious disease, it is prudent to understand the potential phase changes occurring with the complex organic-inorganic media in which pathogens are suspended. Here, we study the phase changes of levitated aerosol particles composed of model respiratory compounds (salt, protein) and culture media (organic-inorganic mixtures commonly used as suspension media in studies of pathogen survival) with decreasing relative humidity (RH). Depending on composition, efflorescence was either not observed or occurred between ~30 and 45% RH (consistent with NaCl efflorescence). Further, we identify humidity-dependent amorphous phase changes at intermediate RH (45-80%). Specifically, we identify (semi-)solid gel and ultra-viscous states, where the organic fraction becomes more viscous with decreasing RH. A higher protein content causes aerosol particles to be (semi-)solid under a wider range of RH conditions. Diffusion, and thus disinfection kinetics, are expected to be inhibited in these observed amorphous (semi-)solid states. Thus, amorphous phase states are likely hindering virus inactivation at moderate to low RH, which may help explain the protective effect of proteins on virus survival. Comparisons of our observations to previous studies of viral survival suggest that formation of a (semi-)solid state can contribute to the recovery of virus viability at intermediate to low RH. We discuss the implications for amorphous phase states of respiratory aerosol for ambient transmission under, as well as a conceptual framework toward predicting the survival of pathogens in varying suspension media and ambient conditions.

2AC.1

Nucleation and Growth of Particulate Matter from Aromatic Hydrocarbons Using a Photooxidation Flow Tube. ISSAK PROAñO LóPEZ, Murray Johnston, *University of Delaware*

The formation of secondary organic aerosol (SOA) via the nucleation and growth of nanoparticles from the photooxidation of anthropogenic volatile organic compounds (AVOCs) is of increasing atmospheric interest. Despite most volatile organic compounds in the atmosphere being of biogenic origin, an increasing presence of AVOCs from human activities during the industrial period has led to a corresponding increase in SOA formation in and around areas where urbanization and industrialization abound. AVOCs exhibit the ability to produce particulate matter of their own while simultaneously enhancing the production of SOA from biogenic precursors.

AVOCs that produce low-volatility products are traditionally of the aromatic hydrocarbon class, and the dominant oxidation mechanism these exhibit in the atmosphere involves the hydroxyl radical (·OH). A flow tube-type photooxidation reactor is designed and constructed to generate ·OH for the study of particle nucleation and growth from AVOCs while approximating real-world atmospheric conditions. Previous work saw the molecular composition of anthropogenic SOA characterized in an online fashion using droplet-assisted ionization (DAI) interfaced with a Waters Synapt G2-S quadrupole ion mobility time-of-flight mass spectrometer. In this study, extractive droplet-assisted ionization (E-DAI) will combine the benefits afforded by electrospray ionization (ESI) with the online abilities afforded by DAI, and interface these with the Waters Synapt G2-S to characterize molecular composition. Particle-phase composition of aerosol produced in the photooxidation flow tube will be reconciled with previous work using traditional DAI, offline analysis using ESI, and gas-phase oxidation products previously reported using chemical ionization mass spectrometry. The results will afford insight on the mechanisms of particulate growth in urbanized environments.

2AC.2

Nucleation Dynamics and Fragmentation Reactions Explain Differences in Secondary Organic Aerosol Formation between Environmental Chambers and Oxidation Flow Reactors. CHARLES HE, Andrew Lambe, Beth Friedman, Delphine K. Farmer, John Seinfeld, Jeffrey R. Pierce, Shantanu Jathar, *Colorado State University*

Environmental chambers and oxidation flow reactors (OFR) are used to study secondary organic aerosol (SOA) formation under a wide range of atmospheric aging times (hours to weeks). While SOA parameters used in atmospheric models are typically developed using chamber data, there is an opportunity to incorporate OFR data to improve their representation, especially over longer photochemical ages. In this work, we use a size-resolved chemistry and microphysics model, updated to represent nucleation, phase-state-limited gas/particle partitioning, oligomerization, wall loss, and heterogeneous chemistry, to simulate SOA formation from the photooxidation of α-pinene in chamber and OFR experiments. We argue that we can develop consistent SOA parameterizations across chamber and OFR data by accounting for, most importantly, nucleation dynamics in OFRs from low-volatility oxidation products, including highly oxygenated organic molecules (HOM). Preliminary OFR simulations show that: (1) nucleation dynamics can significantly affect the simulated SOA mass yield and size distribution and gas-phase fragmentation can decrease the SOA mass yield at longer photochemical ages (>5 days); (2) phase-state-limited gas/particle partitioning has a marginal influence on SOA formation due to the elevated relative humidity (30-40%) that leads to less viscous aerosols; and (3) heterogeneous chemistry has little effect on both the SOA mass yield and size distribution. Furthermore, we find that when the nucleation rate is linked to the concentration of low-volatility species (including HOMs), we can not only reproduce the measured size distributions from the OFR experiments but also reproduce observations of SOA mass and O:C in both the chamber and OFR experiments. Ongoing work is focused on developing OFR-informed parameters for other SOA precursors (e.g., n-dodecane, toluene) and applying these updated parameterizations in chemical transport models to study SOA evolution over longer timescales.

2AC.4

Aqueous SOA Formation from the Photo-oxidation of Vanillin: Direct Photosensitized Reactions and Nitrate-Mediated Reactions. BEATRIX ROSETTE GO MABATO, Yan Lyu, Yan Ji, Yong Jie Li, Dan Dan Huang, Xue Li, Theodora Nah, Chun Ho Lam, Chak K. Chan, *City University of Hong Kong, China*

Vanillin (VL), a phenolic aromatic carbonyl abundant in biomass burning emissions, forms triplet excited states ($^3VL^*$) under simulated sunlight leading to aqueous secondary organic aerosol (aqSOA) formation. This direct photosensitized oxidation of VL was compared with nitrate-mediated VL photo-oxidation under atmospherically relevant cloud and fog conditions through examining the VL decay kinetics, product compositions, and light absorbance changes. The majority of the most abundant products from both VL photo-oxidation pathways were potential Brown carbon (BrC) chromophores. In addition, both pathways generated oligomers, functionalized monomers, and oxygenated ring-opening products, but nitrate promoted functionalization and nitration, which can be ascribed to its photolysis products ($^\bullet OH$, $^\bullet NO_2$, and N(III), NO_2^- or HONO). Moreover, a potential imidazole derivative observed from nitrate-mediated VL photo-oxidation suggested that ammonium may be involved in the reactions. The effects of oxygen (O_2), pH, and reactants concentration and molar ratios on VL photo-oxidation were also explored. Our findings show that O_2 plays an essential role in VL photo-oxidation, and oligomer formation was enhanced at $pH < 4$. Also, functionalization was dominant at low VL concentration, whereas oligomerization was favored at high VL concentration. Furthermore, comparisons of the apparent quantum efficiency of guaiacol photodegradation indicate that in this study, guaiacol oxidation by photosensitized reactions of VL is less efficient relative to nitrate-mediated photo-oxidation. Lastly, potential aqSOA formation pathways via VL photo-oxidation were proposed. This study indicates that the direct photosensitized oxidation of VL and nitrate-mediated VL photo-oxidation may be important aqSOA sources in areas influenced by biomass burning emissions.

2AC.5

Heterogeneous Reactivity of HCl on CaCO3 Aerosols at Stratospheric Temperature. HAN N. HUYNH, V. Faye McNeill, *Columbia University*

Recently proposed as a possible alternative to sulfate particles for stratospheric solar radiation management (SSRM), calcite ($CaCO_3$) aerosols have been modeled to have minimal negative impact on both stratospheric ozone level and temperature. However, the heterogeneous chemistry of $CaCO_3$ aerosols with relevant trace gases, such as HCl, at stratospheric conditions is still underexamined. We previously reported the heterogeneous uptake of HNO_3 and HCl on $CaCO_3$ aerosols at ambient condition as well as the role of water on increasing $CaCO_3$ reactivity. In our recent study, we have further examined the kinetics of HCl uptake on airborne $CaCO_3$ aerosols at stratospheric temperature, 207 ± 3 K, by performing experiments under dry conditions using an aerosol flow tube coupled with a custom-built quadrupole chemical ionization mass spectrometer (CIMS). The reactive uptake coefficient for HCl was measured to be 0.056 ± 0.005, consistent with the negative temperature dependence of gas uptake on solid surfaces in the literature. This finding suggests at least an initial strong reactive uptake of HCl gas on $CaCO_3$ aerosols surface in the stratosphere that we expect to increase with the presence of water vapor in realistic stratospheric conditions. Additional experiments are needed to understand the change in gas uptake coefficient on $CaCO_3$ aerosols over the aerosol lifetime in the stratosphere. Based on a recent 2020 modeling study, our result suggests that the reactions of HCl and HNO_3 with calcite in the stratosphere could still lead to stratospheric ozone depletion, albeit less than sulfate particles.

2AC.7

Photolysis of Atmospherically Relevant Monoterpene-derived Organic Nitrates. YUCHEN WANG, Masayuki Takeuchi, Tianchang Xu, Siyuan Wang, Nga Lee Ng, *Georgia Institute of Technology*

Organic nitrates (ONs) have been detected in atmospheric environments as potential NO_x reservoirs and they can impact the spatial distribution of reactive nitrogen species and subsequently ozone formation. While photolysis of ONs can result in the release of NO_2 back to atmosphere, the rates and mechanisms of photolysis of atmospherically relevant ONs have not been well constrained especially for monoterpene-derived ONs (MT-ONs). In this work, we investigated the photolysis of three synthetic ONs derived from α-pinene, β-pinene and limonene through chamber experiments. The measured photolysis rate constants for these three MT-ONs are in the range of 0.45 – 1.81 10-5 s^{-1} with corresponding photolysis lifetimes ranging from 15.4 – 62.2 hours. With consideration of the difference in solar and chamber light spectra and the absorption cross section of these synthetic MT-ONs measured by ultraviolet–visible spectrophotometry, the ambient photolysis lifetimes for these MT-ONs decreased to 2.0 – 16.2 hours. Photolysis mechanisms are proposed based on major photolysis products identified by high-resolution time-of-flight chemical-ionization mass spectrometer (HR-ToF-CIMS). We found that the NO_x produced via photolysis of MT-ONs can participate in further reactions to produce new ON species with a higher oxidation state. Finally, with our proposed photolysis mechanisms and ambient photolysis rates, we employed a 0D-model to simulate photolysis of α-pinene-derived ON under ambient conditions and found that 90% of α-pinene-derived ON can be converted to NO_x and HNO_3 within 12 hours of irradiation time and ozone was formed correspondingly. These findings show that photolysis is a major atmospheric sink for MT-ONs and highlight their important role in NO_x recycling and ozone formation.

2AC.8

Increased Photochemical Sinks Help Balance the SOA Budget: Experimental Evidence and Modeling Results. KELVIN BATES, James Cope, Tran Nguyen, Daniel Jacob, *Harvard University*

Following the recent implementation of increased secondary organic aerosol (OA) sources, particularly from isoprene, atmospheric models tend to overestimate OA loadings. They also tend not to include photochemical sinks of OA mass, despite mounting evidence for the importance of these reactions in the atmosphere. At the same time, models frequently underestimate atmospheric loadings of small organic acids. Here, we incorporate new photochemical sinks of OA into GEOS-Chem, a global chemical transport model, and find that these chemical pathways bring simulated OA burdens into better agreement with observations from the Southeast United States and the remote troposphere. Based on recent literature, we implement photolytic OA losses with rates and photorecalcitrant fractions specific to each OA precursor; preliminary results suggest that these reactions can decrease the simulated mass of isoprene-, terpene- and aromatic-derived aerosol by up to 50%, 40%, and 18% respectively. We also implement the OH-initiated oxidation of isoprene-derived OA constituents (including 2-methyltetrols and organosulfates) based on our own bulk- and particle-phase laboratory experiments, which show that these fragmentation-dominated reactions can lead to the production and revolatilization of large yields of formic and acetic acids. We show that these pathways can reduce simulated burdens of isoprene-derived OA by up to 40% and increase the global atmospheric formic acid source by up to 23%. The incorporation of photochemical OA sinks into global models can therefore improve both OA and organic acid budgets, although the organic acids remain underestimated in GEOS-Chem.

2AC.9

Photolysis of Aqueous Atmospheric Aerosol Mimics.

MELISSA GALLOWAY, Jacqueline Sharp, Daisy Grace, Shiqing Ma, Joseph Woo, *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 kinetics are determined through spectral decomposition of experimentally measured UV-visible absorbance data; bleaching and browning rates vary with wavelength and aldehyde identity, while mass spectrometry shows that the chemical composition changes significantly upon photolysis.

2AC.11

Variation in Organic Aerosol Volatility Derived from Combined Thermal Desorption and Chemical Composition Measurements in Different Environments across the Globe.

CLAUDIA MOHR, Wei Huang, Cheng Wu, Yvette Gramlich, Sophie Haslett, Joel A. Thornton, Felipe Lopez-Hilfiker, Ben H. Lee, Harald Saathoff, Xiaoli Shen, Ramakrishna Ramisetty, Linyu Gao, Junwei Song, Siegfried Schobesberger, Liine Heikkinen, Sara Blichner, Ilona Riipinen, *Stockholm University*

The development of the filter inlet for gases and aerosols that can be coupled to a time-of-flight chemical ionization mass spectrometer (FIGAERO-CIMS) has enabled the combined analysis of molecular composition and volatility of organic aerosol particles and their precursor gases in real time (Thornton et al., 2020). With the FIGAERO, volatility of particulate compounds is assessed through the analysis of their signal evolution as a function of temperature (called thermograms) when being desorbed from the filter. In addition, the information on molecular composition of particulate and gaseous compounds from the chemical ionization mass spectrometer can be used in volatility parametrizations (Isaacman-VanWertz et al., 2020) to calculate the compounds' saturation vapor pressure, and to establish volatility basis sets (VBS, Donahue et al., 2011) for the bulk aerosol. VBS are used in model frameworks from the process to the global scale (e.g. Mohr et al., 2019; Farina et al. 2010), as they allow for an efficient description of organic aerosol partitioning and chemical aging – albeit with large uncertainties, as volatility measurements and estimates are subject to these.

Here we present a comparison of organic aerosol volatility derived from molecular composition measurements and thermogram analysis for a number of ambient FIGAERO-CIMS datasets across the globe (Mt. Chacaltaya, Bolivia; Alabama, US; Hyytiälä, Finland; Stuttgart and Karlsruhe, Germany; Delhi, India). We will assess the variability of derived volatility, discuss the reasons for differences and similarities in the relationships between volatility and chemical composition for the different locations and environments, compare the FIGAERO-based results to other methods for particle volatility determination, and discuss the limitations of parametrizations. In addition, we will show implications of volatility variation in different model frameworks, such as e.g. the use of VBS in a cloud parcel model.

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2AC.12

Emissions and Secondary Formation of Air Pollutants From Modern Heavy-Duty Trucks in Real-World Traffic – Chemical Characteristics Using on-Line Mass Spectrometry. LIYUAN ZHOU, Christian M. Salvador, Michael Priestley, Mattias Hallquist, Qianyun Liu, Chak K. Chan, Åsa M. Hallquist, *City University of Hong Kong, China*

Complying with stricter emissions standards, a new generation of heavy-duty trucks (HDTs) has gradually increased its market share and now accounts for a large percentage of on-road-mileage. The potential to improve air quality depends on an actual reduction in both emissions and subsequent formation of secondary pollutants. In this study, the emissions in real-world traffic from Euro VI compliant HDTs were compared to older classes, represented by Euro V, using High-Resolution Time-of-Flight Chemical Ionization Mass Spectrometry (HR-ToF-CIMS). Gas phase emissions of several hundred species were observed for 70 HDTs. Further, the particle phase and secondary pollutant formation were evaluated for a number of HDTs. The reduction of primary EFs was evident (~ 90%) and in-line with a reduction of 28–97% in typical regulated pollutants. Secondary production after photochemical ageing in an oxidation flow reactor exceeded the primary emissions (EFAged/EFFresh ratio ≥ 2). Organic acids and byproducts from urea-selective catalytic reduction (SCR) systems had both primary and secondary sources. A non-negative matrix factorization (NMF) analysis highlighted the issue of vehicle maintenance as a remaining concern. However, the adoption of Euro VI has a significant positive effect on emissions in real-world-traffic and should be considered in e.g. urban air quality assessment.

2AP.2

Calculation of the Nanoparticle-Ion Attractive Collision Rate Coefficient by Continuum-Molecular Dynamics Hybrid Simulations. TOMOYA TAMADATE, Takafumi Seto, Christopher J. Hogan, *University of Minnesota*

Nanoparticle charging plays an important role in numerous aerosol measurement applications; for example, the charge distribution is often needed *a priori* in size distribution inversion from mobility distributions. Charge distributions are usually not measured directly, and are instead estimated from ion-particle collision limited reaction models, which are dependent upon the ion-particle collision rate coefficient. While regression equations for the charge distribution based upon a modified version of Fuchs limiting sphere model are almost universally applied in aerosol measurement, these equations have not been rigorously tested for nanoclusters (1-2 nm particles) and recent work suggests they may not be accurate specifically for collisions between nanoclusters and ions of opposite charge. Recently, we developed a “continuum-molecular dynamics simulation hybrid approach”, to determine ion-ion recombination rates. This method is based on the limiting sphere method classically used for transition regime collision phenomena in aerosols, but utilizes molecular dynamics simulation with all-atom models within the limiting sphere. Here, we extend this method to examine nanocluster-ion collisions, specifically for positively charged argon and negatively charged silicon nanocluster composed of 50 to 500 atoms (1 to 3 nm), with changing pressure (10^2 to 10^5 Pa) and different two temperatures (300 and 1,000 K). Results are compared to the classical limiting sphere method, as well as recently developed collision rate coefficients for ion-particle systems.

2AP.3

The Study of Inelastic Collisions in Electrical Mobility by Coupling MD to Kinetic Theory Physical Gas Modelling.

CARLOS LARRIBA-ANDALUZ, Viraj Gandhi, *IUPUI*

One of the least understood problems when trying to calculate electrical mobility in polyatomic ions and charged nanoparticles is the understanding of how the size, mass and structure of the gas and ion affect the momentum transfer. This effect is known to be manifested differently for different gases. For example, He gas tends to have collisions that are more specular and elastic. However, air or N2 tend towards more diffusive and inelastic collisions. While the diffuse vs. elastic nature of the gas collisions can be attributed in part to the potential interaction (4-6-12), the elastic vs. inelastic condition is not that well understood. The reason has to do with the fact that not only the strength of the field must be taken into account, but also the energy transferred into the internal degrees of freedom of the molecule itself.

In this work, we couple the solution of the Boltzmann equation to the ion velocity distribution in a gas environment in the free molecular regime with a Molecular Dynamics simulation in order to study the effect that different gases and ions have on the elastic vs. inelastic nature of the interaction. By considering the two-temperature theory, an effective temperature may also be used to describe how this effect changes at different temperatures and fields. This is the first time that this coupling has been accomplished to this degree of detail, and it can be the basis to better understand nucleation, coagulation, collision induced dissociation, and mobility and diffusion of ions.

2AP.4

The Fractal Characteristics of Atmospheric Coated Soot: Implications for Morphological Analysis.

Jie Luo, Qixing Zhang, CHENCHONG ZHANG, Yongming Zhang, Rajan K. Chakrabarty, *University of Science and Technology of China*

Soot particles, as a major light absorber in the atmosphere, contribute great positive radiative effects to the climate. The radiative effects of soot have gained increasing interest in recent years, while there are still large uncertainties. Multiple modeling studies have shown that various soot morphologies can lead to large uncertainties in the estimations of radiative properties, while the morphological characteristics of soot, especially for coated soot, are still not fully understood. Here we numerically investigate the variation of fractal characteristics of soot particles as they are coated. We find the ideal fractal law can fit the morphologies of coated soot only when the radius of gyration of coated soot is identical to that of the soot core. In that case, the fractal dimension of coated soot is close to that of the soot core, which can explain the unchanged fractal dimension as soot is evenly coated. Our results also show that the fractal parameters of coated soot at different size scales can be varied, so the ideal fractal law does not fit the structures of unevenly coated soot. The results of the Q-space analysis indicate that if soot particles are unevenly coated, the power-law exponent of the structure factor versus the scattering wave vector tends to -4 for heavily coated soot. It implies that heavily, unevenly coated soot exhibits the characteristics of nearly spherical particles. We anticipate our research provides morphological constraints for coated soot particles in further modeling studies.

Citation: Luo et al. (2021): The fractal characteristics of atmospheric coated soot: Implication for morphological analysis. J. Aer. Sci., 157, 105804.

2AP.5

Modeling the Size-Dependent of Mass Absorption Cross-Section of Black Carbon Aggregates.

FENGSHAN LIU, Joel Corbin, Prem Lobo, Gregory Smallwood, *National Research Council Canada*

The mass absorption cross-section (MAC) of black carbon (BC) particles is an important parameter to convert the measured BC aerosol absorption coefficient to BC mass concentration. MAC has often been considered an intrinsic property of BC particles. Several recent ex-situ measurements of MAC of BC aerosols sampled from different combustion sources showed that the MAC displays a fairly strong increasing trend with increasing particle mobility diameter (dm) from about 50 nm to 200 nm by about 30 to 40% and then reaches a plateau at larger dm. On the other hand, the modeled MAC of BC aggregates displays very weak size dependence over the dm range of 50 to 200 nm, regardless of the solution methods (Mie, Rayleigh-Debye-Gans theory, and numerically accurate generalized Mie-solution method), particle morphologies (sphere, fractal aggregates formed by monodisperse or polydisperse spherical monomers in point-contact or with overlap), and refractive index (RI) relevant to mature soot. Therefore, the current theoretical methods and BC particle morphology models fail to reproduce the observed size-dependent BC MAC over the dm range of 50 to 200 nm.

The potential influence of size-dependent refractive index (RI) of BC particles was modeled by using the model of Kelesidis and Pratsinis (2019). This model predicts a rapid evolution of BC RI from nucleation soot to mature soot with increasing dm and there is only small variation in RI over the dm range of 50 to 200 nm, failing to predict the observed size-dependent BC MAC.

A modified size-dependent RI model was proposed to reproduce the strong size-dependent BC MAC. However, the mechanism for the strong size-dependent RI over the mobility diameter range of 50 to 200 nm remains unclear.

2AP.6

Single Particle Light Scattering from Light Beams with Orbital Angular Momentum.

MATTHEW B. HART, Vasanthi Sivaprakasam, Ryan Lindle, Wenbo Sun, Abbie Watnik, *Naval Research Laboratory, Washington, DC*

The solution to Maxwell's equations includes light with an angular component of momentum with respect to the direction of propagation. That is, the Poynting vector of this type of light, which defines the energy flux, has an angular component. Such light is commonly referred to as having orbital angular momentum (OAM). The solution of Maxwell's equation describing this light includes the Associated Laguerre polynomials, L_n^m, which result in OAM beams for all n or m > 0, and Gaussian light for n = m = 0. For all cases where $m \neq 0$, OAM beams will have an intensity minima along the central axis of the beam. This, together with the angular component of the energy flux, can cause the scattering interactions with materials to be very different than that from plane waves. Theoretical angular scattering calculations show that the light scattering maxima occur at different angles from the forward direction of zero degrees [1, 2]. The use of OAM light is being explored in a wide range of fields that include material interrogation, light propagation, sensing and communication.

In this work we investigate the scattering properties of OAM light from single, micron sized spherical particles that are suspended in an electrodynamic trap that we optimized for a previous study [3]. We utilize phase plates and a spatial light modulator to generate the OAM beams (wavelength of 532 nm) that are incident on a suspended particle. We have adapted the particle trap to study the angle resolved scattering signal in a scattering plane that covers over 40 degrees in each of the forward, back and side scattering geometries. We plan to generate OAM beams of varying mode (m = 0 to 8) and collect the angular scattering signal for varying sizes of commercially available particles of varying materials. Preliminary angular scattering calibration measurements from Gaussian beams and varying order OAM modes will be presented. Our future plans and comparison to theoretical measurements will be discussed.

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2AP.7

Direct Observation and Assessment of Phase States of Ambient and Lab-generated Sub-micron Particles upon Humidification. ZEZHEN CHENG, Noopur Sharma, Kuo-Pin Tseng, Libor Kovarik, Swarup China, *Pacific Northwest National Laboratory*

Ambient organic particles (AOP) exhibit a wide range of viscosities and different phase states, altering their roles in atmospheric processes and complicating the prediction of their climate effects. Our current knowledge of phase states of AOP is limited due to challenges in the field measurements. Thus, we present a new analytical platform that uses a tilted stage integrated to the Peltier cooling stage interfaced with an Environmental Scanning Electron Microscope (ESEM) to directly observe and assess the phase state of organic particles as a function of RH. Three types of organic particles have been studied: Suwannee River fulvic acid (SRFA) particles, lab generated soil organic particles (SOP), and field-collected AOP. The chemical composition, morphology, and functional groups of individual particles were probed using Computer-controlled scanning electron microscopy with energy-dispersive X-ray spectroscopy (CCSEM/EDX) and scanning transmission X-ray microscopy with near-edge X-ray absorption fine structure spectroscopy (STXM/NEXAFS). Results show that all three types of particles are organic-rich, but SOP and AOP contain a considerable amount of inorganic species. The phase state can be determined based on the particle's aspect ratio (particle width/height), which we proposed for solid, semisolid, and liquid particles are 1.00-1.30, 1.30-1.85, and >1.85, respectively. We found that solid SRFA particles transition to semisolid state at ~90% RH and to liquid state at ~97% RH, agree with the literature. The solid SOP transition to the semisolid state at ~85% RH and the liquid state at ~97% RH. The solid AOP transition to semisolid state at ~65% RH and liquid state at ~97% RH. Our results indicate that this new platform can directly observe and quantitatively indicate the phase transition of field-collected organic particles at different ambient conditions.

2AP.8

Next Generation UCR Chamber Minimizes Effect of Electrostatics on Particle Wall-loss. CHEN LE, Qi Li, Don Collins, David R. Cocker III, *University of California, Riverside*

Minimal particle wall loss along with accurate particle wall-loss correction is critical for an environmental chamber to be used to determine true aerosol yield. It has been concluded by experimental observations over the previous years that the UCR dual 90-m³ collapsible chambers particle wall-loss behavior was dominated by electrostatic deposition and was significant enough to overwhelm Brownian motion and gravitational settling, which are the other two main driving forces of particle wall-losses (Le et al., 2021; McMurry and Rader, 1985). Possible explanations for the existence of electrostatic effect were speculated to be: 1) the Teflon chamber walls rubbing against each other in the dual-chamber design due to our external mixing system (air handlers) being on during experiments; 2) the Teflon chamber walls rubbing the reflective aluminum surfaces of the chamber enclosure (Le et al., 2021). Understanding the shortcomings of our previous chamber design and operation, a next generation 120-m³ indoor chamber has been recently constructed at UCR to minimize the effect of electrostatics and to lower its particle wall-loss rate. An extra supporting structure for the Teflon chamber was implanted, physically separating the chamber wall and the metal groundings. In addition, a set of soft x-ray external enclosure neutralizing devices was deployed and tested (Hamamatsu Photonics).

A high-flow mono-dispersed particle injection system and a dual-SMPS measurement technique were utilized in the earlier study to characterize the size-dependent particle wall-loss behaviors in the previous generation environmental chamber (Le et al., 2021). In the current study, an identical experimental set-up was applied to the new generation of chamber with or without the using of the additional external neutralizing system. It was observed that the new construction design reduced particle wall loss rate and that the particle wall loss rate became more size dependent. Further neutralization of the chamber walls using the soft x-ray system further reduced particle wall loss rate and also further increased the dependence of particle wall loss rate on size. Particle wall loss correction used for aerosol yield measurement was reduced from 85-90% to ~20% for a 12-hour experiment. Evaluation of the potential side-effects of using these external neutralizing devices on aerosol generating processes during experiments provides guidance for the standard operation processes of the new chamber and provides insights for the future chamber designs.

2AP.9

Comparison of New Particle Formation (NPF) Events in Various Ambient Atmospheres. HAEBUM LEE, Joonwoo Kim, Jiyeon Park, Young-Jun Yoon, Kihong Park, *Gwangju Institute of Science and Technology*

New particle formation (NPF) in the ambient atmosphere has been observed in various locations in the world. The newly formed nanoparticles can grow to the submicrometer particles increasing the number of particles and having a potential to serve as cloud condensation nuclei (CCN). The occurrence of NPF will be affected by several factors such as precursor gases, preexisting aerosols, and meteorological parameters (RH, temperature, and solar radiation). We observed NPF events at the remote (Ny-Alesund, Norway (Arctic)), urban (Gwangju, Korea), and agricultural (Gimje, Korea) sites and examined new particle formation rate (J), growth rate (GR), and dimensionless NPF occurrence criteria (L_Γ). The average NPF occurrence frequency was 23.6%, 45.4%, and 55.9% at the Arctic, urban, and agricultural sites, respectively. The dimensionless NPF occurrence criteria agreed well with the observed NPF events at all sites. The highest formation and growth rates were observed at the agricultural site. The H_2SO_4 played more important roles in new particle formation and growth at the urban site, compared to the Arctic and agricultural sites. More comparison of NPF characteristics among sites will be presented.

2AP.10

Field Directed Assembly of Aerosol Nanoparticles in Free-molecular and Transition Regime. PRITHWISH BISWAS, Pankaj Ghildiyal, George Mulholland, Michael Zachariah, *University of California, Riverside*

Manipulating the fractal dimension of nanostructures in continuum regime to obtain different architectures has been widely explored. However, ballistic dynamics in the free molecular regime, typically observed in aerosol phase, causes nanoparticles synthesized through high temperature aerosol routes, to form aggregates with the universal fractal dimension (D_f) of 1.8. In this study, it has been demonstrated that external field induced interparticle interactions can be utilized to linearly assemble particles and hence tune the D_f of particle aggregates even in the free-molecular regime. Through performing a hybrid ensemble/cluster-cluster aggregation Monte Carlo simulation, we have demonstrated that an ensemble of particles can be made to interact through directional attractive and repulsive forces by inducing dipole moments from an externally applied field, thereby leading to an aggregate structure transition. The fractal dimension of the aggregates can be tuned by changing primary particle size, temperature and the applied field strength and linear chain-like aggregates with D_f~1 can be obtained when the applied field strength is above a certain threshold value for a particular primary particle size and temperature. It has been demonstrated that the threshold magnetic field strength required to linearly assemble 10–500 nm particle sizes are practically achievable whereas the field required to assemble sub-100 nm particles by inducing electrical dipoles, are beyond the breakdown strength of most gases. A correction factor to free molecular and transition regime coagulation kernel, based on magnetic dipolar interactions, has been derived to theoretically account for the enhanced coagulation rates due to attractive interactions. A comparison has been made between the coagulation time-scales estimated by theory and simulation, with the estimated polarization time-scales of the primary particles and the oscillation time period of the magnetic field, to demonstrate that sub-50 nm superparamagnetic primary particles can be magnetized and assembled at any temperature, while below the Curie temperature ferromagnetic particles of all sizes can be magnetized and assembled, given the applied field is higher than the threshold.

2CO.1

A Reactive Molecular Dynamics-based Exploration of Soot Inception Pathways in Combustion. Khaled Mosharraf Mukut, Akaash Sharma, Eirini Goudeli, SOMESH ROY, *Marquette University*

Accurate prediction of the formation of soot in combustion systems is important for many reasons – from better combustion efficiency to combat climate change. Yet, the fundamental physico-chemical processes behind the formation of soot are still not completely understood. In this study, the mechanism of incipient soot formation is investigated in silico by reactive molecular dynamics (MD) simulation using the reactive force field (reaxFF) potentials without making any a priori assumption about the inception pathways or characteristics of incipient soot. Acetylene molecules are allowed to collide at 1500 K to form new species leading to incipient soot. The temporal evolution of precursor species is tracked to understand the pathways to soot and to identify and isolate the key soot precursors. The evolving mixture composition contains small molecules (up to molecular weight, MW < 240 kg/kmol) in the very early stages of nucleation. Later, the gradual formation of distinct clusters of larger molecules and incipient soot (MW > 1000 kg/kmol) are observed. The molecular population can be differentiated into active, abundant small molecules and rare, transitionary large molecules, providing insight into the transition boundary between gaseous precursor molecules and incipient soot. Additionally, the internal structure of the formed soot clusters is quantified based on the aliphatic/aromatic carbon ratio and by the number of 5-, 6- and 7-member rings. The incipient soot shows an aromatic core with a shell made of aliphatic carbons. It is also observed that the aliphatic molecules play a significant role during coalescence. The soot growth rates are found to be closely linked to the chemical structure of obtained incipient soot. The soot clusters that are rich in aliphatic carbon chains are softer and, thus, more prone to coalesce with each other, in contrast to larger clusters that are rich in aromatic rings.

2CO.2

Achieving Sampling Parameter-Independent Measurements of Incipient Soot in Laminar Flames with High-Resolution Differential Mobility Analysis. FARNAZ KHOSRAVI, Francesco Carbone, *University of Connecticut*

The detailed analysis of the transition from the gas to the particle phase that occurs in flames and causes soot formation and emissions is one of the major challenges faced by the combustion community. This study investigates the size distribution function (SDF) and charge-state of the nanometer-sized products of one premixed and one diffusion, ethylene-fueled, laminar flames experimentally. A sampling orifice drilled in a horizontal tube probe under small constant suction pressure extracts the samples to be analyzed, including incipient soot, from the flames while the nitrogen dilution flow enforces them to a Half-Mini High-Resolution Differential Mobility Analyzer (DMA). We investigate the effects of the nominal DMA resolution, the sampling orifice diameter (i.e., the dilution ratio, DR), and the transport time (Δt) to the DMA inlet separately. We implemented several flow patterns to bring the sample at the entrance of DMA to control Δt independently of all other parameters and reduce its values down to 30 ms. The results determine the conditions under which one can measure the shape of the sample SDFs independently of the sampling and analysis parameters. Increasingly larger values of DR/Δt are necessary to avoid distortions of the SDF shape as the sample ages in the flames when the sampling orifice positioning is further downstream. On the other hand, changes in DR may affect the measured total number concentrations even when they do not affect the SDF shape. We are performing additional experiments to try to rationalize this peculiar finding.

2CO.3

Santoro Flame: The Volume Fraction of Soot Accounting for Its Morphology & Composition.

GEORGIOS A. KELESIDIS, Sotiris Pratsinis, *ETH Zurich, Switzerland*

Laser diagnostics for on-line monitoring of soot mass or volume fraction, f_v, from combustion sources are calibrated using co-flow diffusion flames, such as the miniCAST generator [1]. In this regard, the soot f_v measured by Santoro and coworkers [2] in an ethylene diffusion flame by light extinction is used widely to validate soot formation and growth models. This f_v has been obtained using constant absorption function, $E(RI) = 0.16$ or 0.19, for soot spheres neglecting the evolving soot morphology and composition. The f_v obtained that way is 2 times larger than that measured by thermocouple particle densitometry (TPD) [3] at identical conditions.

Here, the evolution of f_v in the above flame is derived accounting for the realistic soot morphology and composition [4] by coupling discrete dipole approximation [5] with discrete element modeling for soot surface growth and agglomeration [6]. The soot f_v derived using light extinction data with this variable $E(RI)$ accounts for the realistic soot morphology and composition, in excellent agreement with TPD data [3] at the centerline and maximum f_v path of the Santoro diffusion flame. So, the evolving soot morphology and composition are essential to determine the soot f_v and close the mass balance of models for soot formation and growth.

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2CO.4

Retrieving Pre-factor and Fractal Dimension of a Single Soot Aggregate.

Divjyot Singh, LAURENCE LU, Alexei Khalizov, *New Jersey Institute of Technology*

Combustion soot aggregates have a complex morphology which influences their radiative forcing, surface chemistry, cloud nucleation efficiency, and atmospheric lifetime. The morphology is commonly described by the fractal law, using the scaling prefactor and fractal dimension. These fractal parameters are usually calculated from the dependence of aggregate monomer counts on the radius of gyration across an ensemble of differently sized aggregates. This approach returns the average fractal parameters for the ensemble rather than for a single soot aggregate.

In some applications, like investigating soot restructuring, it is necessary to retrieve fractal parameters of a single aggregate. Such analysis has been performed on 3D electron tomography images using the common cube-counting method, which discretizes an aggregate into voxels of a certain size and counts the number of voxels forming the aggregate. This process is repeated several times with different voxel sizes and the fractal parameters are then derived from the linear regression of a log-log plot of the voxel counts against the voxel sizes. This cube-counting method is computationally expensive. Therefore, we explore the application of a monomer-based approach, in which a large number of sub-aggregates are randomly chosen in a range of sizes inside the aggregate. We derive the fractal parameters from the linear regression of a log-log plot of the monomer counts of the sub-aggregates against their radii of gyration.

We test both methods on aggregates of varying sizes and morphology, generated via a diffusion-limited cluster-cluster aggregation algorithm, and compare their speed and accuracy. We illustrate how the monomer-based approach is computationally fast and can be used in simulations of soot aggregates where fractal parameters need to be found frequently.

2CO.5

Turbulence Impacts upon nvPM Sizes. MADHU SINGH, Akshay Gharpure, Randy Vander Wal, Prem Lobo, Joel Corbin, Gregory Smallwood, *Penn State University*

In a multi-partner collaboration led by NASA and DLR, the field campaign ND-MAX/ECLIF2 was conducted between January 14 and February 3, 2018 from Ramstein Air Base in southwest Germany. Ground-based particle and gas measurements were performed on the DLR A320 “Advanced Technology Research Aircraft (ATRA)” with IAE V2527 engines as the emissions source. A series of reference and blended fuels were studied in order to vary aromatic concentration, H-content, sulfur content and naphthalene content. Results presented here are results from TEM analysis of non-volatile particulate matter (nvPM). Collected directly upon TEM film grids, aggregate, primary particle and nanostructure scales were analyzed for selected conditions.

A striking observation is the range of primary particle size. Projected particle diameter range is 5 – 100 nm. Notably this range of primary particle sizes is that repeatedly found within a single aggregate. This range of particle size is interpreted as describing the corresponding ensemble of fuel rich pockets in the combustion zone in terms of phi and residence time. Some parcels are sufficiently diluted or short-lived by turbulent action to allow only small primary particles to form. Subsequently aggregation of varied particles from different fuel-rich regions then occurs (also due to turbulence) – effectively remixing these fuel-rich pockets. In this manner the soot particles provide forensic insights into the turbulent mixing dynamics. As a consequence and unlike laboratory soot sources, there is no single streamline or trajectory describing particle growth and no single condition in equivalence ratio or temperature for particle nucleation. Given the different trajectories of small/large particles and growth histories and species origins, a difference in H-content would be expected. This is reflected in the relative contributions of sp2/sp3 content within the particles as confirmed by EELs analysis.

2CO.7

Laboratory Evaluation of the Volatility of Nanoparticles Generated from Jet Engine Lubrication Oil. NOBUYUKI TAKEGAWA, Anna Nagasaki, *Tokyo Metropolitan University*

The characterization of particle emissions from jet aircraft is an important issue in the assessment of the aviation impacts on climate and human health. In the method for measuring non-volatile particles from turbofan engines, a volatile particle remover (VPR) heated to 350°C is generally employed to vaporize volatile compounds such as sulfate and organics. Tetracontane (C40) is used as a test compound for evaluating the removal efficiency of volatile particles in VPRs. Recent studies have shown that the formation of nanoparticles from jet engine lubrication oil could be an important source of aerosol particles in aircraft emissions under real-world operating conditions. We investigated the volatility of nanoparticles generated from unused jet engine lubrication oil (Mobil Jet Oil II), triacontane (C30), and C40. The particle number fraction remaining downstream of a custom-made evaporation tube was measured using an ultrafine condensation particle counter (UCPC; Model 3776, TSI) and a condensation particle counter (CPC; Model 3771, TSI) for initial particle diameters of 30 and 50 nm. The temperature of the evaporation tube was varied from room temperature (~20°C) to 400°C, and the temperature dependency of the particle number fraction remaining was derived for the C30, C40, and jet engine lubrication oil particles. The experimental results suggest that the volatility of the lubrication oil particles was comparable to that of the C40 particles, and that the lubrication oil particles could be entirely removed at the tube temperature of >250°C. The temperature profile of sample air inside the evaporation tube was measured separately from the volatility experiments. The evaporation time scale of the C40 particles was simulated using the measured temperature profile and a simple mass transfer equation to interpret the experimental data.

2CO.8

The Effect of Sodium-laden Solutions on Particulate Emissions from Gas Flares. CAMERON ROTH, Bradley Conrad, Matthew Johnson, *Carleton University*

Flaring in the upstream oil and gas industry (UOG) is the process by which unwanted gases are disposed through combustion in an open-atmosphere flame. During and after flowback operations at hydraulically fractured wells, gas must be separated from produced oil and other liquids prior to combustion. Field experiments have shown that this separation process is imperfect, allowing liquids to be entrained in the gas stream and subsequently combusted. These liquids vary spatiotemporally but are typically composed mainly of formation water. Despite this variability, ions such as sodium and chlorine are consistently present in strong concentrations. Previous experiments studying lab-scale flames doped with sodium aerosols have shown that sodium can significantly disrupt the combustion process, strongly influencing the production of particulate emissions and carbon conversion efficiency (CCE) of the flare. Recent research has also identified that the morphology and, hence, optical properties of carbonaceous particles emitted from sodium-doped flames differ from dry flames.

This work presents an investigation into the effects that entrained sodium-laden formation water may have on particulate emissions from flares in the UOG industry. Experiments using a hydrocarbon gas mixture representative of UOG flaring in Alberta, Canada are conducted at the Carleton University Flare Facility. Aqueous solutions containing NaCl or NaOH at 0.25−8.0%m/m are atomized into the flare gas stream prior to combustion. Particle mass concentrations and optical coefficients in the diluted combustion products are simultaneously measured to infer relative emission rates and optical properties of emitted particulate. Gas-phase instrumentation permits simultaneous calculation of flare CCE and gas-phase emissions. These studies identify significant, and sometimes contrasting effects of NaCl and NaOH solutions on the propensity of a flare to emit particulate matter and the CCE of the flare. The implications of the effective single scattering albedo of emitted particulate and concomitant emissions of greenhouse gases are discussed.

2CO.9

Quantifying Smoke Detector Performance for Spacecraft Applications. CLAIRE FORTENBERRY, Marit Meyer, Thomas Cleary, David Urban, Gary Ruff, *Universities Space Research Association*

Smoke detection presents a unique challenge for the future of human space flight. In a confined cabin where fire suppression and escape options are limited, early fire detection is critical to ensure crew survival and safety. Several factors challenge early fire detection in spacecraft. In microgravity, smoke plumes are unaffected by buoyancy and therefore do not rise as they would on Earth, so smoke detectors are commonly placed within air intakes rather than on ceilings. Additionally, high particle filtration rates typical of spacecraft life support systems may extend a smoke detector's time to alarm, allowing more time for a fire to progress and for toxic combustion products to accumulate in the spacecraft cabin. While different particle-based smoke detector designs have been used in spacecraft throughout the years, each design has distinct advantages and disadvantages. A critical factor in detector performance is particle size, motivating recent studies to characterize particles from the combustion of various spacecraft-relevant materials. These studies demonstrated that smoke particle size widely varies depending on fuel composition and combustion characteristics, further complicating the selection of an optimal detector design.

We present results from laboratory studies to compare the performance of different smoke detector designs with various types of aerosol. Smoldering lamp wick and a soot generator were used to generate aerosol representative of oxidative pyrolysis and flaming combustion, respectively. Diethylhexyl sebacate and mineral oil reference aerosols enabled evaluation of detector performance based on particle sizes. Because quantified relationships between ionization and light obscuration/extinction detectors depended heavily on particle size distributions, these results will inform spacecraft detector design and help predict performance under different potential spacecraft fire scenarios. Finally, we will discuss the applicability of these findings to the development of detectors for future long-duration and lunar missions.

2CO.10

Characterization of Gas and Particle Emissions from Solid Waste Combustions. XIAOLIANG WANG, Hatef Firouzkouhi, Matthew Claassen, Judith Chow, John Watson, Gerhard Fourie, Mabu Mamadi, *Desert Research Institute*

Open burning of household waste is a common practice in many rural areas in developing countries. Due to limited resources for collection and proper disposal, household and municipal solid waste is often disposed in neighborhoods and open burned in piles to reduce odors and create space for incoming waste. Emissions from these ground-level and low-temperature burns cause air pollution, leading to adverse health effects among community residents. This study conducted a laboratory chamber combustion experiment to characterize gas and particle emissions from eight waste categories representative of those burned in South Africa: paper, leather/rubber, textiles, plastic bottles, plastic bags, vegetation, food discards, and combined materials. Carbon dioxide (CO_2) and carbon monoxide (CO) were measured in real-time to calculate modified combustion efficiencies (MCE), which is used to determine emission factors (EFs) during flaming and smoldering phases as well as the entire combustion process. Fuel elemental composition and moisture content have strong influences on emissions. Plastic bags have the highest carbon content and the highest combustion efficiency, leading to the highest EFs for CO_2. Textiles have the highest nitrogen and sulfur contents, resulting in the highest EFs for nitrogen oxides (NO_x) and sulfur dioxide (SO_2). Emissions are similar for vegetation with 0% and 20% moisture contents; however, EFs for CO and particulate matter (PM) from the vegetation with 50% moisture content are 3 and 30 times, respectively, of those from 0% an 20% moisture contents. Particle size distributions (6 nm – 10 µm), light scattering, and absorption properties vary among the fuels and during the burning cycle. Results from this study are applicable to emission inventory improvements as well as air quality management to assess the health and climate effects of household waste open burning.

2RA.1

Stationary and Mobile Measurements of NO2 Vertical Column Density at an Agricultural Site. TAEWOONG GONG, Joonwoo Kim, Haebum Lee, Kihong Park, *Gwangju Institute of Science and Technology*

Nitrogen dioxide (NO_2) plays a role in generating catalytic ozone through a photochemical reaction in the atmosphere. High concentration of NO_2 can cause problems in the human respiratory system and vegetation. The NO_2 is known to be mainly emitted from automobiles, and can also be generated through agricultural and livestock activities (Melynda et al., 2016). At an agricultural site near swine and chicken farms, the NO_2 slant column densities (SCDs) and the vertical column densities (VCDs) were determined by using the Multi Axis Differential Optical Absorption Spectroscopy (MAX-DOAS). The stationary measurement was performed near the swine and chicken farms, and mobile measurement was conducted to determine the spatial variation of NO_2 VCD along the route near the site in Gimje, South Korea (35.83°N, 126.98°E) during June-July of 2020 (summer) and January-February of 2021 (winter). For determination of the VCDs of NO_2, the NO_2 air mass factor was retrieved by a geometric approximation. The NO_2 VCDs from 2°, 4°, 8°, 15° and 30° elevation angles were retrieved from stationary measurement in summer, 20° and 45° elevation angles were retrieved from mobile measurement in summer, and 0°, 1°, 2°, 3°, 4°, 5°, 6°, 7°, 8°, 10°, 15°, 20° and 30° elevation angles were retrieved from stationary measurement in winter. Seasonal and spatial variations of NO_2 VCD around swine and chicken farms will be presented. Also, the relations of the NO_2 VCD to NO_2 concentration at ground level and chemical characteristics of fine particles will be discussed.

2RA.2

Composition and Concentrations of Ambient PM in an Oil and Gas Production Region. KRISTI MCPHERSON, Catherine Masoud, Nirvan Bhattacharyya, Kanan Patel, Leif Jahn, Pearl Abue, Daniel C. Blomdahl, Pawel K. Misztal, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Oil and gas development in the Eagle Ford Shale (EFS) has undergone rapid growth since it began in 2008. Several aspects of oil and gas production have impacts on air quality, including volatilization of wastewater, leaks, and flaring. To investigate these impacts, instrumentation was deployed to Karnes City, TX, located in the EFS, in the spring of 2021. Instrumentation included an ACSM, SEMS, iodide mode FIGAERO-CIMS, Vocus-2R-PTRMS (with a VIA inlet), a microaethalometer, and monitors for O3, NOx and NO2 to measure aerosol and gas-phase concentrations and composition.

The maximum NR-PM1 concentration was 15 µg m-3 and the average concentration was 4 µg m-3. Particulate sulfate was the largest fraction of PM1 and several episodic plumes for sulfate were observed. The plumes were associated with wind direction and somewhat correlated with hydrogen sulfide concentrations, an emission associated with oil and gas production. Episodic plumes were also observed for organic PM1. While most organic plumes coincided with sulfate plumes, some did not. The average fraction of organic PM at m/z 44 (f44) was 0.17, which is comparable to the f44 in the reference PMF factor for oxidized organic aerosol, suggesting that organic aerosol in the region was highly oxidized. Black carbon concentrations exceeded 1 µg m-3 at times, with an average concentration of 0.5 µg m-3. Data from FIGAERO-CIMS and Vocus-2R-PTRMS provide further insight into the molecular composition of the aerosol, and gas-phase data provide insight into the atmospheric chemistry influencing aerosol concentration and composition. Due to the intermittent nature of emissions from oil and gas activity, especially flaring, this characterization of regional and episodic aerosol is important for better understanding impacts on air quality, exposure, and health.

2RA.4

Refining Ammonia Emissions Estimates with Satellite-based Observations Using a Novel Framework and an Air Quality Model. CONGMENG LYU, Shannon Capps, Mark W. Shephard, Daven Henze, Matthew Lombardo, Shunliu Zhao, Amir Hakami, Steven Thomas, Jeremy Silver, Peter Rayner, *Drexel University*

The Community Multiscale Air Quality (CMAQ) model calculates the impact of emissions on atmospheric composition, including inorganic aerosols, while considering the transport and reactions of chemical constituents. Adjusting emissions by comparing modeled concentrations with observations is justified when the science processes are well understood as is the case for inorganic species such as ammonia (NH_3). The Finite Difference Mass Balance (FDMB) method and four-dimensional variational (4D-Var) data assimilation leverage differences in simulated and actual observations to revise estimates of emissions with spatial specificity. In this study, we evaluate the capability of a CMAQ-based data assimilation system to improve NH_3 emissions, which are relatively uncertain given the diversity of emissions processes in the agricultural sector. To do so, the iterative FDMB and a Python-based four-dimensional variational framework (py4dvar) are integrated with CMAQ and its adjoint to constrain NH_3 emissions with observations from the satellite-based Cross-track Infrared Sounder (CrIS). Observing System Simulation Experiments (OSSEs) are conducted with the CrIS observation operator to evaluate the extent to which emissions are expected to be recovered with the hybrid assimilation framework. The OSSE conducted with the 2007 modeling platform and 2016 CrIS data on a regional domain in Georgia results in promising recovery of the true emissions. The framework is then ported to a 2017 modeling platform for assimilation of 2017 CrIS NH_3 observations to mitigate the mismatch between modeling platform and satellite observation years. Three suitable periods are selected from April through October 2017 for assimilation. Independent surface measurements are used to evaluate posterior modeled concentrations.

2RA.5

PM2.5 Characteristics in the Ammonia-Rich Agricultural Environment. JOONWOO KIM, Haebum Lee, Taewoong Gong, Jiho Jang, Dahye Oh, Kihong Park, *Gwangju Institute of Science and Technology*

Gas-phase NH_3, which is emitted from agricultural areas, plays a key role in atmospheric chemistry as the major basic gas. The NH_3 neutralizes acidic gases, promotes secondary aerosol formation, and is converted to particulate NH_4^+ which contributes to the increases of $PM_{2.5}$ mass and nanoparticle number concentrations. To characterize $PM_{2.5}$ in the NH_3-rich agricultural environment, we performed field measurements (point and mobile measurements) of aerosols and gases downwind of an intensive animal farming area in the summer of 2020. The average NH_3 concentration was 81.7±84.3 ppb. The NH_4^+ completely neutralized anions in aerosols, indicating that the atmosphere was NH_X-rich ($NH_X = NH_3 + NH_4^+$). The mass fraction of particulate NO_3^- in $PM_{2.5}$ was as high as 21.9%, which is contrary to the sulfate-dominant $PM_{2.5}$ in summer at urban sites. During the $PM_{2.5}$ events, the nitrate oxidation ratio (NOR = $[NO_3^-]/([NO_2] + [NO_3^-])$) doubled to ~0.5 and the ratio of water-soluble organic carbon to organic carbon increased. Excess NH_X was likely to promote the formation of secondary aerosols, especially NO_3^-, and contributed to the increase of $PM_{2.5}$ mass concentration. Further analyses on NH_3 emissions from the source area, spatial distribution of fine particles, and their physical and chemical properties are in progress and will be presented.

2RA.6

Understanding Ambient Trends in Particle Phase Nitrate Contributions from Inorganic & Organic Species. JESSICA HASKINS, Colette L. Heald, Douglas Day, Pedro Campuzano-Jost, Jose-Luis Jimenez, *Massachusetts Institute of Technology*

There is conclusive evidence from field studies across the globe showing that organic nitrate aerosols ($pRONO_2$) are important components of fine mode total particle nitrate (pNO_3) on a continental scale in Europe and of ambient organic aerosols (OA) on a global scale. $pRONO_2$ have been shown to be responsible for > 50% of the OA production in the southeast US during summer. However, the broader regional contribution of $pRONO_2$ to total particle nitrate and, the variability in that contribution throughout North America in different seasons, and chemical regimes remains in question. We present data compiled from 10+ field campaigns across North America showing the large-scale trends in spatial and temporal variability in ambient measurements of $pRONO_2$ under various conditions utilizing simultaneous measurements of assorted biogenic volatile organic compounds (BVOCs), nitrogen oxides (NO_x), and other gas phase species. We highlight how both the total mass of $pRONO_2$ and fraction of total pNO_3 that is organic vary in polluted verses rural areas, in the vertical, across different temperature and relative humidity schemes, diurnally, and as a function of measured BVOCs.

2RA.7

Chemical Signatures of Fire and Urban Influenced Secondary Aerosol Formation in the Central Amazon.

EMILY FRANKLIN, Lindsay Yee, Rebecca Wernis, Gabriel Isaacman-VanWertz, Nathan Kreisberg, Robert Weber, Brett Palm, Weiwei Hu, Pedro Campuzano-Jost, Douglas Day, Paulo Artaxo, Rodrigo Souza, Jose-Luis Jimenez, Scot T. Martin, Allen Goldstein, *University of California, Berkeley*

Biogenic secondary organic aerosol (SOA) plays a critical role in atmospheric chemistry and climate in the tropics, a region where increasing anthropogenic activities (urbanization and fires) perturb natural processes of oxidation chemistry. While SOA formation in the tropics has been observed and modeled to increase in the presence of anthropogenic pollutants, the mechanisms by which these enhancements occur and implications for particle chemistry remain unclear. During the Green Ocean Amazon (GoAmazon) field campaign of 2014/5, over 200 submicron aerosol samples were collected over periods spanning both the wet and dry seasons of 2014 at the “T3” Manacapuru rural site, located 70km downwind of urban Manaus. Utilizing TD-GCxGC-EI-HRToFMS (thermal desorption two-dimensional gas chromatography with electron ionization time-of-flight mass spectrometry), ~1500 unique organic compounds from these samples are separated, cataloged, and traced. Using dynamic time warping hierarchical clustering and time series correlation with established tracers of biomass burning and urban influence, the chemical signatures of anthropogenically influenced SOA formation are extracted from background measurements representing a range of natural conditions. These chemical signatures reveal that biomass burning activity accounts for ~50% of dry season organic signal and ~10% of wet season organic signal. Urban plume influence, consisting of both primary emissions from the city as well as products that are uniquely produced when biogenic precursors are exposed to anthropogenic oxidants, accounts for approximately one quarter of wet season organic signal and less than one fifth of dry season organic signal. Mass spectral comparisons to compounds in the NIST/EPA/NIH mass spectral database and those in samples collected from single precursor oxidation experiments conducted under a variety of oxidizing conditions reveal the presence of previously unpublished monoterpene oxidation products which are observed in the field exclusively under urban plume influenced conditions. These new tracers provide mechanistic insights into how human activity alters biogenic secondary aerosol formation.

2RA.8

Characterizing the Atmospheric Processes of Brevetoxins in Sea Spray Aerosols Generated from Florida Red Tide.

KAREN SEM, Myoseon Jang, Zechen Yu, Richard Pierce, Patricia Blum, *University of Florida*

Florida red tide consists of high-biomass blooms of the dinoflagellate *Karenia brevis*, which emits polyether brevetoxins that cause neurotoxic shellfish poisoning. Sea spray aerosols (SSA) generated via wave motion during red tide events can be transferred by wind to coastal areas and can cause respiratory irritation in humans after short-term exposure. Atmospheric conditions can affect the longevity of brevetoxin contained in SSA and resulting adverse human health effects. This study characterizes the environmental conditions that lead to brevetoxin degradation in SSA during red tide events. Samples of seawater collected during a *K. brevis* bloom in Manasota Key, Florida are nebulized into a large outdoor photochemical chamber to mimic the atmospheric processes of aerosolized toxins. The aerosols are then atmospherically aged under various environmental conditions, including the presence or absence of sunlight, O_3, OH radicals, and organic matter. Aerosols are collected during the aging process using a Particle-to-Liquid Sampler. The aerosols’ brevetoxin concentrations are measured using a conventional enzyme-linked immunoabsorbent assay (ELISA) to assess the rate and extent of their degradation. Brevetoxin decay is also confirmed by measuring concentrations with high-resolution liquid chromatography–mass spectrometry (LC–MS). Exploratory results indicate that brevetoxin concentrations in SSA decreased more rapidly in the presence of sunlight than in its absence, suggesting that reactions with OH radicals contribute largely to the algal toxin degradation. Additionally, nighttime chamber studies showed that brevetoxin decay also occurs in the presence of O_3. Chamber data will be used to obtain kinetic constants for the reaction of brevetoxin with major atmospheric oxidants (O_3 and OH radicals) and applied to the development of a model to predict atmospheric process of brevetoxin in SSA. This model can then assist in the development of a risk model to protect coastal communities from brevetoxin exposure during red tide events.

2RA.9

New Particle Formation over the Western North Atlantic Ocean: Results from the NAAMES Field Campaign. JIAOSHI ZHANG, Xianda Gong, Qian Xiao, Armin Wisthaler, Markus Müller, Sven Arne Philipp Schiller, Richard Moore, Luke Ziemba, Ewan Crosbie, Ryan Bennett, Jian Wang, *Washington University in St. Louis*

New particle formation (NPF) in the remote marine environment can contribute substantially to aerosol and CCN population, therefore influencing the marine clouds and climate. In this study, we investigate the new particle formation over the Western North Atlantic Ocean (WNAO) in different seasons (winter, late spring and summer) using airborne measurements during the North Atlantic Aerosol and Marine Ecosystem Study (NAAMES) field campaign. The WNAO region is impacted by a variety of synoptic regimes that lead to different atmospheric transport among ocean, North American continent, and the Arctic. The airmasses sampled are classified into four representative categories (i.e., background, biomass burning, biogenic and continental pollution) using trace gas and VOCs measurements including CO, acetonitrile, benzene, acetone, and methanol.

NPF events were observed at a wide range of altitudes, from near ocean surface to upper free troposphere above 6 km. Vast majority of the NPF events were observed under background conditions with minimum influences from continental emissions. The newly formed particles in the background airmass coincided with elevated dimethylsulfide (DMS) mixing ratio, especially during late spring and summertime when ocean biological activities are relatively high. NPFs inside the marine boundary layer were mostly observed under postfrontal conditions, when airmasses originated from the Arctic. NPFs in the upper free troposphere were observed in the outflow of convective clouds with reduced aerosol surface area and elevated RH and DMS mixing ratio. Oxidation products of DMS are likely the major precursors during these NPF events. Newly formed particles were also observed in continental outflows from North America inside free troposphere, suggesting impact of continental emissions on NPF. The potential precursors and mechanisms for these NPF events, which occurred in different airmasses and at a range of altitudes, will be compared and summarized.

2RA.10

A Global-scale Mineral Dust Equation. XUAN LIU, Jay R. Turner, Randall Martin, Bret Schichtel, Jenny Hand, *Washington University in St. Louis*

A robust method to estimate mineral dust mass in ambient particulate matter (PM) is essential, as the dust fraction cannot be directly measured but is needed to understand dust impacts on the environment and human health. In this study, a global-scale dust equation is developed that builds on the widely used Interagency Monitoring of Protected Visual Environments (IMPROVE) network's "soil" formula that is based on five measured elements (Al, Si, Ca, Fe, and Ti). We incorporate K, Mg, and Na into the equation using the mineral-to-aluminum (MAL) mass ratio of $(K_2O+MgO+Na_2O)/Al_2O_3$ and apply a correction factor (CF) to account for other missing compounds and adsorbed water, based on which we develop a global-scale dust equation with region-specific coefficients (Dust = $[1.89Al\times(1+MAL)+2.14Si+1.40Ca+1.36Fe+1.67Ti]\times CF$). For desert dust in major global source regions, the estimates from the global equation are consistent with the total mineral mass (calculated by summing all the oxides of dust) with a small normalized mean bias (NMB within ±1%). For $PM_{2.5}$ with high dust content from the U.S. IMPROVE Network, the global equation estimates the dust mass well (NMB within ±5%) at most sites. For desert dust transported to non-source regions, the global equation still performs well (NMB within ±2%). The global equation can also represent paved road, unpaved road, and agricultural soil dust well (NMB within ±5%). This global-scale dust equation provides a promising approach for characterizing mineral dust of different types from various regions.

2RA.12

Indoor Environment Air Quality Evaluation in a High Elevation Metropolitan Area in the Andes.

RUBEN MAMANI-PACO, Mihai Chiruta, *Atmospheric Physics, Univ. Mayor de San Andrés La Paz Bolvia*

The emergence of Coronavirus disease 2019 disease (COVID-19) with its airborne transmission nature of the virus responsible for the SARS-CoV-2 coronavirus put into sharp focus the indoor air quality and the necessity to monitoring it.

In the past year indoor workspace environments had become unusable due the poor air quality. Many organizations using office spaces took different measures trying to limit the spread of COVID-19.

A simple way to increase air quality in closed environments is through natural ventilation. This would also reduce the probability of contagion by COVID-19 in such environments. It requires the monitoring of key parameters to ensure proper ventilation is achieved. In this work we plan to monitor the air quality of different indoor workspaces using the newly developed “My Air” integrated environmental monitoring system. The parameters that we will monitor are: barometric pressure, temperature, relative humidity, CO2 concentration, total volatile organic compounds concentration, and particulate matter concentration in four channels PM1, PM2.5, PM4, PM10. Additionally, we want to evaluate the effect of living at high elevation (low atmospheric pressure) on the performance of the system.

Subject headings: COVID-19 – closed environments – indoor air quality

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2SI.1

Recovery of Airborne SARS-CoV-2 Virus Surrogate Captured by Filtration: Effect of Sampling and Storage Stress.

NIRMALA THOMAS MYERS, Taewon Han, Mei-Ling Li, Gary Brewer, Martin Harper, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Occupational and community exposures to the SARS-CoV-2 virus via the aerosol transmission route is a major concern worldwide. Currently there are no standardized protocols to sample airborne viruses, including SARS-CoV-2, and identify potential exposures. Furthermore, there is limited knowledge on how sampling and storage stress impact the recovery of captured airborne viruses.

Our study analyzed the impact of sampling and storage stress on Human Coronavirus OC43 or HCoV-OC43, a surrogate of SARS-CoV-2 virus, captured by filtration. The HCoV-OC43 virus was aerosolized and then captured by a PTFE filter with PTFE lamination (Zepore) on polypropylene support pad in a conductive plastic cassette (VIRA-PORE, Environmental Express). The effect of sampling stress was evaluated by varying sampling flow rate (3 and 10 L/min) and sampling time (10 and 60 mins). Additional stress was added in a few tests by passing clean air through a filter with the virus on it for 1, 5, and 15 hours. Experiments to determine the effect of storage stress were designed to simulate 2-day transportation of the filter samples to a laboratory (stored at 25°C) and storage up to one week before analysis (stored at room temperature at 25°C and refrigerated conditions at 4°C).

The mode diameter of the aerosolized OC43 virus was 50-60 nm as determined by SMPS and CPC system (TSI Inc.) and MiniWRAS (Grimm Inc.) measurements – to the best of our knowledge, the first reported airborne particle size distribution of HCoV-OC43. Our results showed no significant difference between the virus recovery for the two sampling flow rates, the additional stress of being exposed for 15 hours, and different sampling times ($p > 0.05$). However, the RNA yield after seven days of storage at room temperature (25°C) was ~2x less compared to storage at refrigerated conditions (4°C). Based on these results, to avoid RNA degradation during transport and storage, we recommend shipping filter samples in a cold container within a week from sampling and store short-term in a laboratory refrigerator (4°C) before analyses. The general recommendations from our study can apply to other filter types as well when used for virus sampling, and we plan to investigate other filter types in our prospective studies.

2SI.2

Exploring Approaches to Characterize Respiratory Droplets >20 µm Diameter. JOSHUA HARRISON, Henry Symons, Justice Archer, Jonathan P. Reid, Bryan R. Bzdek, *University of Bristol*

Respiratory aerosol emissions are likely key to elucidating the transmission of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). These emissions span a wide size range, from < 1 µm diameter to >> 100 µm diameter, with significant variability in number concentration with droplet size. The current view of these emissions is that they consist of three distinct modes. The bronchiolar mode is centered around < 1 µm diameter and arises from aerosol produced in the bronchioles during breathing. The laryngeal mode is centered around 1-2 µm diameter and is associated with vocalization. These two modes represent the vast majority of the aerosol number concentration. The oral mode is generated in the oral cavity, is associated with significantly larger droplet sizes (~200 µm diameter), and contributes relatively few droplets but most of the mass. Whereas the droplets in the bronchiolar and laryngeal modes are well within the size range accessible by commercial aerosol measurement equipment, robust approaches to measure the oral mode do not currently exist. This contribution describes efforts to characterize the robustness of two new approaches to characterize the oral mode. In one approach, droplets are deposited onto water-sensitive paper and droplet size inferred from a color change. In the other, a fluorescein rinse is used before respiratory maneuvers, and droplets deposited onto target paper are then imaged using ultraviolet light to reveal the droplets. Both approaches are highly sensitive to spreading coefficients on their respective substrates. To calibrate these approaches, droplets reproducibly ejected from a microdroplet dispenser were deposited onto the appropriate substrate, permitting quantification of the relationship between deposited spot size and droplet diameter. Challenges of interpreting these measurements and their limitations will also be discussed.

2SI.3

High-Resolution Detection of Aerosols Produced During Breathing and Speech with an Electrical Low-Pressure Impactor. PAUL TUMMINELLO, Caleb Everett, Marva Seifert, Chantal Darquenne, Jonathan Slade, *University of California San Diego*

Aerosols produced from speech and breathing are thought to contribute to airborne pathogen transmission, which has become a focal point of the SARS-CoV-2 pandemic. Previous studies have measured aerosols produced during speech using laser-based detection and analysis with an aerodynamic particle sizer. These techniques have elucidated relationships between particular words and vocal amplitude in the production of aerosols. However, these measurements have been limited regarding the size (>0.5 µm) and timescales (1 s) of aerosol detection. In English, individual words and certain sounds may last only a fraction of a second. Here we utilize an electrical low-pressure impactor (ELPI) for detecting aerosols, one not previously applied to speech, which offers a greater range of detectable aerosol size (0.006 µm – 10 µm) and heightened temporal resolution (100 ms) compared to other methods. Participants in the study read stimuli while speaking and breathing with and without an N95 mask into an aluminum funnel connected to the ELPI. The results demonstrate significantly more aerosol production from human speech and breathing than previously thought, with a majority of the number of particles with diameters comparable to single viruses (between 0.07 µm and ~0.2 µm). Combined phonetic and aerosol analysis enabled detection of aerosols from some sound types lasting only ~100 ms. To simulate the aerosol concentrations one may be exposed to from speech in real conversation, participants read a paragraph for ~30 s, producing nearly 106 particles cm^{-3} cumulatively and volume concentrations ~105 $µm^3$ cm^{-3}. Nasal breathing alone produced about half the concentration of aerosols as speaking while wearing an N95 mask effectively removed nearly all particles generated from speaking and breathing. These results provide novel insights into aerosol production by human speech as well as the efficacy of masks in reducing aerosol transmission. Given the relatively greater buoyancy of fine aerosols and inordinate volumes of aerosol produced, these results can help inform transmission risks of airborne pathogens not accessible from previous methods.

2SI.4

Filtration Efficiency and Inhalation Resistance of Cloth Mask Combinations and the Effects of Washing and Drying On Performance. SUMIT SANKHYAN, Karen Heinselman, Peter Ciesielski, Hannah Teed, Teresa Barnes, Sameer Patel, Marina Vance, *University of Colorado Boulder*

In this study, filtration efficiency of different respirators, masks, and face coverings for particles in the size range of 60 nm - 4 µm was investigated under a "perfect fit" condition using two experimental setups. The filtration efficiency at the most penetrating particle size of 0.3 µm on average ranged from 90-99% for N95 and KN95 respirators, 40-88% for surgical masks, and 9-51% for cloth masks and a 2-ply bandana. We also investigated the effects of doubling surgical masks or layering a cloth mask over a variety of surgical masks, as this seems to have become a popular approach during the COVID-19 pandemic. For most combinations, the filtration efficiency improved by ~25% for particles 0.3-1 µm in diameter without any substantial change in the filter quality factor. To investigate the reusability of cloth masks, 2-layer cotton fabric samples were washed and dried for 52 cycles and, while this process led to an increase in inhalation resistance (~20 Pa), the size-resolved filtration efficiency did not change noticeably. Electron microscopy analysis revealed that washing and drying led to a deconstruction of individual fibers at the scale of several microns to hundreds of nanometers in the form of delamination of the fiber wall and fibrillation of the nanofiber constituents. The results from this study can be useful for understanding the sustainability of cloth masks and the relative protection of different masks and layering strategies to reduce both $PM_{2.5}$ exposure the risk of respiratory disease transmission.

2SI.5

Practical Considerations of Cloth Facemask Performance Versus Insert Areal Coverage. JAMES RADNEY, Christopher Zangmeister, *National Institute of Standards and Technology*

The CDC and WHO recognized that wearing cloth face coverings can slow transmission of respiratory diseases; specifically, the Severe Acute Respiratory Syndrome Coronavirus-2 (SARS-CoV-2). Adding a layer of material with a high filtration efficiency (FE, e.g. polypropylene sheets that meet the HEPA standard) as an inset in the mask can potentially provide the wearer with additional personal protection; however, data on the insert areal coverage necessary to realize benefits is sparse. The relationship between insert area ratio (IAR, relative to fabric area), FE, differential pressure (ΔP, a surrogate for breathability) and quality factor (QF, a ratio of FE to ΔP) utilizing two fabrics (rayon and 100 % cotton lightweight flannel) and three insert materials (HEPA vacuum bag, sterilization wrap and paper coffee filter) was investigated. It was found that: 1) The relationship is complicated, and a tradeoff exists between personal protection from filtration during inhalation and source control from leakage during exhalation. 2) The addition of any insert to a cloth mask assemblage will increase both FE and ΔP, but not necessarily QF. 3) FE, ΔP and QF of the composite mask scale with IAR. 4) Improvements in the QF of the composite assemblage require inserts with a higher QF than the cloth and larger differences yield greater gains. However, the converse is also true with lower QF inserts decreasing the QF of the system. 5) The increased ΔP from an insert results in increased leakage during exhalation and 6) to minimize leaks, ΔP must be as low as possible.

2SI.6

How You Test Matters: Respiratory Filtration Testing Using Common Aerosol Instruments. TIM JOHNSON, Greg M. Olson, Justin S. Koczak, Andrea J. Tiwari, *TSI Incorporated*

During the COVID-19 pandemic, the expertise of aerosol researchers has been called upon like never before. Many members of the aerosol science community have dedicated time and resources to testing face masks of various kinds in the interest of protecting medical personnel, other essential workers, and the general public. Numerous papers describing such results have been published by this community since the onset of the pandemic.

When testing filter efficiency, the first decision that must be made is whether the filter will be tested according to a standard method. If a standard method is not followed, decisions pertaining to instrumentation used in testing, face velocity, particle characteristics (size, neutralization, composition), and loading conditions must all be made. In the context of the pandemic, aerosol researchers made these decisions according to what was achievable with the resource they had available. Each of those decisions impact the filtration efficiency test results.

This presentation will illustrate the effects of those important decision on the measured efficiency of filters. This will be done using a dataset collected by testing a well-characterized control media, as well as a variety of barrier face covering materials (and combinations thereof). This testing used an experimental matrix that explores the influence of several variables (instrumentation type, face velocity, and particle size) on the final measurement of filtration efficiency. The effects of particle neutralization and loading will also be discussed.

Having illustrated the influence of each of those variables, this presentation will then review the literature to examine the range of choices made in recently published papers and infer the comparability of results among studies.

2SI.7

Optimized Hospital Ventilation to Reduce Virus Aerosol Transmission. MEIYI ZHANG, Tatiana Baig, Brooke Smith, Maria King, *Texas A&M University*

Most hospital rooms have ventilation designs that do not effectively maintain a virus-free environment. The problem became even more important during the COVID-19 pandemic as patients already suffering from diseases and injuries are more vulnerable to SARS-CoV-2 virus infection. The objective is to design an optimized hospital room ventilation system that will reduce virus aerosol transmission. In a ¾ scale hospital chamber airflow was simulated as a function of different room configurations using ANSYS Fluent. Out of five room configurations, the most optimal computational flow models were obtained from two designs. Configuration #1 consisted of an air inlet above the bed, with the air exhaust at the lower right corner, the bed at its standard position with the monitor next to it, and chair against the wall at the end of the room. Configuration #2 had the items at the same positions as #1 with an air curtain operating at the door. Experimental results based on the quantification of aerosolized bacteriophage PRD1 as virus simulant collected with twelve filter samplers at predetermined locations validated the flow models. For Configuration #1, the highest phage concentration was collected at higher levels near the bed, indicating that the phages released from the nebulizer at patient’s head were carried by the air currents first over the bed then towards the foot of the bed in agreement with the computational flow model. Higher phage concentrations were collected near the door. Experimental data show that adding air curtain to Configuration #2 results in overall lower phage concentrations at all locations, with the highest phage numbers observed at the nebulizer location and lowest counts near the door. In conclusion, optimized design with air curtain can be implemented to effectively reduce virus aerosol transmission in hospital rooms and lower the risks of viral infections.

2SI.8

Effectiveness of a Negative Pressure Airway Chamber in Reducing the Exposure of Healthcare Providers to Aerosol Generating Medical Procedures. ALBERTO BALDELLI, Kevin Heieis, Steven Rogak, Andrew Poznikoff, Matthias Görges, Robert Purdy, *The University of British Columbia*

Aerosols carry airborne viruses, such as SARS-CoV-2; this is a concern for healthcare providers (HCP) when working in close proximity to patients undergoing aerosol-generating medical procedures. The negative pressure airway chamber (NPAC), a Plexiglas enclosure fitted securely over a patient's head and shoulders with applied high-volume suction, was developed to shield HP from airborne particles generated while performing airway manipulation tasks at induction of anesthesia. Results from both a physical simulation study on baseline performance and a trial with human participants during simulated clinical use are presented.

The NPAC efficacy in trapping aerosols was investigated using a manikin in a regular hospital room with minimal ventilation. When applied to a manikin emitting 10 lpm of saline aerosols (median dried size ~ 1 µm), the NPAC reduced particulate matter concentrations (PM) at the HCP location by an average of 89 ± 5%, when compared to its absence. When performing common anesthetic tasks: preoxygenation, bag-mask ventilation and high flow oxygen therapy, the levels of PM at the HCP location never exceed the baseline (no aerosol source). Removing the chamber after performing these tasks was also shown to not cause a surge in PM at the HCP location.

With ethical approval and informed consent, a within-subject, block-randomized, study comparing intubation of a manikin with and without the NPAC was conducted. Simulated intubation trials involved: a) an aerosol generator being started and the HCP placing their hands and arms into the attached NPAC sleeves and gloves, b) bag-mask ventilation for 3 min, c) termination of aerosol generation, d) mask removal and airway instrumentation with an endotracheal tube, e) auscultation following removal of the NPAC. PM were reduced 84% for the overall clinical trials; PM peaks while performing bag-mask ventilation and auscultation were reduced by 82%.

2SI.9

Aerosolisation and Transmission of SARS-Cov-2 in Healthcare Settings (AERATOR). Florence Gregson, Sadiyah Sheikh, Fergus Hamilton, Mark Gormley, Jules Brown, Nick Maskell, Bryan R. Bzdek, JONATHAN P. REID, *University of Bristol, U.K.*

The transmission of respiratory diseases such as SARS-CoV-2 is known to occur through inhalation of aerosols or larger droplets containing respiratory secretions. Certain medical procedures, wherein high air flow travels over respiratory mucosa, are thought to generate viral aerosol and pose transmission risk to people in the vicinity when performed on infected patients. Through the study AERosolisation And Transmission Of SARS-CoV-2 in Healthcare Settings (AERATOR), we set out to quantify the aerosol generated during such procedures, classified as Aerosol Generating Procedures (AGPs). We cover a broad range of medical specialities, such as anaesthesia, orthopaedic and ophthalmic surgery, respiratory medicine and dentistry. Sampling the aerosol generated in real clinical procedures involves working around a series of environmental constraints, such as a high aerosol background concentration and positioning instrumentation as close to the source as possible around clinical staff. In all measurements we consistently sample aerosol with either an optical particle sizer (Dp = 0.3-10 µm) or Aerodynamic Particle sizer (0.5 – 20 µm) to measure both the aerosol concentration and the size distribution. However, we adapt our protocol for each clinical speciality for as reliable measurements as possible. Some studies, such as delivery of non-invasive ventilation (NIV) in respiratory medicine, involve healthy volunteers performing procedures in an ultra-clean background to unequivocally assign the sampled aerosol to the procedure. For dental procedures, plumes of aerosol are generated by the drills or ultrasonic scalers themselves, so we compare the modes within the generated size distribution from phantom controls with patient data. Our results suggest that patient coughing poses greater risk of aerosol generation than many NIV procedures (Hamilton et al, Lancet Resp. Med., 2021) and that policy of PPE, ventilation strategies and the use of patient facemasks in some medical procedures should be re-evaluated.

2SI.10

Lethality Caused by Small Particle Aerosols of H5N1 Influenza Virus in Cynomolgus Macaques Is Highly Dose Dependent. DOUGLAS REED, Katherine O'Malley, Mengying Xia, Morgan Midgett, Emily Olsen, Gwenddolen Kettenburg, Michelle Marti, Priscilla da Silva Castanha, Jacqueline Corry, Masaru Kanekiyo, Barney Graham, Simon Barratt-Boyes, *University of Pittsburgh*

We have previously demonstrated that exposure of cynomolgus macaques to aerosols containing high (106-107 pfu) doses of highly pathogenic H5N1 (A/Vietnam/1203/2004) avian influenza virus triggered a rapid acute respiratory distress that was lethal within 3-4 days. Fever and increased respiratory rate were noted within the first day of exposure and PET/CT imaging found evidence of an enormous inflammatory response in the lungs two days after exposure. There was a substantial depletion of the alveolar epithelium as well as elevated levels of inflammatory cytokines and chemokines in the blood and lungs. To evaluate whether the pathogenicity and lethality would be virus dose dependent, we performed a study exposing cynomolgus macaques to lower doses of H5N1. Even at the lowest dose tested, 102 pfu, macaques developed a fever response within 24 hours of infection. Substantial respiratory changes were only seen at the highest doses tested, 105 pfu. Four of the six macaques exposed at the dose in the 105 pfu range succumbed to the disease within 4-6 days. At lower doses, no macaque succumbed to infection. Surviving macaques had largely recovered by 7 days post-infection and were euthanized and necropsied at 14-15 days post-infection. Although tissues from survivors were negative for virus by plaque assay and there was no obvious gross pathology, both immunohistochemistry and PCR assays found evidence for residual viral infection in the lungs at study endpoint. In addition, all surviving macaques had anti-NP antibody at study endpoint. Analysis of these results as well as our prior data established an inhaled dose of 2.51 x 105 pfu as the LD50 for aerosolized H5N1 in the cynomolgus macaque model. This model will be useful for studying the underlying pathogenesis of lethal disease caused by H5N1 as well as evaluation of potential vaccines, prophylactics, or therapeutics.

2SI.11

Presence of SARS-CoV-2 Aerosol in Homes of COVID 19 Patients. GEDIMINAS MAINELIS, Robert Laumbach, Kathleen Black, Nirmala Thomas Myers, Pamela Ohman-Strickland, Shahnaz Alimokhtari-V, Adriana De Resende, Alicia Legard, Leonardo Calderón, Shirin Hastings, Howard Kippen, *Rutgers, The State University of New Jersey*

The ongoing COVID-19 pandemic, caused by coronavirus SARS-CoV-2, has already killed over 3 million people worldwide, with over 500,000 deaths in the U.S. alone, and the toll is still climbing. One key challenge is to reduce secondary attack rates among household contacts, which are estimated by the CDC to be as high as 50%. In addition to close interpersonal contact, emerging evidence suggests that airborne transmission is important for spreading SARS-CoV-2 infections in enclosed and/or poorly ventilated spaces, such as homes.

Here we provide the first assessment of the prevalence of airborne particles containing SARS-CoV-2 viral RNA in the homes of infected, self-isolating individuals. Subjects were recruited in fall/winter of 2020-2021 through an email flyer delivered at the time of notification of test positivity. Saliva screening at the time of the first visit verified continued positivity for all reported subjects. 24-hr air samples were collected in the isolation room (the primary room used by the subject) and the common room (an adjacent room) on PTFE filters (SKC Inc., Eighty Four, PA) using filter holders and Leland Legacy pumps (SKC Inc.) operated at 10 L/min. The samples were eluted from the filters by vortexing them 3x for 10 seconds in RNA grade water and then analyzed by RT-PCR for the presence of three SARS-CoV-2-specific genes. The study is ongoing, but so far, in air samples of nine homes out of fifteen, at least one gene was detected with Ct values < 37. The proportion of homes with detection for a particular gene ranged from 27% to 50%. Our results show that SARS-CoV-2 RNA is common in the home air of COVID-19 patients. Therefore, in addition to social distancing, hand hygiene, and face covering, mitigating airborne viral loads by other or additional means should be seriously considered to minimize disease transmission in homes.

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2SI.12

Disease Presentation is Dose-Dependent in a Nonhuman Primate Model of Inhalational COVID-19.

PAUL DABISCH, Katie Beck, Jennifer Biryukov, Jordan Bohannon, John Yeager, Brian Green, Jeremy Boydston,
BNBI / DHS NBACC

In order to understand the hazard posed by aerosols containing SARS-CoV-2, information on a number of parameters are needed, including the emission rate and size distribution of particles from an infected individual, the ability of infectious virus contained within those particles to survive in the air, and the infectivity following inhalation by a susceptible host. The aim of the present study was to assess the dose-dependence of infection for aerosolized SARS-CoV-2 in a nonhuman primate model of COVID-19. The results demonstrate that host response, specifically the presence of fever and seroconversion, is dose-dependent. The median dose for seroconversion was significantly lower than that for fever, suggesting that lower doses are able to induce an immune response without other overt signs of disease. A subset of animals that seroconverted without other signs of disease also shed virus in nasopharyngeal and oropharyngeal swabs, suggesting that these animals may also be able to spread disease. These data will be useful to inform disease transmission modeling related to COVID-19, and also reinforce the need for public health measures that minimize aerosol concentration and exposure dose, such as masking, distancing, and increased ventilation.

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All research was conducted in compliance with the Animal Welfare Act and other federal statutes and regulations relating to animals and experiments involving animals and adheres to principles stated in the Guide for the Care and Use of Laboratory Animals (National Research Council, 2011). The facility where this research was conducted is fully accredited by the Association for Assessment and Accreditation of Laboratory Animal Care International.

3AC.1

Airborne Microplastics in a Suburban Location in the Desert Southwest. KANCHANA CHANDRAKANTHAN, Pierre Herckes, *Arizona State University*

Microplastics are rapidly emerging anthropogenic stressors that pose a potential threat to ecosystems and human health. They are defined as plastic particles that are less than 5 mm in size. Microplastics are either intentionally manufactured at a microscopic size or result from the fragmentation of larger plastic litter. While the ubiquitous nature of microplastics in water has been well documented, studies on their distribution in the air are limited. Microplastics in suspended particulate matter in the atmosphere are important in assessing microplastic contamination within a breathing zone. Owing to their small size and low material density, microplastics can be easily inhaled and pose a potential threat on humans. Apart from the adverse effects caused due to the mere presence of microplastics, a concern arises from the additives used in plastic manufacturing and adsorbed hydrophobic organic pollutants such as Polycyclic Aromatic Hydrocarbons (PAHs). In addition to the concentration, it is important to understand the chemical composition of microplastics. Chemical characterization will yield information on the nature of the microplastics present and therefore provide an insight into their origin and toxicity.

Here we present results on the occurrence of microplastics in suspended particulate matter in a suburban location in the desert Southwest, and thereby aim to contribute to the limited existing knowledge of their occurrence in the air. Samples were collected, processed and microplastics were counted under an optical microscope to obtain quantitative information of their distribution in air. Microplastics were present in all collected suspended particulate samples ranging from 0.1 to 1.1 microplastics/m^3 with an average concentration of 0.5 microplastics/m^3. Micro-Raman spectroscopy was used to identify the chemical composition of microplastics in suspended particulate matter. Chemical characterization results revealed Polyvinyl Chloride (PVC) as the most abundant identified polymer.

3AC.2

Contribution of Organic Aerosol to PM2.5 in Bogotá, Colombia. KAREN BALLESTEROS, Ricardo Morales Betancourt, Amy P. Sullivan, *Universidad de los Andes*

Organic aerosol (OA) is one of the major components of fine atmospheric aerosol particles. Recent fields campaigns and simulations studies in Colombia have demonstrated a significant contribution of OA to urban and rural aerosols. In this work we focus on constraining the sources associated with OA and its precursors over the city of Bogotá, Colombia. We used PM$_{2.5}$ chemical speciation data from field campaigns carried out during 2018 to evaluate the ability of a regional transport model to reproduce and explain the observed OA. The samples were collected at three sites during high- and low aerosol concentration seasons in the region. We used The Weather Research and Forecasting Model coupled with Chemistry (WRF-Chem) with two different chemical mechanisms and aerosol schemes, RACM/MADE-VBS and MOZART/MOSAIC, in conjunction with the detailed in-situ observations of chemical PM$_{2.5}$ to analyze the seasonality of OA over in the city of Bogotá, and to establish the most relevant sources (local vs. regional) for this component. Simulations were carried out for the same periods were data is available, spanning a high biomass burning season (February 2018) and a low biomass burning season (September 2018). The temporal and spatial distribution of meteorological variables in are well captured by both model configurations. The two aerosol schemes utilized in this work reproduce the observed seasonal variations in aerosol concentration, with a difference between February and September of 10 µg/m^3. However, when MOZART was used, modeled PM2.5 was 30% higher than in the RACM experiment. Both schemes show that unspeciated PM2.5 and OA are the most prevalent aerosol in the city, in agreement with field observations. SOA concentration dominates the OA fraction by 66% for RACM-MADE-VBS and 74% for MOZART-MOSAIC during February and 69% for RACM-MADE-VBS and 71% for MOZART-MOSAIC during September consistently showing that MOZART-MOSAIC simulates more SOA than RACM-MADE-VBS. This differences between SOA within mechanisms may be attributed to MOZART-MOSAIC contains a simple SOA gas/particle partitioning scheme and has more biogenic specifies included.

3AC.4

Accelerated Chemical Reaction in Ultrafine Droplets: Effect of Droplet Size on Product Formation.

YAO ZHANG, Murray Johnston, *University of Delaware*

Reaction acceleration in ultrafine (<100 nm diameter) droplets is reported for the first time using droplet assisted ionization (DAI) to monitor product formation. Previous work has shown that DAI is an effective ionization technique to study the kinetics and mechanisms of reactions in droplets since it is able to decouple processes intrinsic to the droplet environment from those unique to the mass spectrometer ion source. The reaction of Girard's T (GT) reagent with carbonyls, which are abundant functional groups in secondary organic aerosol, is used as a model system. Reaction mechanisms are elucidated based on the droplet size dependence of product formation. Three types of experiments were performed: 1) size selected, dry GT particles reacting with pinonaldehyde vapor; 2) size selected droplets containing GT reacting with pinonaldehyde vapor; 3) Size selected droplets containing both GT and SOA from α-pinene ozonolysis. In the first experiment, the reaction occurs only at the air-particle interface. In the second and third experiments, the reaction occurs at both the interface and in the droplet volume, and the relative importance of the two changes with droplet size. For small droplets, the reaction occurs primarily at the interface. In this case, rapid product formation at the interface, followed by diffusion of the products into the droplet volume allows product formation to build up beyond what is possible by reaction in the droplet volume alone. The reaction occurs on the surface. Products formed at the interface can diffuse to the interior. This process continues until a droplet size-dependent equilibrium state is reached. When the droplet size increases, product formation eventually becomes independent of droplet size and is determined just by reaction in the volume. The accelerated reaction occurs because the free energy of binding of the reactants to the interface compensates for the increase in free energy of droplets compared to the bulk liquid. The mechanism of reaction acceleration was found to be similar no matter it is of a reaction between gas-phase and droplets (experiment 2) or a reaction in droplets (experiment 3). This work gives insight into how accelerated chemistry in droplets might influence the growth of atmospheric aerosol.

3AC.5

Influence of Structure and Functionality on Uptake of Semivolatile Organic Compounds to Surfaces.

GRAHAM FRAZIER, Gabriel Isaacman-VanWertz, John Morris, *Virginia Tech*

Mineral compounds, both on the ground and suspended as aerosols, present unique surfaces for deposition and chemical reactions of reactive organic gases. To date, the many of uptake studies have focused on inorganic species and oxidation studies. However, most organic carbon is emitted to the atmosphere as reduced carbon from a small subset of terpenoid compound classes. Many of these compounds are semivolatile, and even the more volatiles compound classes (e.g., monoterpenes) have been shown to reversibly partition to surfaces under typical ambient conditions. Small differences in the molecular structures of organic compounds can have substantial impacts on their physicochemical properties, so it is critical to understand the role of molecular structure on the uptake and surface chemistry of reactive organic compounds. We explore the influence of structure by measure surface uptake and interactions for a range of benzyl substituted compounds with systematically varied functionality, including aromatic monoterpenes. Uptake is measured on several compounds chosen to represent a selection of environmentally relevant surfaces by flowing sub-ppb concentrations through a flow tube with varied lengths of coated material. In addition, key interactions responsible for surface uptake were interrogated via transmission infrared spectroscopy. Together, these techniques provide new insights into the role of adsorbate electronegativity, molecular structure, and acid-base interactions on the uptake of organic compounds by environmentally relevant surfaces.

3AC.7

Kinetics and Products of Heterogeneous Hydroxyl Radical Oxidation of Isoprene Epoxydiol-Derived SOA.

JIN YAN, Yue Zhang, Yuzhi Chen, N. Cazimir Armstrong, Zhenfa Zhang, Avram Gold, Andrew Lambe, Barbara Turpin, Andrew Ault, Jason Surratt, *University of North Carolina at Chapel Hill*

In isoprene-rich regions, acid-catalyzed multiphase reactions of isoprene epoxydiols (IEPOX) with inorganic sulfate ($Sulf_{inorg}$) particles form secondary organic aerosol (IEPOX-SOA), extensively converting $Sulf_{inorg}$ to lower-volatility particulate organosulfates (OSs), including 2-methyltetrol sulfates (2-MTSs) and their dimers. Recently, we showed that heterogeneous hydroxyl radical (OH) oxidation of particulate 2-MTSs generated multifunctional OS products. However, atmospheric models assume that OS-rich IEPOX-SOA particles remain unreactive towards heterogeneous OH oxidation, and limited laboratory studies have been conducted to examine the heterogeneous OH oxidation kinetics of full IEPOX-SOA mixtures. Hence, this study investigated the kinetics and products resulting from heterogeneous OH oxidation of freshly-generated IEPOX-SOA in order to help derive model-ready parameterizations.

First, gas-phase IEPOX was reacted with acidic $Sulf_{inorg}$ particles under dark conditions in order to form fresh IEPOX-SOA particles. These particles were then subsequently aged at RH of 56% in an oxidation flow reactor at OH exposures ranging from 0~15 days of equivalent atmospheric exposure. Aged IEPOX-SOA particles were sampled by an online aerosol chemical speciation monitor (ACSM) and collected onto Teflon filters for off-line molecular-level chemical analyses by hydrophilic liquid interaction chromatography method interfaced to electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (HILIC/ESI-HR-QTOFMS). Our results show that heterogeneous OH oxidation only caused a 7% decay of IEPOX-SOA by 10 days exposure, likely owing to the inhibition of reactive uptake of OH as fresh IEPOX-SOA particles have an inorganic core-organic shell morphology. A significantly higher fraction of IEPOX-SOA (~37%) decayed by 15 days exposure, likely due to the increasing reactive uptake of OH as IEPOX-SOA become more liquid-like with aging. Freshly-generated IEPOX-SOA constituents exhibited varying degrees of aging with 2-MTS-dimers being the most reactive, followed by 2-MTSs and 2-methyltetrols (2-MTs), respectively. Notably, extensive amounts of previously characterized particle-phase products in ambient fine aerosols were detected in our laboratory-aged IEPOX-SOA samples.

3AC.8

Condensed Phase Reactions of Carboxynitrates with Alcohols to Form Esters: Measurements of Kinetics and Equilibria.

HANNAH MABEN, Paul Ziemann, *University of Colorado Boulder*

Organic aerosols decrease visibility and negatively impact human and environmental health. Secondary organic aerosol (SOA) is formed from the partitioning of the oxidation products of volatile organic compounds (VOCs) that are emitted into the atmosphere from biogenic or anthropogenic sources. These products can undergo particle-phase reactions, which impact the formation, composition, and chemical-physical properties of aerosols. While these reactions are known to occur in the atmosphere, models and data describing their kinetics and equilibria are sparse. To investigate one of these reactions, a synthesized probe compound was used to measure the kinetics and equilibria for the formation of an ester from the reaction of a C_{11} carboxynitrate with 1-octanol. The disappearance of the carboxynitrate and the formation of products was monitored using HPLC-UV, and product identity was confirmed using ESI-MS and ATR-FTIR. The probe compound was mixed with 1-octanol and the reaction was monitored over 24 hours to determine the rate and equilibrium constants. Then, to study the effects of an acid catalyst, the same experiment was conducted with added sulfuric acid, first diluted in acetonitrile to maintain a single organic phase and then in water for an organic/aqueous phase-separated reaction. The carboxynitrate did not react with 1-octanol in a single organic phase reaction, but ester formation was observed when sulfuric acid was added both in a single organic phase and in a phase-separated reaction. Based on the results, the forward and reverse rate constants and equilibrium constant were determined. These results provide useful insights into the types of oligomerization reactions that are likely to occur in atmospheric aerosols, and rate and equilibrium constants that can be added to models to better predict transformations of SOA in the atmosphere.

3AC.9

Multiphase Heterogeneous OH Oxidation of a Long Chain Alkyl Sulfate. SZE IN MADELEINE NG, Rongshuang Xu, Man Nin Chan, *The Chinese University of Hong Kong*

Atmospheric organosulfur species are ubiquitous in aerosols. Among these species, organosulfates are one of the major classes. A large variety of alkyl sulfates has been found but their sources and transformation pathways are poorly understood. We carried out an laboratory experiments on the heterogeneous OH oxidation of sodium dodecyl sulfate (SDS) aerosol, which investigates how this long chain alkyl sulfate chemically transformation in the atmosphere by identifying the reaction products before and after oxidation using an aerosol flow tube coupled with an atmospheric pressure soft ionization source (Direct analysis in Real Time, DART) and a high resolution mass spectrometer. From aerosol-DART spectra, we found that SDS decays at a faster rate (an effective OH rate constant of 2.65×10^{-12} cm^3 $molecule^{-1}$ s^{-1}) than that of smaller alkyl sulfates (e.g. methyl- and ethyl sulfate). Product analysis show that a number of more oxygenated functionalization products were formed upon oxidation. Inorganic sulfate was also formed, but with a lower abundance. We postulate that the small sulfate yield might attribute to the longer carbon chain and the morphology of SDS near the aerosol surface, which may unfavor fragmentation processes and the generation of sulfate radicals upon oxidation. This limits the formation of inorganic sulfate via sulfate radical chemistry. The results of this work provide greater insights into the heterogeneous OH chemistry of organosulfates and their atmospheric fates.

3AC.10

Chemical Characterization of Stratospheric Particles with the Next Generation of Airborne Laser Mass Spectrometer: PALMS-NG. JUSTIN JACQUOT, Xiaoli Shen, Kyra Slovacek, Gregory Schill, Michael Lawler, David Thomson, Karl Froyd, Daniel Murphy, Daniel Cziczo, *Purdue University*

The Particle Analysis by Laser Mass Spectrometry - Next Generation (PALMS-NG) instrument has been designed and tested for use on NASA’s ER-2, a stratospheric research aircraft, to characterize in-situ the chemical composition of particles. The strong convective storms that generally occur during the summertime over North America carry out particles from the troposphere to the stratosphere. The NASA DCOTSS research project aims to get a better understanding of the chemistry and composition of the stratosphere seeded with water and pollutants originally from the troposphere.

PALMS-NG is an evolution of the existing laboratory and aircraft PALMS instruments. The main new feature consists of a bipolar time-of-flight mass spectrometer, which has a dual S shape and is named sTOF. In addition, optical improvements have led to a higher detection efficiency and larger size range of measurable particles than the original instruments. It can detect particles below 150 nm and up to several micrometers in diameter. PALMS-NG can be decomposed in two distinct parts: (1) particle detection and size estimation and (2) chemical analysis. A particle enters the instrument under vacuum through a multiple stage inlet tube to allow control of particle speed while maximizing particle transmission. First, two 405nm continuous laser beams enable an estimate of the particle size from the scattering signal analysis. Second, a 193 nm ultraviolet (UV) pulsed laser ionizes the particle. PALMS-NG bi-polar mass spectrometer has two high voltage electrodes - one positive and one negative - that separate and extract the positive and negative ions resulting from the UV pulse hit. The ions enter the sTOF mass spectrometers and ultimately impact microchannel detection plates located at each side of the instrument. The measured time-of-flight of the ions gives a mass spectrum for the identification of the chemical components that composed the detected particle.

3AC.11

Characterization of Hydroxymethanesulfonate (HMS) and Sulfate in Fairbanks, Alaska using Ion Chromatography (IC).

KAYANE DINGILIAN, Michael Battaglia, James Campbell, Jingqiu Mao, Rodney J. Weber, *Georgia Institute of Technology*

Sulfate comprises a significant portion of atmospheric particulate matter (PM 2.5), but its chemistry is still not understood well under extremely cold temperatures and low oxidant concentrations. These conditions are prevalent in the winter in Fairbanks, Alaska, where several campaigns to understand the severe air pollution in the area are underway. Recent experiments in the laboratory have suggested that much of the sulfate being measured is, under certain conditions, actually hydroxymethanesulfonate (HMS), which is formed from the reaction of dissolved species of sulfite and formaldehyde. Analysis with ion chromatography (IC) is evolving to assess the relative importance of HMS and sulfate, both in sample collection and sample preparation. In our work, we perform experiments on samples taken from both premade standards containing sulfur compounds as well as real data from filters to develop methods for the accurate quantification of HMS vs. sulfate as well as identify any loss of HMS due to conversion to sulfate during sample preparation. These methods will also be integrated into the upcoming Alaskan Layered Pollution and Chemical Analysis (ALPACA) research initiative taking place in Fairbanks, Alaska, where we will be deploying not only filters but a continuous particle-into-liquid sampler (PILS) system coupled to IC. We hope to use this data to gain a better understanding of low-temperature atmospheric sulfur chemistry as well as improve current atmospheric models to better reflect real mechanisms and phenomena.

3AC.12

Secondary Organic Aerosol Formation from Photooxidation of Acyclic Terpenes in an Oxidation Flow Reactor.

SHAN GU, Farzaneh Khalaj, Véronique Perraud, Celia Faiola, *University of California, Irvine*

One challenge in predicting secondary organic aerosol (SOA) formation is an incomplete representation of biogenic volatile organic compounds (BVOCs) emitted by plants, particularly those that are emitted in response to plant stressors. Plant emissions of acyclic monoterpenes, such as β-ocimene and β-myrcene, and acyclic sesquiterpenes, such as α-farnesene, are commonly induced or present at elevated concentrations under stress conditions (e.g. water, ozone, and herbivores stress) – conditions that are becoming more frequent in a rapidly changing climate. In this study, we investigated SOA formation from the photooxidation of acyclic terpene standards in an oxidation flow reactor (OFR). VOC concentrations were measured at the OFR inlet and outlet by sampling the air stream onto multi-bed adsorbent cartridges composed of Tenax TA and Carbopack. The cartridges were analyzed offline with a thermo-desorption gas chromatograph mass spectrometer (TD-GC-MS). At the outlet of the OFR, continuous monitoring of ozone, particle size distributions, and particle bulk composition was conducted using an ozone monitor, custom-built scanning mobility particle sizer (SMPS), and time-of-flight aerosol chemical speciation monitor (TOF-ACSM), respectively. SOA particles were also collected on Teflon filters and analyzed offline for detailed SOA chemical composition using an ultra high performance liquid chromatography system equipped with a heated electrospray ionization source and a high resolution Q Exactive Plus orbitrap mass analyzer (UPLC-HESI-HRMS). SOA chemical composition and mass yields will be compared across acyclic terpene systems, and will also be compared to the more typically studied, α-pinene SOA system.

3AP.1

Possible, Impossible and Expected Diameters and Flow Rates in Droplet Aerosols.

MAKSIM MEZHERICHER, Howard A. Stone, *Princeton University*

In our recent work we demonstrated a novel liquid atomization technique producing aerosols of submicron-diameter droplets for pure solvents, suspensions, and solutions. Our aerosol generation process is based on disintegration by gas jets of thin liquid films formed as bubbles on a liquid surface. For this system and, in general, for any other aerosol generation system, one of the arising questions is how to theoretically predict possible, impossible and expected droplet diameters and flow rates which the system will produce at different regimes. And another question is how to compare our aerosol generation method with other techniques, and in general how to compare between different aerosol production methods.

In this work we show that the diameters and flow rates of the produced droplets are governed by the interplay of process timescales including capillary breakup, liquid viscosity, and gas jet pressure.

Timescale ratios can be converted into the ratios of specific energies and into the ratios of specific energy rates provided by the gas jets and dissipated by the atomized liquid. Using those ratios, we developed a new theoretical approach to determine an upper limit of droplet diameters and flow rates in droplet aerosol generation and introduce atomization diagrams. The theoretically predicted and measured droplet diameters and droplet flow rates for various liquids (water, gasoline, diesel) were a good agreement for our aerosols of submicron-diameter droplets.

Using the developed theoretical analysis to compare between our droplet generation method with conventional pressure nozzle, we demonstrate that our approach can also serve as a theoretical framework for comparison between different aerosol and spray production techniques.

3AP.2

Process Level Modeling of Vertically Resolved New-particle Formation at the Southern Great Plains Observatory.

O'DONNELL SAMUEL, James Smith, Ali Akherati, John Shilling, Fan Mei, Hubbe John, Stephen Springston, Joel A. Thornton, Siegfried Schobesberger, Emma D'Ambro, Ben H. Lee, Charles Long, Chongai Kuang, Jerome Fast, Anna Hodshire, Charles He, Michael J. Lawler, Jeffrey R. Pierce, Shantanu Jathar, *Colorado State University*

New particle formation (NPF) is a significant source of cloud condensation nuclei and aerosol number concentrations in the atmosphere. Many studies investigate NPF at the surface, but fewer studies examine the vertical profile of NPF across the boundary-layer mixed layer (ML) and residual layer (RL). The upper ML and RL can have favorable conditions for NPF, such as low condensation/coagulation sinks, low temperatures, high relative humidity, rapid photochemistry, and elevated concentrations of precursor species.

To investigate the driving processes and vertical profile of NPF, we used a model of the boundary-layer column along with aircraft- and ground-based observations from the two Holistic Interactions of Shallow Clouds, Aerosols, and Land Ecosystems (HI-SCALE) campaign deployments in 2016 at the Atmospheric Radiation Measurement, Southern Great Plains observatory. During HI-SCALE, 8 sustained NPF events were observed at the ground, 2 of which were observed by the aircraft as starting near the top of the boundary-layer prior to being observed by surface instruments. The SOM-TOMAS column model simulates gas-phase oxidation reactions, thermodynamics, gas-particle partitioning, aerosol microphysics, vertical mixing, and nucleation using two state-of-the-art organic and inorganic nucleation schemes.

The model is able to predict the occurrence of nucleation and generally can predict the subsequent aerosol mass and number concentrations. Additionally, for several of the modeled nucleation events during HI-SCALE, vertical mixing of freshly nucleated particles from the upper ML or RL (where precursor concentrations were elevated) to the surface model layer was necessary to explain the observed aerosol size distribution at the surface. Finally, we find that the vertical profiles of temperature and precursor concentrations as well as the dynamic evolution of the ML with time can explain much of the vertical profile of nucleation in the model.

3AP.3

A Machine Learning Based Aerosol Dynamics Model for Log-Normal Aerosols.

ONOCHIE OKONKWO, Rahul Patel, Ravindra Gudi, Pratim Biswas, *University of Miami*

Aerosol reactors play a crucial role in industrial-scale synthesis of advanced ceramics powders and commodity particles including carbon blacks and titania. The product properties – which include light scattering, and photo-catalytic properties for titania – depend on the aerosol product characteristics such as particle size, size distribution, morphology, and crystal phase. These characteristics are determined by various aerosol dynamics phenomena, including, reaction, nucleation, condensation, sintering, coagulation, and charging occurring in the reactor systems. For optimal design and control of aerosol reactors, an understanding of the evolution of particulate systems which accounts for the dynamics phenomena is required. The aerosol dynamics phenomena are described by the general dynamics equation (GDE). The GDE is a non-linear partial integro-differential equation which, therefore, requires the development of efficient numerical solution methods. The complexity and computational burden associated with solving the GDE lies in the coagulation term [1].

Artificial neural networks (ANN) have been shown to accurately describe highly complex phenomena in a computationally efficient manner [2]. This presentation shows the first step in the development of an accurate and highly computationally efficient solution method for the GDE using a simplified coagulation term based on ANN. The ANN model, which is trained by the particle size distribution obtained from the log-normal moment model solution at the coagulation time, is used to evaluate a proxy coagulation kernel. Using the proposed ANN solution approach, simulations are done for three scenarios 1) pure coagulation; 2) nucleation, condensation, coagulation; and 3) nucleation, sintering and coagulation. The results from the proposed model are compared with the moment model, bi-modal model and experimental results from previous works to demonstrate its accuracy and superior computational performance.

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3AP.4

Multiple Wavelength Digital Holography for Color Micro-particle Imaging.

RAMESH GIRI, Gorden Videen, Matthew J 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 different material compositions can be differentiated.

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3AP.5

Design of a Multi-Angle Light Scattering Setup Covering the Whole Scattering Angle Range (0.32° to 177.6°) and Interpretation of Light Scattering Data Under Q-Space Analysis.

PRAKASH GAUTAM, Justin Maughan, Christopher Sorensen, *Kansas State University*

We designed and built a laboratory light scattering apparatus for aerosols based on a novel optical scheme covering the scattering angle range 0.32º ≤ θ ≤ 177.6º, an extreme forward to the backscattering regime, involving 46 angles. The apparatus allows for a quick and efficient procurement of data, ensuring the elimination of the effects of possible in-homogenous of the aerosols. The experimentally observed scattered intensity is plotted in terms of scattering wave vector q on a double logarithmic scale, i.e., Q-space analysis, in addition to the conventional linear plot versus θ. Scattering data for hematite (Fe2O3) aggregates and molybdenum disulfide (MoS2) particles, both having large real and imaginary part of the refractive index, were plotted under Q-space analysis that uncovered an extended Guinier regime with two Guinier crossovers for hematite and a single regime for MoS2 particles, consistent with the microscopic pictures. The hematite showed an anomalous enhanced backscattering [1, 2]. In addition, scattering data we will be presented for irregularly shaped Al2O3 abrasive and Arizona road dust particles for whole scattering angle range with an emphasis on the backscattering regime.

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3AP.6

Morphological Characterization and Classification of Aerosol Aggregates through Multispectral Light Scattering Simulations.

STEPHEN HOLLER, Jaeda Mendoza, Emily Shipley, Sequoyah Waters, Kevin Aptowicz, *Fordham University*

Light scattering from non-spherical particles and aggregates produces complex speckle patterns that result from interference among the constituent particles. Experimental results have indicated that information contained within the two-dimensional speckle pattern is related to morphological characteristics of the aerosol, which can be used for the classification of the particles. We performed a series of multispectral light scattering simulations to control for the aggregate parameters to better understand the influence of the morphological characteristics on the speckle pattern and how those same descriptors could be employed to classify the particles. This talk will focus on the descriptors and their relation to the simulated aggregates and how one may use the multispectral information for classifying various particle types, including those of biological origin.

3AP.7

Super-droplet Method to Simulate Lagrangian Microphysics of Fallout Particles.

DANA MCGUFFIN, Donald Lucas, Joe Morris, Kim Knight, *Lawrence Livermore National Laboratory*

Nuclear detonations produce hot clouds that quickly cool and rise, forming dangerous ultrafine to coarse aerosol (fallout) that can potentially disperse over long distances and deposit. Therefore, the ability to predict aerosol size, chemical components, and location is necessary to inform public officials and determine guidance for the public. Quickly predicting these quantities is vital to protecting the public in these scenarios, so this work presents a computationally efficient way to model particle microphysics in a hot, turbulent cloud.

The super-droplet method (SDM) is an efficient way to model cloud microphysics without losing accuracy. SDM represents the particle size distribution by sampling it with a set of computational particles called “super-droplets”. Each super-droplet represents several real particles, and its size is adjusted as condensation and coagulation evolve. In the Lagrangian framework, each super-droplet acts as a computational particle with aerosol-specific attributes (size, composition, shape) in addition to the typical Lagrangian attributes of particle position, velocity, and mass.

Previously, SDM has been developed and applied to ice nucleation and cloud microphysics simulating precipitation. In this talk, we present the preliminary results of particle nucleation and growth in a hot cloud that represents a homogeneous cooling fireball. We apply SDM to evolve fallout microphysics in a zero-dimensional model, with plans to incorporate SDM into high-resolution large eddy simulations. The simulated processes include homogeneous nucleation, condensation, and coagulation.

Between 1945 and 1970, about two hundred atmospheric nuclear tests were performed by the United States. Several of these tests were airbursts that did not interact with the ground, which are ideal to validate the SDM model. We compare size distributions for airburst nuclear tests from the SDM simulation, previous theoretical calculations, and field measurements taken during the tests.

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3AP.9

Sintering of Lignin-based Particles During Fast Pyrolysis: A Kinetic Study Using Furnace Aerosol Reactor And Tandem Differential Mobility Analysis.

SUJIT MODI, Onochie Okonkwo, Pratim Biswas, *Washington University in St. Louis*

A major operational challenge of industrial large-scale utilization of lignin through fast pyrolysis is the plugging of the reactors [1]. This is due to the growth of lignin-based particles by sintering that leads to the formation of oversized agglomerates and subsequent plugging. The growth of particles is also the basis for imprecise control of size and decrease in the specific surface area of particles [2]. Presently, there is a dearth of knowledge about the sintering phenomenon in lignin-based particles. Using the approach described previously by Cho and Biswas [3], the present study investigates the sintering kinetics of lignin-based particles. Briefly, experiments are carried out in FuAR followed by characterization of size and morphology using tandem differential mobility analyzer and SEM, respectively. Further, the effect of techniques used for preventing lignin sintering: thermal stabilization and lignin pretreatment with calcium and magnesium hydroxide is investigated using the same approach. Additional compositional analysis using FTIR and XPS will help to understand the underlying mechanism for inhibition of sintering. The overall results presented will provide novel insights to lignin sintering which will help in optimization of existing and development of new methods to effectively deal with the agglomeration.

Keywords: Sintering, reactor plugging, furnace aerosol reactor, tandem differential mobility analysis

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3AP.10

Prediction of Ion Mobility at High E/n Using the Two-Temperature Theory to Maximize Selectivity. VIRAJ GANDHI, Carlos Larriba-Andaluz, *IUPUI*

The ability to separate ions in the gas phase using electrical mobility has become ubiquitous in the field of aerosol science. In particular, when coupled to a Mass Spectrometer (MS), a mobility analyzer can give information of mass over charge and shape of the molecules. One of the shortcomings of mobility is its low resolution which many times is insufficient to separate similar molecules. To overcome this problem, higher fields may be used to provide non-linear correlations that may allow to separate ions which would be otherwise non-separable at low fields. Here we use experimental results at high fields together with theory and numerical calculations to show that the mobility of non-spherical ions may be calculated quite accurately even at high fields. The two-temperature theory at the fourth order approximation is used to estimate the mobility from all-atom models showing errors of less than 3% with respect to experiments over the whole field range. This is the first time that these calculations have been attempted with this degree of accuracy. Moreover, by mixing different field strengths with different temperatures and gases, the mobility of an ion may be tailored. The effect of these parameters may be greatly enhanced by potential interactions, especially at low temperatures, making the method extremely unique and possibly a candidate for much higher mobility separation than exists at this time.

3AP.11

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 an environmentally friendly way to remove heavier alkanes from natural gas. Understanding the non-equilibrium vapor-liquid phase transitions of n-alkanes is therefore essential to the development of these devices. Homogeneous nucleation rates have been measured in supersonic Laval nozzles for n-alkanes down to n-pentane, and, thus, n-butane and propane are the next logical candidates from both the experimental and theoretical points of view. A second goal of our research is to determine the critical cluster sizes from isothermal nucleation rate measurements. Working with these short-chain alkanes should then let us compare our nucleation results to those determined via direct mass spectrometric sampling in post-nozzle flows carried out at ETH Zürich. In particular, we can follow the nucleation process as it changes from one controlled by a free energy barrier to the barrier-free, collisional limit. All experiments use argon as the carrier gas. Pressure Trace Measurements (PTMs) provide estimates of 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. Classical Nucleation Theory (CNT) fails to describe the particle formation process under our conditions because of its incorrect description of the smallest clusters. The determination of experimental nucleation rates requires the combination of PTMs results and number densities measured by Small Angle X-ray Scattering (SAXS) experiments. Correlation functions between number densities and initial partial pressure of n-pentane and n-hexane were used to estimate the number densities of propane and n-butane. Further SAXS experiments will be conducted once the Advanced Photon Source is again available for outside researchers.

3AP.12

Investigations on Air Ion Properties and Their Connections to Atmospheric Radioactivity and Electricity.

XUEMENG CHEN, Heikki Junninen, Jussi Paatero, Susana Barbosa, Joonas Vanhanen, Tuukka Petäjä, Veli-Matti Kerminen, Markku Kulmala, Carlos Larriba-Andaluz, *University of Tartu / IUPUI*

Air ions refer to airborne charge carriers present in air. These range from small molecules (<1nm) to clusters (1-3nm) to nanoparticles (>3nm). Their production is closely related to ionization processes caused by atmospheric radioactivity, including radon, cosmic and terrestrial radiation[1]. Air ions are a fundamental player in atmospheric electricity. Being the charge carriers, air ions respond to the Earth-atmosphere electric field by drifting towards different directions depending on their polarities. Air ions (in particular molecules and clusters) are also observed frequently taking part in atmospheric new particle formation (NPF)[2-3], through which they modify atmospheric aerosol properties. Atmospheric aerosol particles can impact air quality, weather and climate. Via cloud processes and space charge formation, aerosol particles can also interact with atmospheric electricity and radioactivity[4-5]. Moreover, many aerosol measurement techniques are based on pre-charging of sampled particles. Therefore, it is crucial to have a thorough knowledge of ion properties to link all these disciplines. The connections of air ions to atmospheric electricity and radioactivity will be presented based on ambient measurements conducted in Finland and Estonia. We will also introduce a new Marie-Curie project —MaSMob-Lion, where we investigate the mass-size-mobility relationship of ions aiming to facilitate a smooth interconversion of the three properties to assist intercomparisons of ions and aerosol particles measured by different techniques.

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3IA.2

Successfully Lowering Exposure to Air Pollutants in Public Transport.

BORIS GALVIS, Ricardo Morales Betancourt, Daniela Mendez, Yadert Contreras Barbosa, Alejandra Montejo-Barato, Diego Roberto Rojas-Neisa, *Universidad de La Salle*

Commuters are often exposed to higher concentrations of air pollutants than those reported by urban monitoring sites. Despite the recent transformation of urban transport towards zero or low-tailpipe emission alternatives, the assessment of these transformations over commuter exposure are limited by the paucity of such studies. In this work, we use a unique data-set of personal exposure to traffic related air pollutants (TRAP), collected over the span of 5 years to assess changes due to the new the fleet of Bogota's Bus Rapid Transit System. The renewal process started in 2019 and up until 2020 replaced 1440 Euro-II and III diesel-powered buses with a mix of Euro-VI compressed natural gas (CNG) and DPF-equipped Euro-V diesel buses. We measured the change in personal exposure to Black Carbon, PM2.5 and ultra fine particles before, during, and after the retirement of the old buses and the introduction of the new ones. We used data collected by the researchers during 2015 and 2017, and new measurements performed over two campaigns between 2019 and 2020. Significant drops in the concentrations of PM2.5 and BC were observed during the 2019 campaign, with a mean 50% decrease for PM2.5(176 to 92ug m^{-3}) and BC (90 to 45ug m^{-3}). Further reductions were observed during the 2020 measurement campaign, even after accounting for effects of the COVID-19 pandemic related mobility restrictions. Nevertheless we found that commuters were exposed to higher concentrations inside the stations and buses and in the central and southern areas of the city and even more if they are inside vehicles with more than 682 $x10^3$ vehicle kilometers traveled. This evidence of positive effects of urban transport interventions can be used as input for decision-makers to put forward policies aimed at improving the quality of life of city commuters related to air pollution.

3IA.3

Assessment of PM2.5 Concentration and Transport in Indoor Environments Using Low-Cost Sensors.

SUMIT SANKHYAN, Julia Witteman, Steven Coyan, Sameer Patel, Marina Vance, *University of Colorado Boulder*

Fine particulate matter ($PM_{2.5}$) 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 (OPS 3330, TSI Inc.) by deploying them in four 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 $PM_{2.5}$ levels. A range of home activity sensors (Samsung SmartThings) was also deployed to detect the opening of doors and windows as well as the operation of the air purifier. Preliminary results show a range of correlation levels between low-cost monitors and the OPS, with R^2 values ranging from 0.75 to 0.94, and among pairs of the same low-cost monitor models, with R^2 values between 0.60 and 0.99.

3IA.4

Estimation of PM2.5 Exfiltration Factor from Biomass Cooking.

Jyoti Jyotsana, Gupta Anurag, CHIMURKAR NAVINYA, Harish C Phuleria, *Indian Institute of Technology Bombay*

The Particulate matter (PM) emissions from the biomass burning is known to adversely affect human health as well as climate. Most climate models and national/regional emission inventories assume complete exfiltration of the emitted PM from the indoor spaces, however in real scenario exfiltration depends on the type of biomass fuel used, stove types and kitchen ventilation. In this study, we examine the exfiltration factor for $PM_{2.5}$ from different biomass fuels used for cooking in households. As part of the NCAP-COALESCE project (https://ncapcoalesce.iitb.ac.in/) field surveys were conducted across rural India for obtaining the biomass fuel usages, kitchen and homes characteristics. The simulated cooking experiments are conducted in the laboratory condition (mock kitchen) as well as in resident indoor kitchens using different biomass inside IIT Bombay campus in Mumbai, India. The real time concentration of pollutants before, during and after the cooking event are measured using portable gas and PM analysers. Exfiltration factor is determined based on the difference in decay slope estimated by using mass balance for various fuel-device combinations. The field survey data revealed 79% households in four districts in Western rural India (out of 588 total households surveyed) cook indoors. As a result of different government schemes such as “PMUY” and “Give It Up” campaign in 2016, the biomass fuel use had dropped but 30% still use traditional stove (TS) for primary cooking while 37% use it for secondary cooking in Western India. We find that $PM_{2.5}$ during cooking is 28 times higher than the background concentration (65 ± 16 ug/m^3) while CO exceeds 6 times the background levels (1 ± 0.04 ppm). $PM_{2.5}$ exfiltration factor for mock kitchen using firewood, dung cake and crop residue fuels is 73 ± 16 %, 60 ± 8 % and 49 ± 27 %, respectively. $PM_{2.5}$ exfiltration for the actual residential homes is 45 ± 23 % and 35 ± 16% for traditional and improved stoves, respectively. Thus, range of exfiltration vary with different fuel-stove combinations. Subject to conducive conditions for field measurements, the exfiltration factor will be estimated in rural households in Maharashtra and Gujarat as well.

3IA.5

Nerves Impact Following Short-Term Exposure to Cooking Ultrafine Particles. Motahareh Naseri, MEHDI AMOUEI TORKMAHALLEH, Mojtaba Jozizadeh, Sahar Sadeghi, Reza Khanbabaie, Flemming Cassee, *Nazarbayev University, Nur-Sultan, Kazakhstan*

This abstract summarizes a controlled clinical study investigating the impact of cooking (frying chicken and fries) ultrafine particles using a gas stove on the human brain and alzheimer biomarkers. At least thirty healthy volunteers over 25 years old are currently being recruited for this study. The experiments is presently being conducted in two consecutive days in a fully furnished apartment. The first day is a control day when no cooking is conducted and the second day is the exposure day when cooking is performed. The study participant will stay in the experimental apartment for the whole 2 days including control and exposure experiments. Each volunteer is experienced the first day as a control experiment (without cooking) and the second day as an exposure experiment (with cooking). An Electroencephalograph (QEEG) is used to measure the brain wave pattern. Volunteers enter the apartment at 8:00 am. The brain EEG is measured in 21 steps starting one h after arrival (9 am) and ending 49 hours after the arrival. The cooking is conducted 25 and half hours after arrival (at 9:30 am the second day) for 20 minutes. Interleukin-6 (IL-6) as an Inflammatory marker, beta-amyloid, and alpha-synuclein were measured in plasma or serum in five steps (one h after arrival (9 am), 2 hours after arrival (10:00 am), 25 hours after arrival (9:00 am), 26 hours after arrival (10:00 am) and 49 hours after arrival (09:00 am)). So far we examined 10 volunteers and we continue the measurements until at least 30 volunteers are studied. The results will be presented at the upcoming AAAR conference.

Keywords: Electroencephalography, Inflammatory markers, blood biomarkers.

3IA.6

Kitchen Area and Personal Exposure Measurements of Carbon Monoxide and Particulate Matter in Rural and Urban Malawi. STEPHANIE PARSONS, Joseph Pedit, Andrew Grieshop, Pamela Jagger, *North Carolina State University*

Almost 4 million deaths annually are attributable to household air pollution (HAP) from using traditional biomass (wood, dung, crop residues) fuels, which are prominent in sub–Saharan Africa (SSA). However, HAP observations collected in SSA are sparse, particularly those comparing urban and rural exposures. The Malawi Forest and Livelihoods Household Survey, conducted in 2002, 2006, and 2009, focused on use of forest resources. Here, we present data from follow-up studies conducted in 2013 and 2014 that measured fuel use and exposures for different cooking technologies. We collected kitchen and personal exposure measurements of carbon monoxide (CO) and particulate matter ($PM_{2.5}$) in 2013 in 100 households in two rural districts. In 2014, data was collected in 148 households in urban Lilongwe. CO and $PM_{2.5}$ monitors in cooking areas provided kitchen concentrations while monitors were simultaneously worn for 24-hour exposure measurements. Personal exposure was driven by contrasts in fuel use: 99% of rural cooks primarily used biomass and had 2.5 times higher 24-hour average $PM_{2.5}$ exposure (433 +/- 484$\mu g\ m^{-3}$) than urban cooks (172 +/- 164$\mu g\ m^{-3}$), while 82% of urban cooks used charcoal primarily and had CO exposures (7.1 +/- 7.0ppm) almost three times greater than rural cooks (2.7 +/- 2.0ppm). Cooks with separate kitchens had double the $PM_{2.5}$ exposure of those cooking in their primary dwelling or outdoors. Cooks using half-walled kitchens had CO and $PM_{2.5}$ exposures 50% and 42% higher than cooks using enclosed kitchens. We observe poor correlations between kitchen and personal CO and $PM_{2.5}$ averages in both settings. CO diurnal trends were similar between settings, peaking at mealtimes; however, urban cook nighttime peaks doubled those of rural cooks. This study contributes to the sparse data on HAP exposures in SSA and demonstrates the influence of fuel and household characteristics on exposure.

3IA.7

Insights into the Strategies of Reducing the Aerosol Particle Concentration in Indoor Environments Using Mobile Air Purifiers - Experimental and Numerical Analyzes.

ADRIAN TOBISCH, Lukas Springsklee, Lisa-Franziska Schaefer, Nico Sussmann, Martin Lehmann, Raoul Zoellner, Jennifer Niessner, *Heilbronn University of Applied Sciences*

Aerosols are generally recognized as one of the main routes of transmission of COVID-19. In order to reduce the risk of infection indoors, mobile air purifiers are used. We focus on the effects of a filtrating air purifier. Specifically, we report results of ongoing work applying a sensor network of 12 sensors (PM 1) measuring and simulating particle concentration at head height and taking thermal effects into account.

In an auditorium, simple-made setup of “thermal dummies” were placed at some seats to simulate the effect of persons being in the room. In this work, we investigate the transport of aerosol particles from a dummy equipped with an aerosol generator (“infected dummy”) to receiving thermal dummies. Experimental and numerical methods are used to investigate how the risk of infection suggested by the particle concentration in an exemplary lecture hall can be reduced by a clever choice of the location and orientation of the air purifier. For analyses, we use optical particle counters and a sensor network to monitor the particle concentration and particle size spectrum with high spatial resolution. A computational fluid dynamics (CFD) model is set up and validated based on the measurement data.

At the recommended air exchange rate of 5.1 /h, the cumulated PM 1 mass at head level was reduced by 75 %, independently of the location of the infected dummy, compared to the “no air purifier” case. It turns out that a corner installation of the air purifier with a blow out against the wall may be particularly advantageous. In this best case, the particle mass at head height throughout the lecture hall was reduced by approximately 13 % points more than compared to the worst case location and orientation. We will discuss further results of spatially resolved particle measurements and simulations.

3IA.8

Effect of Low-Cost Air Purification on Aerosol Dispersion and Droplet Deposition in a Conference Room.

LINHAO LI, Stephanie Eilts, Zachary Pope, Meng Kong, Clay Maranville, John Jaranson, John Elson, Rainer Vogt, Christopher J. Hogan, *Well Living Lab*

Respiratory particles and droplets exhaled when an infected individual coughs, sneezes, or speaks, as well as during normal breathing, can result in indoor virus transmission. A portable air purification unit can reduce virus transmission risk by decreasing the overall aerosol concentration in a room by filtering and recirculating the air that passes through the unit. This is important in rooms with poorer ventilation and an inability to be ventilated with adequate amounts of fresh outdoor air. The whole-room and localized impact of portable air purification on aerosol dispersion and deposition has not been well studied. We conducted a series of experiments in a simulated conference room (6.04m × 2.31m × 2.6m) assessing the particle removal rate and deposition change owing to the presence of a low-cost portable air purifier comprised of a Lasko Model 3733 box fan and TriDim MERV 13 filter placed within a custom-built cardboard frame. A breathing simulator manikin was developed to provide physiologically correct inhalation and exhalation, with the manikin itself being anatomically correct. During operation, this breathing simulator ejected fluorescein-tagged particles in the 1-3 um size range. We measured deposition flux on upward- and downward-facing horizontal surfaces throughout the room and discerned aerosol mass concentration using impingers. The collected data enabled us to calculate surface-specific deposition velocity using deposition flux mass concentration measurements. Aerosol size distributions within the room were also quantified using a TSI 3330 Optical Particle Sizer. Two conditions were investigated: (1) Normal HVAC operation (44 CFM supply; Baseline), and (2) Normal HVAC operation + low-cost air purifier with filter. Results suggested this low-cost air purifier increased effective air exchange rate by 3.3x over baseline (15.6 vs. 4.7 h-1), but also introduced greater deposition to surfaces near the breathing simulator manikin versus baseline.

3IA.9

Using a High-Flow Extractor to Reduce Aerosol Exposure in Medical Environments. BOWEN DU, Tianyuan Li, Clyde Matava, Vincent Collard, Simon Denning, John Fiadjoe, Pierre Fiset, Thomas Engelhardt, Jeffrey Siegel, *University of Toronto*

The transmission modes of the severe acute respiratory syndrome SARS-CoV-2 include droplets and droplet nuclei (aerosols). Thus, aerosol-generating procedures, in addition to normal breathing, coughing, and sneezing of patients, pose an elevated infection risk to healthcare workers especially in confined spaces such as operating rooms and dental operatories. Some clinicians are using transparent plastic barriers to reduce aerosol spread, but these barriers may limit access to the patient and mobility of the clinician and may offer limited protection depending on room airflow patterns. As an alternative, this work proposed using high-flow extractors which combines local suction and high-efficiency filtration to capture and remove aerosols generated by patients and medical procedures. Using a test dust (1 – 20 µm) in a coughing mannequin and emissions from an essential oil diffuser (0.01 – 1 µm) to simulate abrupt coughing aerosols and continuous breathing aerosol, respectively, we carried out experimental investigation of the particulate matter removal efficiency of a portable high-flow air extractor with an exhaust rate of up to 235 L/s. A wide range of aerosol equipment was used to characterize size distributions and spatial variation in concentrations. We found approximately 76% and 97% reductions in PM_1 concentration near the source and at the clinician's head, respectively, when the extractor was on during the coughing tests. For PM_{10}, we saw similar reduction rates of 80% and 97% at the two locations, respectively. In the continuous emission scenario, the extractor achieved a 99%-100% reduction in PM concentrations near the source, resulting in a complete reduction of detectable concentrations at the clinician's head. Therefore, the use of high-flow extractors should be considered in medical environments where strong sources of aerosols are present.

3IA.10

Children's PM2.5 Indoor Exposures in Mongolian Kindergartens. ZHIYAO LI, Munkhbayar Buyan, Rufus Edwards, Bat-Amgalan Gantumur, 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. The poor ambient air quality leads to high indoor $PM_{2.5}$ exposure because of infiltration, especially for those who live or study in or near the "ger" (yurt) neighborhoods that surround Ulaanbaatar's urban core. A monitoring study is being conducted to quantitatively evaluate Mongolian indoor air quality with a focus on children's exposure inside kindergartens and hospitals in the Bayanzurkh District of Ulaanbaatar. The 28-site network, deployed in February 2020 and operating through at least spring 2022, includes 24 kindergartens and 4 healthcare facilities using AirVisual Pro low-cost sensing devices to assess the indoor $PM_{2.5}$ and CO_2 concentrations. A subset of sites has PurpleAir PM devices outdoors. Adjustment factors for several PM low-cost sensing devices, including AirVisual Pro and PurpleAir, were developed from a winter 2019/2020 outdoor pilot study in Bayankhongor, Mongolia, that included collocation with a MetOne Model 2010 Beta Attenuation Monitor (BAM). In Bayanzurkh District, kindergarten indoor concentrations were highest in and near the ger areas. Across the District, large variations of indoor concentrations were sometimes observed over relatively small spatial scales. Indoor air quality and detailed building characteristics data are being used to rank kindergartens for potential interventions. The presentation will summarize results for indoor $PM_{2.5}$ spatiotemporal variability across the network and both $PM_{2.5}$ and CO_2 variations related to building characteristics and occupancy.

3IA.11

Particle Emissions from Fused Filament Fabrication 3D Printers and Their Impacts on Indoor Air Quality in School Environments.

QIAN ZHANG, Aika Davis, Marilyn Black, *Underwriters Laboratories Inc.*

Material extrusion fused filament fabrication (FFF) 3D printers with thermoplastics as print materials have been widely used in school environments. However, studies have shown that FFF 3D printing emits high levels of ultrafine and fine particles, which could deteriorate indoor air quality and adversely affect human health, especially for susceptible population like children. This study aims at understanding particle emissions from 3D printers used in school environments, estimating their effects in classroom air quality and occupants, and suggesting mitigating strategies if needed. Particle emissions from various commonly used print materials will be characterized by concentration levels and size distributions, in different school classroom settings. Air quality in classrooms with 3D printers will be compared to controlled classrooms without 3D printers to evaluate the effects of 3D printing. Field measured results in this study will be compared to model estimated exposure levels with classroom conditions and the emission results obtained from a chamber study. The potential health impacts associated with particles will also be discussed.

3IA.12

Investigation of the Size Resolved Fluorescent Bioaerosol in School Buildings with and without Upper-Room UVGI.

CHUNXIAO SU, Josephine Lau, *University of Shanghai for Science and Technology*

The adverse effect of bioaerosols has been one of the main concerns for human in highly occupied buildings such as classrooms. After the outbreak of COVID-19, investigation of behavior and effective intervention technology of indoor bioaerosols, especially for smaller size ones, have been urgent and critical.

To demonstrate the decay rates of bioaerosols by upper-room UVGI and room conditions, a field experiment was developed. Settings of the UVGI and non-UVGI classrooms were switched weekly through as eight-week measurement. In the measurement, samples were collected in two classrooms serving as UVGI and non-UVGI control rooms in an elementary school. The two classrooms shared the same schedules through the entire measurement. The size resolved concentrations of fluorescent bioaerosol were measured as the primary parameter for the analysis.

Our result shows that the decay rates of fluorescent bioaerosol concentrations for the smaller sizes of bioaerosols (0.5 and 3 micro meter) have shown consistent higher susceptibility than these for the larger sizes of bioaerosols. The fluorescent bioaerosol concentrations in UVGI room show higher decay rates than the larger fluorescent bioaerosols. The higher decay rates of small size bioaerosols indicates potential better application of air cleaning technology such as UV light, especially at where small size bioaerosols are the main source of pollutions. This will help further prevent the transmission of disease by bioaerosols such as COVID-19 in indoor environment.

3SI.1

Viral Shedding from Persons Infected with SARS-CoV02: Aerosols, Droplet Spray, and Fomites. Oluwasanmi Adenaiye, Jianyu Lai, Filbert Hong, Sheldon Tai, Jennifer German, Somayeh Youssefi, Paul Jacob Bueno de Mesquita, Barbara J. Albert, Tianzhou Ma, Stuart Weston, Matthew B. Frieman, DONALD K. MILTON, *School of Public Health, University of Maryland, College Pk*

Background: Characterization of viral shedding into aerosols, droplet spray, and onto fomites is important for understanding SARS-CoV-2 transmission.

Methods: We recruited participants infected with SARS-CoV-2 starting 8 May 2020 through advertising, intensive contact testing, and weekly testing of a community cohort. We collected exhaled coarse (>5µm) and fine (≤5µm) aerosol from cases using a Gesundheit-II (G-II) exhaled breath sampler, mobile phone and mid-turbinate swabs, saliva, and sera; large droplet spray deposited on G-II inlet cone was sampled for cases studied starting 10 September 2020. Samples were tested for viral RNA and cultured for the presence of infectious virus.

Results: As of 30 April 2021, we enrolled 80 persons with presumed or confirmed infection, collected a second sample from 76 on a subsequent day, and have complete qRT-PCR data for 45 confirmed PCR positive cases, seronegative at enrollment, who gave 69 G-II sample visits on days -1 to +7 relative to symptom onset (mean 3.8). Culture data is pending. All cases were ambulatory and mildly symptomatic or asymptomatic at the time of observation. Overall, 36% of cases had viral RNA detected in one or more fine and 29% in coarse aerosol samples, 26% in droplet-spray, and 58% in fomite samples (mobile phone swab) at or above the limit of detection (~75 copies). Most positive samples had only a trace of viral RNA. Samples above the limit of quantification (250 copies) were observed for 18% of cases in fine and 9% in coarse aerosols, 8% in droplet-spray, and 38% in fomite samples.

Conclusion: We observed aerosol shedding in a small fraction of cases, similar to the proportion responsible for the majority of secondary infections. Viral RNA was more frequently observed in aerosols than droplet spray.

3SI.2

Measurements of Exhaled SARS-CoV-2 and Human Respiratory Droplets Using an Infectious Aerosol Capture Mask. JOSHUA SANTARPIA, Nicholas Markin, Steven Lisco, Gabriel Lucero, Danielle Rivera, Vicki Herrera, Sarah Stein, *University of Nebraska Medical Center*

There are several remaining unanswered knowledge gaps regarding the details of the mechanisms of aerosol transmission of SARS-CoV-2, the virus that caused the COVID-19 pandemic. One of these gaps is an understanding the range of infectious virus that are emitted by an infected individual as an aerosol. The present work focuses on the utilization of an Infectious Aerosol Capture Mask (IACM), originally employed as system to isolate COVID-19 patients, and in the present study repurposed to collect exhaled aerosols from infected individuals. The system consists of an oxygen delivery mask and filter cartridge attached to either hospital suction or an independent vacuum pump. The efficacy of the mask in capturing exhaled breath aerosols was evaluated using a mannequin attached to a nebulizer and simulated using computational fluid dynamics. To quantify the viral content of exhaled breath from COVID-19 patients, a gelatin filter was used to capture aerosol particles from the mask and the interior surface was swabbed and subsequently assayed by PCR. Test with inert aerosols indicated that at vacuum flow rates of at least 1 SCFM the mask captured at least 99% of the aerosol generated through the mouth and nose of the mannequin. CFD simulations were run with the mask vacuum flow rate at 1 SCFM and initial aerosol velocities representative of breathing, speaking, and coughing. During breathing and speaking, all particles between 0.5 and 20 µm were captured either on the surface of the mask (0-1% for breathing, 71-84% for speaking) or in the filter (99-100% for breathing, 16-29% for speaking). During coughing, a small fraction of particles (1-8%) may escape the mask, but the remaining are either impacted on the mask surface (81-91%) or collected at the filter (8-11%). Exhaled aerosol samples from eight patients, previously diagnosed with COVID-19, were collected using the IACM. Total exhaled virus concentrations ranged from below the limit of detection to 1.1x106 RNA copies/hr of the viral E gene of SARS-CoV-2. No SARS-CoV-2 aerosol was detected in air samples collected adjacent to the patient when the mask was being worn. These data indicate that the IACM is both useful for containing the exhaled aerosol of infected individuals and can be used to quantify the viral aerosol production rates during respiratory activities.

3SI.3

SARS-CoV-2 RNA Contaminated HVAC Filters and Indoor Surfaces in the Built Environment during Both Isolation and Quarantine Stages.

JIN PAN, Seth Hawks, Aaron Prussin II, Nisha Duggal, Linsey Marr, *Virginia Tech*

There are relatively little data about the presence of SARS-CoV-2 in the built environment, except for hospitals, which accommodate only the sickest patients. To investigate the level of contamination on different surfaces, we collected heating, ventilation, and air conditioning (HVAC) filters and surface swab samples from university dormitory rooms housing students who were exposed and tested positive for COVID-19. Because patients shed more viruses earlier in the course of infection, we hypothesized that we would find more viruses in the quarantine dormitory, which housed students who had been exposed and were waiting for their test results, than in the isolation dormitory, which housed students who had already tested positive. We detected viral RNA from 9/21 (42.9%) filters, 49/125 (39.2%) surface samples, and 4/6 (66.7%) exhaust grilles in the public bathrooms of the two dormitories combined. We found no significant differences ($p>0.05$) in the positivity rate between quarantine and isolation rooms except for the floor swabs ($p<0.05$), which may be attributed to the difference between the hard vinyl floor in the quarantine rooms vs. the carpeted floor in the isolation rooms. Viral RNA was present in all five surface sample types, including the sink handle, sink floor, sink countertop, door handle, and thermostat panel, among which the sink floor exhibited the highest positive rate (14/28), followed by the thermostat panel (12/28). Viral RNA levels on surfaces varied widely, from 10 to 10^4 genome copies per swabbed area of $\sim 10 \times 10$ cm^2. We also tested the infectivity of samples with a Ct value lower than 33, and none of them were positive. Positive samples from the HVAC filters and bathroom exhaust grilles indicate that the virus was in the air, either directly from exhaled respiratory aerosols or resuspension of dust.

3SI.4

Aerosol Generation from Flute Playing.

KARIN ARDON-DRYER, Lisa Garner Santa, Michael San Francisco, Emily Bailey, *Department of Geosciences, Texas Tech University*

The current covid-19 crisis brought into question the safety of musical rehearsal and performance. Aerosol spread in flute playing occurs as the flutist’s airstream splits crosses the lip-plate and as air exits the flute through the foot joint. The flutist’s air also escapes through the tone holes, though at a much slower speed. Our study examined the emission of aerosol particles (concentration and size distribution) and emission of biological particles related to flute playing. The potential of two mitigation devices was included in the experiment. These mitigation devices were the Win-D-Fender™, originally designed to block wind from interfering with the flutist’s airstream when playing outdoors, and the Rose Johnson attachment, or Flute Boot, a lightweight cloth “sock” attached to a silicone ring that slides over the end of the foot joint.

Particles in a size range of 10 nm up to 10 micrometers were captured using TSI NanoScan SMPS (Scanning Mobility Particle Sizer) and Optical Particle Sizer (OPS) devices. The presence of biological particles including (SARS-CoV-2, Influenza A virus, Staphylococcus aureus, Streptococcus pneumonia, and RNAse P) was examined using real-time reverse transcriptase-polymerase chain reaction (rRT-PCR).

Aerosol emissions from ten different players were measured in this study, half female and half male. Flute players' ages ranged from 22 to 52, and their years of playing ranged from 9 to 40 years. Some participants did not show a significant increase in aerosol emission while playing the flute, while others (referred to as super-emitters), had a high aerosol emission even with the mitigation devices. We found that the Win-D-Fender helped to reduce emissions, but the Rose attachment was not as effective. To our surprise, no biological particles were detected.

3SI.5

Quantification of Expiratory Particulate Matter Generated from Singing, Speaking, Breathing, Cough and Playing of Musical Instruments.

JUSTICE ARCHER, Henry Symons, Natalie Watson, Christopher Orton, Pallav Shah, James Calder, Bryan R. Bzdek, Declan Costello, Jonathan P. Reid, *University of Bristol*

The coronavirus disease-2019 (COVID-19) pandemic continues to heighten the awareness of aerosol generation by human expiratory events and their potential role in viral respiratory disease transmission. Sufficient knowledge of expiratory particulate particle size, number concentration, and sites of origin is therefore of great importance for understanding respiratory disease transmission via the aerosol route.

In this work, we expand on our previous study (Gregson et al., 2021), which informed changes in UK government policy on musical performances in the summer 2020 to include a wider cohort of professional musicians (adult and children), to quantify the number concentration and size distributions of expiratory particulate matter generated during vocal activities (singing, speaking, breathing and coughing) and playing woodwind and brass instruments. We carried out measurements in a laminar flow operating theatre, with a near-zero background aerosol concentration allowing us to quantify relatively the small amounts of expiratory particulate matter produced from the expiratory activities. We used an aerodynamic particle sizer (APS, Model 3321, TSI Inc.) at 1s scan time to quantify the number concentration and size distribution of particles with diameters in the range of 0.5 – 20 µm. For expiratory droplets >20 µm, we used water-sensitive paper placed at a distance of 10 cm from a participant's mouth level to assess differences in the prevalence of droplets produced from singing and coughing. We will present measurements of expired aerosol size distributions and number concentrations generated by adults and children singers during vocal activities (singing, speaking, breathing, and coughing) and playing woodwind and brass instruments.

3SI.6

Bioaerosols in the Performing Arts: Quantifying Aerosol Emissions from Speech, Song, and Wind Instruments.

Kristen Fedak, Nicholas Good, Christian L'Orange, Ky Tanner, Amy Keisling, Emily Morton, Dan Goble, Rebecca Phillips, JOHN VOLCKENS, *Colorado State University*

Airborne transmission, whether by large droplets or smaller aerosols, is considered the primary mode of infection for COVID-19. Several “super-spreading” events have been linked to performing arts activities, presumably due to the close proximity of people and the increased bioaerosol emission rates from speech, song, and wind instruments. Prior to the pandemic, little was known about bioaerosol emissions (and exposures) in the performing arts. The objective of this work, therefore, was to quantify aerosol emission rates from a panel of human volunteers who participate in performing arts activities. We recruited 100 participants of both sexes and ranging in age from 12 to 63 years; participants were limited to those who practice within the performing arts (either acting, dance, vocal, or wind instruments). Over a ~2hr study session, participants performed a series of maneuvers within a cleanroom environment (e.g., talking, singing, playing an instrument) while aerosol emission rates were quantified using a constant-volume dilution system with isokinetic sampling. We employed an ensemble of measurement techniques to characterize size-resolved emission rates of particles ranging from ~7 nanometers to 500 microns in diameter. We also characterized sound pressure levels (i.e. volume), CO2 mixing ratio, temperature, and humidity continuously. Linear models were developed to examine trends in number emission rates by maneuver and participant characteristics. To our knowledge, this is the largest controlled laboratory study of human bioaerosol emissions to date. We found that aerosol emission rates vary logarithmically (by up to a factor of 20x) between participants. Sex is an important determinant of particle number emissions, and volume is confirmed as a driving factor for vocal emissions. When normalized to exhaled CO2, the effect of sex is attenuated, which suggests that monitoring of both CO2 and volume can provide important feedback for control of infection risk indoors.

3SI.7

Simulations of Infection Risk for Indoor Transmission of COVID-19.

Gregoire Labat, Haider Allawi, Isaac Flores Espinoza, SHERYL EHRMAN, *San Jose 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. Airborne transmission is now believed to be a significant route. To estimate risk of indoor transmission via aerosols for unvaccinated individuals, we developed a box model of aerosol generation, removal and exposure, assuming well mixed conditions. Infectious aerosol generation rates (quanta/time) are estimated based upon activity level and quanta emission rates reported in literature, removal rates are estimated based upon ventilation parameters, filtration efficiencies and deposition, and exposure risk is estimated using a modified Wells-Riley approach. The model was evaluated by comparison to case studies of outbreaks reported in the literature: choir practice, cycling class, long distance bus ride, and recreational hockey game. Predictions were reasonably close to the observed attack rate in all cases. Effects of masking of both the infectious and susceptible individuals were estimated, incorporating viral load and mask efficiencies as a function of aerosol/droplet size obtained from literature. Results suggest that while mask wearing does not completely prevent transmission, it significantly reduces it, reinforcing the importance of masks as a non-pharmaceutical intervention.

3SI.8

Respiratory Droplet Emissions and Transport Estimates Using CFD for a Nine-Person, Cubicle-Style Office.

Sohaib Obeid, Mahender Singh Rawat, Paul White, Jacky Rosati Rowe, Andrea Ferro, GOODARZ AHMADI, *Clarkson University*

There has been strong evidence that the airflow patterns significantly affect the transmission of airborne infectious diseases in indoor environments (Li et al., 2007). Computational fluid dynamics (CFD) can be used to evaluate infectious droplet transport from source to receptor. For example, Bjorn and Nielsen (2002) and Topp et al. (2002) studied the dispersal of exhaled air and personal exposure in ventilated rooms using this approach. For this study, we used an improved CFD modeling approach to predict airborne concentrations of virus-laded droplets from one infected individual in a representative nine-person, cubicle-style office environment. A transition three–equation k-kl-ω turbulence model suitable for application to low Reynolds number flows developed by Walters and Cokljat (2008) was used in the simulations. A user-define-function (UDF) accounting for the turbulent diffusion of droplets and their gravitational sedimentation was developed and used to evaluate the infected droplet concentration in the office space. Instantaneously-mixed mass balance modeling, which assumes that the concentration is the same everywhere in the room, was also conducted for comparison. Assuming that one infected individual is present in the simulated workspace, we assess the concentration and exposure level at the other eight office workstations. Depending on which individual was “infected,” the concentrations in the room predicted by the CFD modeling varied widely, even for the steady-state condition. Scenarios that resulted in the largest differences in exposure estimates for the occupants in the room occurred when the infected person sat within a recirculation zone produced by the ventilation system. The impact of increasing the room ventilation rate and increasing the divider height above the top of the desk from 54” (1.37 m) to 64” (1.63 m) were also evaluated.

This document has been reviewed in accordance with U.S. Environmental Protection Agency policy and approved for publication.

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3SI.9

Design-Aided Mitigation of the Spread of Virus Aerosols. SUNIL KUMAR, Maria King, *Texas A&M University*

The fast spread of the COVID-19 pandemic compelled countries to impose lockdown, restrict movement of people, limit the industrial production, impacting supply chains to control the spread of the coronavirus. However, production cannot be shut down for extended time as closing of industries would lead to food and health crisis. Depending on the type of the work employees are either required to work alone or stand in queue. Processing food, packaging items and processing meat require workers to stand next to each other around the conveyor belts. In general, these facilities are ventilated by central heating and air conditioning units. The air streams generated from ventilation ports are complex and long, which can transport the virus aerosols from one corner of the food processing plant to another corner. In a closed environment of this kind, a single sneeze from an asymptomatic worker can potentially spread the virus to the whole facility and turn it to be a super spreader for the community. In general, the fabrication rooms or packaging units are not designed to effectively reduce the risk of virus transport under the influence of HVAC system. Therefore, necessary design modifications are needed to control the spread of virus aerosols in closed workplaces. This study presents an efficient and economic design modification of the common space at a fabrication facility, by preventing the development of long air streamlines to reduce the spread of sneeze droplets. The modified design includes installation of optimal size transparent plastic sheets around the employees' workspace. The improved design has been tested for different environmental conditions and ventilation rates. The study provides a comprehensive insight into understanding the role of ventilation system and presents possible pathways to reduce the spread of virus aerosols in any industry irrespective of its size and type of work.

3SI.10

Quantification of Expiratory Aerosol and Droplets Produced during Exercise. Henry Symons, Justice Archer, Christopher Orton, Natalie Watson, James Calder, Declan Costello, James Hull, Pallav Shah, BRYAN R. BZDEK, Jonathan P. Reid, *University of Bristol*

The COVID-19 pandemic has brought considerable attention to the role of different human expiratory events in airborne pathogen transmission. Concern and uncertainty surrounding these issues led to widespread suspension of sporting events and closure of gyms and other venues. Quantification of respiratory aerosol and droplets will aid in assessing the relative risks of different activities and inform mitigation strategies to minimise exposure risk. In this work, we aim to quantify the emission rate and size distributions of respired aerosol generated during differing levels of physical activity. We used cardiopulmonary exercise testing (CPET) as a means of standardising the intensity of exercise undertaken across a cohort of participants covering a broad range of athletic abilities and other demographics. After an initial test that quantifies the athletic ability of participants, we measured aerosol generation by breathing at three relative levels of activity: resting, moderate exercise and heavy exercise. To detect the relatively small amounts of aerosol produced by respirable activities, we carried out measurements in a laminar flow operating theatre, with a near-zero background aerosol concentration. Two aerodynamic particle sizers quantified the number concentrations and size distribution of particles with diameters in the range of 0.5 – 20 µm. The total particle flux is estimated by combining measured aerosol number concentrations with participant ventilatory data. Additionally, the production of large droplets >20 µm was assessed. Clear increases in the concentration of aerosols generated by breathing as a function of exercise intensity were observed. These increased concentrations are compounded by a concurrent increase in ventilation rate during greater levels of physical activity. The results highlight the need for careful consideration of mitigation strategies to minimise the risks of airborne pathogen transmission during exercise, particularly in indoor spaces such as gyms and sports halls where ventilation rates are relatively low.

3SI.11

Pathogens and Size Characterization of Aerosols Generated during Aerosol Generating Procedure in COVID 19 Positive Patient Intensive Care Units. SHRUTI CHOUDHARY, Tracey Bach, Meghan Wallace, Carey-Ann Burnham, Michael Durkin, Jennie Kwon, Hilary Babcock, Stephen Liang, Pratim Biswas, *Washington University in St Louis*

The airborne transmission of infectious diseases in the health care settings especially in Intensive care units during commonly identified aerosol-generating procedures (AGP) such as Bronchoscopy, High Flow Nasal Cannula (HFNC), Opti flow, Tracheostomy always remains a concern for health care workers. There are a limited number of studies that report possible pathogens and number concentration of aerosols present in the air during the AGPs in COVID 19 positive patient ICUs. Aerosol capture and real-time size characterization of aerosols were performed in the ICU for 15 minutes during Bronchoscopy (n=2), HFNC (n=6), Opti flow (n=5), Tracheostomy (n=3), patient on Ventilator (n=10), Bilevel Positive Airway Pressure (BiPAP) (n=1), changing HFNC to BiPAP (n=1), changing BiPAP to AIRVO (n=1). The bacterial culture analyses of the collected samples reported Staphylococcus epidermidis, Staphylococcus capitis, Staphylococcus haemolyticus, Aspergillus fumigatus, Bacillus subtilis during bronchoscopy; Staphylococcus capitis during HFNC; corynebacterium coyleae during opti flow; Corynebacterium tuberculostearicum, Staphylococcus hominis, Staphylococcus epidermidis during patient on Ventilator. Number size distribution and mass concentration of the aerosols generated during the AGPs were compared with the baseline level among which Bronchoscopy emitted highest number of aerosols in the size range 10 nm to 1µm. Procedures such as HFNC, Opti flow, changing from BiPAP to AIRVO also reported an increase in certain size range of 20-100nm and 200 to 500nm. Thus, the results show that viable pathogens generated from the AGPs are present in the ICU rooms and that increase in number concentration of the aerosols can be an indicator for the pathogens present in the ICU room when compared with the baseline measurements. Cloud-based distributed real-time PM sensing of the aerosols in ICU and other health care settings are also described.

3SI.12

Detection of Non-infectious SARS-CoV-2 from Aggregated Samples of Bioaerosols Produced during Expiratory Activities. Tyler J. Johnson, ROBERT T. NISHIDA, Ashlesha P. Sonpar, James Lin, Kimberley Watson, Stephanie Smith, John Conly, David Evans, Jason S. Olfert, *University of Alberta*

The COVID-19 pandemic is caused by transmission of SARS-CoV-2 from person-to-person. At the time of writing, SARS-CoV-2 RNA has been detected in samples of ambient air and surfaces in clinical settings, including in aerosols smaller than 5 µm in diameter, likely produced by patients nearby. The limited number of studies to date which include samples of air directly exhaled by study participants have not reported attempts to culture the virus. In this work, participants identified by a recent positive oro- or naso-pharyngeal (NP) swab were asked to breathe, speak and cough into a single-use, medical-grade mask placed directly over their nose and mouth and the bioaerosols they emitted were continuously sampled from air in the mask by bioaerosol samplers (i.e. BioSampler® and Andersen Cascade Impactor) for ex situ virological analyses. Cycle thresholds (Ct) from quantitative reverse-transcriptase polymerase chain reaction (RT-qPCR) analyses indicate RNA of SARS-CoV-2 was present in samples of air emitted by participants (in aggregate samples of breathing, speaking and coughing), including in bioaerosols smaller than 10 µm in aerodynamic diameter. Despite detecting SARS-CoV-2 RNA in air samples (e.g. from BioSampler, n=17; Ct: 26.4-36.6), previous data shows those samples were unlikely to culture. Indeed, all attempts to culture the virus from samples of bioaerosols have been negative to date (0 of 27; limit of detection, 5 PFU/mL) despite sampling air directly emitted by participants who carried infectious virus as detected by viral culture of their NP swab (positive by plaque assay: 53%, 9 of 17, Titer: 15 PFU/mL - 18,000 PFU/mL; positive by RT-qPCR: 100%, 17 of 17, Ct: 16.2-30.3).

3ST.1

Droplets and Aerosols in Infectious Disease Transmission: History of the 5-µm Cutoff and the 6' Rule. Katherine Randall, E. Thomas Ewing, LINSEY MARR, Jose-Luis Jimenez, Lydia Bourouiba, *Virginia Tech*

The COVID-19 pandemic has exposed major gaps in our understanding of the transmission of viruses through the air. These gaps slowed recognition of airborne transmission of the disease, contributed to muddled public health policies, and impeded clear messaging on how best to slow transmission of COVID-19. In particular, current recommendations have been based on four tenets: 1) respiratory disease transmission routes can be viewed mostly in a binary manner of “droplets” versus “aerosols”; 2) this dichotomy depends on droplet size alone; 3) the cutoff size between these routes of transmission is 5 µm; and 4) there is a dichotomy in the distance at which transmission by each route is relevant. Yet, a relationship between these assertions is not supported by current scientific knowledge. Here, we revisit the historical foundation of these notions, and how they became entangled from the 1800s to today, with a complex interplay among various fields of science and medicine. This journey into the past highlights potential solutions for better collaboration and integration of scientific results into practice for building a more resilient society with more sound, far-sighted, and effective public health policies.

3ST.2

Ventilation in Schools and Universities. V. FAYE MCNEILL, Richard Corsi, J. Alex Huffman, Do Young Maeng, Shelly Miller, Nga Lee Ng, Atila Novoselac, Paula Olsiewski, Krystal Godri Pollitt, Rachel Segalman, Alex Sessions, Todd Squires, Sabrina Westgate, *Columbia University*

Ventilation is of primary concern for maintaining healthy indoor air quality and reducing the spread of airborne infectious disease, including COVID-19. However, for many universities and schools, ventilation data on a room-by-room basis are not available for classrooms and other key spaces. We present an overview of approaches for measuring air exchange along with their advantages and disadvantages. We also present data from case studies for a variety of institutions across the United States, with various building ages, types, locations, and climates, highlighting their commonalities and differences, and discuss best practices.

3ST.3

An Openly Available Database for Public Education and to Combat Misinformation about Respiratory Aerosols.

J. ALEX HUFFMAN, *University of Denver*

The global COVID-19 pandemic forced life-saving health decisions into the public arena like no time in recent history. Broad confusion about the nature of the respiratory disease, combined with historical misunderstandings of aerosol physics within many public health-related fields, led to further chaos in the roll-out of education about COVID transmission and associated prevention. Rather than relying on public health agencies, many scientists with direct aerosol experience strategized to inform and educate the public more directly using traditional media, social media, and other publicly accessible platforms. As a result of these efforts, a deluge of information became available from scientists, engineers, and science journalists.

As one vehicle to provide reliable information about the transmission and prevention of COVID-19 and other respiratory diseases, I built a Google spreadsheet to share as a central and openly available repository for a broad range of online resources. The sheet was released in July 2020 and has been curated near-daily to provide constant, up-to-date sources for scientists, journalists, and other individuals looking for reliable information and guidance.

The page consists of nine individual tabs and a total of >1,500 individual links (as of Apr 30), with information ranging from entry-level videos on aerosol education to interactive aerosol modeling tools and a repository of peer-reviewed science. The tabs include: (1) reports, guides, and tools; (2) media articles; (3) infographics; (4) videos; (5) threads, blog posts, and podcasts; (6) science articles and preprints; (7) webinar recordings and associated slide decks; (9) related media articles and a list of Twitter-active scientists to follow for trustworthy information.

The spreadsheet is shared as an example strategy to directly inform the public and scientists, along with a brief discussion of challenges and lessons learned. Direct spreadsheet link: https://bit.ly/3fzmB16.

3ST.4

Building an Aerosol Sensing Sensor Network and Inspiring Citizen Scientists.

KERRY KELLY, Anthony Butterfield, Wei Xing, Katrina Le, Tofigh Sayahi, James Moore, Tom Becnel, Miriah Meyer, Ross Whitaker, Pierre-Emmanuel Gaillardon, *University of Utah*

Short-term exposure to fine particulate matter (PM2.5) is linked to numerous adverse health effects. Salt Lake City, Utah periodically experiences some of the highest PM2.5 levels in the nation, yet it has historically been sparsely instrumented and often experiences delays of hours until air-quality information is publicly available. Since 2018, the AQ&U network has been collecting aerosol measurements from a growing number of low-cost sensors (more than 200) in the Salt Lake Valley. AQ&U integrates low-cost, research-grade, and reference measurements with robust data screening, event-specific calibrations, and a Gaussian Process model to understand neighborhood-scale PM2.5 concentrations. It provides near-real time visualizations of PM2.5 concentration along with uncertainty estimates through a public-facing website. AQ&U also provides a rich framework for citizen science. Here, we discuss AQ&U’s community engagement strategies, particularly those to encourage participation of under-served communities, and highlight two of our most successful efforts to engage students as citizen scientists. The first effort centers around a hands-on activity to build and test an aerosol sensor from LegosTM and simple microelectronics. It emphasizes the underlying principles of aerosol light scattering. This has been our college’s most requested outreach activity and has been successfully demonstrated at hundreds of high-school classrooms, numerous STEM tabling events, and the National Science and Engineering Fair. The second effort focuses on an interactive, team-based teaching module using local real-world measurements. This activity's goal is to engage students in generating and testing hypotheses while also encouraging citizen scientists to use real-world air quality data for their own interests, such as exploration, science fair projects, or environmental oversight. This second activity has been a successful strategy for virtual learning. Finally, we also discuss lessons learned.

3ST.5

Social Science in Community Air Monitoring. ELISA LAZZARINO, Sherri Hunt, *EPA*

This review of six EPA STAR-grant funded community-focused projects highlights the value of integrating social scientists at the beginning stages of work. Several social science themes relevant in communicating complex scientific information to the public emerge including advancing environmental literacy, developing trusting relationships with diverse communities, and building the capacity necessary to effect real change. Low-cost air quality sensors remain a focal point for researchers and community action organizations alike in recent years for their potential to cover temporal and spatial gaps in monitoring from conventional sensor networks, as well as their potential to maximize benefits to communities that experience poor air quality. However, researchers and sensor developers continue to face immense challenges to make the devices and the complex data they generate accessible to the public. While still infrequent, collaborations between aerosol scientists, social scientists, and community and citizen scientist collaborators present opportunities to advance science, generate more useful results, and make a greater impact with their research. Social science methods and thoughtful engagements with communities informed the development of several tools, apps, and guidance materials that respond to the needs of their intended communities. While likely more costly in time and resources than traditional aerosol research, these interdisciplinary projects also illustrate how researchers can overcome the challenges and pitfalls of communicating across scientific disciplines and working with communities, ultimately leading to positive change and making the devices more useful.

3ST.6

Multi-Modal Data Sharing and Synthesis for Low-Cost Sensors. ALIAKSEI HAURYLIUK, R. Subramanian, Carl Malings, Ashley Angulo, Randy Sargent, Ana Hoffman, Albert Presto, *Carnegie Mellon University*

A network of Real-Time Affordable Multi-Pollutant (RAMP) sensors has been continuously operating in the Greater Pittsburgh Area since August 2016. In an effort to publicly disseminate the collected data, we developed or partnered in developing several methods of presenting the data. Each method addresses a different use case and target audience, with the consideration of the audience's level of engagement and comfort with data analysis.

The methods include:
1. Sending location-specific air quality alerts based on data from the sensors
2. Displaying interpolated air quality data on a publicly-accessible map
3. Publishing aggregate data in weekly and monthly reports
4. Sharing processed data with OpenAQ and CREATE Lab's Environmental Sensor Data Repository (ESDR) platforms
5. Making freely available the software tools for collecting and processing the raw data from the sensors, and providing documentation and tutorials for their use.

The alerts and map are targeted at the general public, while the reports are most suited to answer questions from sensor hosts and community groups. Processed data are intended for power users, while raw data and software tools have researchers in mind.

This approach utilizes multi-modality in an attempt to answer different questions regarding the current or past state of air quality in the region. It relies on aggregated historical data for providing context and analysis on near-real-time readings to address more immediate concerns about pollutant levels. Tools like recurring reports provide a line of communication with the sensor hosts and community groups, who are concerned with air pollution trends in their area. Furthermore, data aggregation can be used to identify undesirable sensor operation or conditions which result in poor corrective model performance. This is useful both for quality control internally and communicating uncertainties to the consumers of data from low-cost sensors.

3ST.7

Engaging Residents in Community Science to Address Air and Noise Pollution Exposure. MARISA WESTBROOK, Nicholas Clements, Esther Sullivan, *University of Colorado Denver*

Low-income communities of color are disproportionately subject to environmental injustice and inequity. Historically marginalized neighborhoods suffer the negative environmental impacts of major construction projects - including noise and air pollution, traffic disruption, and individual and community health effects. Many such urban communities criticize academic researchers for their lack of engagement beyond the extraction of data and for their failure to translate research findings into knowledge, solutions, and practical changes for impacted communities. Community science has emerged as a popular method for engaging residents throughout the research process. This research project applies community science to aerosol exposure research within three geographically-adjacent communities in Denver, Colorado - recently assessed as the most polluted in the United States - to understand and help mitigate disruption and air pollution emissions from two major construction projects. Through a phased process of engaging with local community organizations, facilitating focus groups with community members, and implementing a field study, we seek to gather and integrate resident input into the process of monitoring and mitigating air pollution in their community through a smartphone app, surveys and environmental sensors. Through this study, we ask: a) what are the primary barriers to aerosol research and science, data, and technology literacy for the community, b) what are the key contradictions between the needs of a community-based aerosol study and the wishes of community members, and c) how can social science principles contribute to communicating science and ensuring equity in the scientific process? Our research findings point to a sample of approaches and tools that academics can employ for equally beneficial community partnerships to ensure that environmental justice research projects are successful and that aerosol research findings are accessible and useful in advancing environmental justice.

3ST.8

IndoorChem: Building a Science Community in the Chemistry of Indoor Environments. MARINA VANCE, Delphine K. Farmer, Julia Bakker-Arkema, Sameer Patel, *University of Colorado Boulder*

Indoor chemistry is a relatively new field that combines expertise from atmospheric chemistry, indoor air quality, building science, and other areas, to further our understanding of the spaces where we spend the vast majority of our time. The IndoorChem community was launched in 2017 to foster the growth of this research community and to communicate its findings with the world. In this presentation, we describe the community building strategies developed for this project, activities performed for each strategy, and major outcomes so far. IndoorChem incorporates two main strategies: (1) internal community building, which aims to bring together researchers in the field to multiply the potential for scientific discovery through collaboration, and (2) external community building, which aims to communicate the science in this program with adjacent scientific fields, other stakeholders, and the public. Activities promoting internal and external community building ranged from science meetings and scientific field campaigns to social media presence, a website and blog, a newsletter, a YouTube channel, and more. This work will quantify the rate of community building through a variety of metrics, such as the growth of the scientific network in terms of the diversity of co-authorships and the outreach to the public in terms of social media reach metrics, over the past 4 years, plans for the continued growth of the network, and lessons learned so far.

3ST.9

Exploding Interest: Air Quality Messaging during and after a Refinery Explosion. PETER F. DECARLO, *Johns Hopkins University*

In the early morning on June 21, 2019 the longest continuously operating refinery in the US exploded. Despite the visible smoke and the acrid smell in the air, official messaging from city officials was that there was no impact to local air quality with minimization of the risks associated with emissions from the fire. Academics and environmental groups disagreed with that and responded. Nearby communities most affected by the explosion were issued stay-at-home orders and remained in the area during the subsequent fire. In the weeks and months following the explosion an Advisory group convened by the Mayors office initiated a series of public conversations about the future of the refinery and the land on which it sits. These meetings brought together a variety of stakeholders from economic, environmental, workers, and community groups. Following the public meetings a report summarizing findings from these conversations was issued by the Mayor's office. This report again minimized air quality impacts on the local community. This presentation will discuss conflicting air quality messaging from public officials and other stakeholders, and ways to effectively engage with community groups and provide assistance for messaging and advocacy.

3ST.10

Historic Redlining and Modern Disparities in U.S. Urban Air Pollution Exposure. HALEY LANE, Julian Marshall, Rachel Morello-Frosch, Joshua S. Apte, *University of California, Berkeley*

Racial-ethnic minorities in the US are systematically exposed to higher levels of air pollution. We explore here how redlining, a racist mortgage appraisal practice started in the 1930s, affects present-day intra-urban air pollution disparities in 202 US cities. In each city, we integrated two data sources: 1) detailed Security Maps drawn by the Home Owners' Loan Corporation (HOLC) that assigned neighborhood investment risk grades of A (‘best’, green), B (blue), C (yellow), and D (‘hazardous’, red, i.e., redlined); and 2) year-2010 estimates of NO_2 and $PM_{2.5}$ concentrations by US Census block derived from a national integrated empirical geographic air pollution model. Three findings are especially noteworthy. (1) We find large present-day intra-urban disparities in air pollution exposure which are consistently associated with historical redlining. Specifically, residents in historically redlined (grade “D”) neighborhoods experience air pollution levels that are 7% [NO_2] and 1% [$PM_{2.5}$] higher than city-wide mean concentrations, on average. Meanwhile, air pollution levels for residents in grade A neighborhoods are 15% [NO_2] and 3% [$PM_{2.5}$] lower than city-wide means. The contrast between NO_2 and $PM_{2.5}$ likely reflects the difference between a largely traffic-related, nearly-primary pollutant [NO_2] versus a secondary, regional pollutant [$PM_{2.5}$] which is attributable to multiple sources. (2) Within individual cities, average NO_2 exposure disparities associated with redlining were double those associated with race and ethnicity. (3) Within each separate historical HOLC classification code, racial- and ethnic exposure disparities persist. Our findings illustrate how the legacy of racially exclusive housing policy and urban planning continues to shape systemic environmental exposure disparities in the US.

3ST.11

Air Quality Monitoring with Low-Cost Sensors in Greater Springfield, MA: Citizen Science and Air Quality Monitoring. Dong Gao, Mahea Heimuli, Kayla Fennell, Anna Woodroof, Mark Chandler, David Bloniarz, Alexander Sherman, Samantha Hamilton, Yoni Glogower, Sarita Hudson, KRYSTAL GODRI POLLITT, *Yale University*

Air pollution continues to be a global public health threat. With the development of sensor and internet technologies, low-cost air sensors (LCS) have emerged as an effective tool for air quality monitoring at a high time and spatial resolution. The use of LCS is of main interest for citizen science initiatives and can help answer community-driven and locally motivated questions. A collaborative air quality monitoring project has recently been conducted to build up a LCS network across Greater Springfield region in Massachusetts, aimed at measuring air pollution levels and providing data to inform public health responses in the city known as having the highest rates of asthma in the country. Public outreach and stakeholder engagement are critical to the success of the project. To raise awareness and establish specific opportunities for the public to collaborate with researchers on topics related to air pollution and the environment, multiple visual interactive community discussion sessions were held. The feedback and concerns, such as air quality information needs, uses, sources, and barrier, were collected during discussions and through feedback forms from the community and incorporated to develop strategies for sensor deployment, data visualization, and other key activities. This community-engaged process enables the generation of community-relevant air quality data which complement the regulatory networks.

4AC.1

Modeling Sulfuric Acid Nucleation of Complex Mixtures.

JACK JOHNSON, Sandra Fomete, Coty Jen, *Carnegie Mellon University*

Aerosol particles form in the atmosphere when gas phase compounds react to form stable clusters in a process known as nucleation. In recent decades, 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 atmospherically relevant 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 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 and mixtures of compounds for sulfuric acid nucleation. Using a parameterization technique, we can determine the effective concentration of stabilizing compounds by reacting a known amount of sulfuric acid to form measurable particles. Our results show that the parameterized concentration is correlated with the measured concentration of stabilizing compounds and reflects the effectiveness of each compound in stabilizing sulfuric acid particles. In addition, sulfuric acid reacted with mixtures of stabilizing compounds to demonstrate how synergistic nucleation mechanisms are captured by our model. The simplicity and accuracy of the model to estimate stabilizing compounds will help improve nucleation rate predictions in diverse regions around the world.

4AC.2

AMORE: Automated Mechanism Reduction in Atmospheric Chemistry.

FORWOOD WISER, Siddhartha Sen, Daniel Westervelt, Daven Henze, Arlene Fiore, V. Faye McNeill, *Columbia University*

There is a need for new approaches for the systematic reduction of complex atmospheric chemical mechanisms for use in large-scale models. We have developed the Columbia University Atmospheric Chemistry Model Reduction (AMORE) algorithm, an automated tool for flexibly generating accurate condensed chemical mechanisms. Using the principles of graph theory, without running the model, AMORE analyzes a reaction network and eliminates reaction pathways with throughputs that do not meet a specified threshold. Those pathways are discarded, along with species left unconnected to the rest of the network, until the desired model size or error tolerance is reached. Species of particular interest are protected from elimination. Inputs for AMORE are sampled from a range of conditions relevant to the continental U.S., generated using GEOS-Chem. We have applied AMORE to develop an updated condensed gas-phase isoprene oxidation mechanism and tested its performance against the full mechanism of Wennberg et al. (2018) in the photochemical box model, F0AM.

4AC.3

Reactive Uptake of Monoethanolamine (MEA) by Sulfuric Acid Particles.

XIAOMENG TIAN, Yangxi Chu, Chak K. Chan, *City University of Hong Kong, China*

The wide application of monoethanolamine (MEA) in post-combustion CO2 capture technology results in CO2 capture plants as a significant MEA emission source.1 As a potentially competitive MEA sink pathway in the atmosphere, the heterogeneous uptake of MEA by sulfuric acid (SA) particles via acid-base reaction might play a role in the formation of particulate MEA sulfate. We investigated the reactive uptake of ppm level MEA by sulfuric acid particles in an Electrodynamic Balance (EDB), in which the uptake changes the hygroscopicity of the particles. Hence, the hygroscopicities of MEA salts including MEA sulfate at different MEA to sulfate ratios over a wide range of RH were studied using an EDB and the Aqualab. Other salts studied include MEA oxalate, nitrate and chloride. Empirical functions were fitted to the experimentally measured hygroscopicity data of MEA sulfate of different MEA to sulfate molar ratios and applied to the analysis of composition change of the particle during MEA uptake and hence the uptake kinetics. The uptake coefficients γMEA were estimated as $(3.23\pm0.64)\times10^{-3}$ and $(9.89\pm 2.62)\times10^{-4}$ at 40%RH and 70%RH, respectively. MEA reactive uptake by acidic particles could be competitive to gas-phase oxidation by ozone as an atmospheric MEA sink process, especially near power plants with high concentrations of fresh SA particles.

Acknowledgment

We would like to acknowledge the Hong Kong Research Grants Council (grant #11302318) for their support.

Reference

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4AC.4

Dynamic Surface Tension of Surfactant Containing Droplets by the Oscillating Droplet Method.

LARA LALEMI, Bryan R. Bzdek, Rachael E.H. Miles, *University of Bristol*

Atmospheric aerosols cool the Earth’s climate by serving as cloud condensation nuclei. The extent of this cooling represents both the most uncertain and largest negative radiative forcing (countering the warming due to greenhouse gases) when predicting the Earth radiative budget. The barrier to cloud droplet activation is influenced by a particle’s surface tension. Surfactants are an important component of atmospheric aerosol mass, with recent atmospheric aerosol analyses in different regions showing the presence of surfactants at estimated concentrations as high as 27 ± 6 mM, resulting in predicted aerosol surface tensions <40 mN m-1. In this presentation, we explore the surface tensions of surfactant-containing microscopic droplets across a range of surfactant concentrations, droplet sizes, and surfactant types, quantifying the extent of surface tension reduction in droplets due to the presence of surfactants.

We use the oscillation approach to quantify the surface tension of aqueous surfactant solution droplets. 30-80 µm diameter droplets are reproducibly dispensed from a microdroplet dispenser with a surface age <1 ms. The resulting oscillations in droplet shape are characterised with 1 µs time resolution. The surface tension is inferred from the frequency of droplet oscillations, which are monitored in a time-resolved manner by stroboscopic imaging. The temporal development of the dynamic surface tension will be compared to bulk solution measurements to determine the effects of confinement on surface-bulk partitioning timescales. For 30 µm diameter droplets containing sodium dodecyl sulfate (SDS), surface tension reduction becomes more significant with increasing surfactant concentration. However, the magnitude of surface tension reduction is smaller than expected for a droplet at equilibrium owing to the short timescale of the measurement. The results provide valuable information about the timescales for surfactant partitioning in microscopic systems.

4AC.5

Optical Properties of Brown Carbon Aerosol in Levitated Droplets.

CHELSEA PRICE, James F. Davies, *University of California Riverside*

Widespread wildfires and biomass burning release aerosol particles containing brown carbon into the atmosphere. These aerosol undergo physical and chemical transformations that influence their effects in the environment. Brown carbon chromophores absorb solar radiation and contribute to atmospheric warming, and may also act as cloud condensation nuclei due to the presence of hygroscopic material. Knowledge of the physical and optical properties of brown carbon aerosol as a function of relative humidity (RH) is limited and needs to be further studied to thoroughly understand their role in the atmosphere.

In this work, a linear quadrupole electrodynamic balance with a broadband light source is used to illuminate suspended aqueous brown carbon particles for Mie resonance spectroscopy. The back scattered light from the particle is then used to determine the size, refractive index, and dispersion properties simultaneously. The broadband light source spans 420-680 nm allowing higher wavelengths (non-absorbing region) to be used for sizing and lower wavelengths (absorbing region) to explore light-absorbing properties. From these methods, we measure the hygroscopic growth and optical properties of pure 4-nitrocatechol (4NC) as well as mixtures of 4NC containing a non-absorbing inorganic component (ammonium sulfate) over a range of mixing ratios. These methods can be applied to other brown carbon species to further classify their hygroscopic and optical properties in order to understand their complex interactions in the environment.

4AC.6

Surface Tension Depression of Aqueous-Phase Glyoxal/Ammonium Sulfate Hanging-Droplet Aerosol Mimics via Direct Photochemistry.

Daphna Fertil, JOSEPH WOO, *Lafayette College*

Carbonyl-containing volatile organic compounds (CVOCs) are present in a wide range of atmospherically relevant contexts and can contribute significant portions of water-soluble organic carbon in aqueous aerosols, forming a variety of heterocyclic and/or oligomeric products under dark conditions. However, condensed-phase chemistry is much less understood, resulting in potential increases and decreases to extent of CVOC oligomerization. This study reports in-situ surface tension measurements of glyoxal/ammonium sulfate hanging-droplet aqueous aerosol mimics, exposed to direct UV-induced photochemistry. While dark chemistry products of glyoxal and ammonium sulfate do not exhibit significant surfactant properties, direct photochemistry results in the immediate formation of products capable of statistically significant surface tension depression. Extent of surface tension depression is measured across multiple bulk-phase concentrations and exposure times, and compared to mimic solution bulk-phase UV/visible absorbance under similar conditions.

4AC.7

Comparison of Hygroscopic Properties of Fresh and Aged Rice Straw and Pine Stem Burning Particles.

ILHWA SEO, Minhan Park, Kihong Park, *Gwangju Institute of Science and Technology*

The biomass burning is a major source of the fine particulate matter ($PM_{2.5}$). Fine particles emitted from biomass burning can lead to adverse health effects and degradation of local and regional air quality. Those particles can also contribute to cloud formation by serving as cloud condensation nuclei (CCN). A laboratory-scale biomass burning chamber was constructed to produce fine particles by the burning of biomasses (rice straw and pine stem). For aging of the biomass burning particle, the Potential Aerosol Mass - Oxidation Flow Reactor (PAM-OFR) was used to simulate the atmospheric photochemical aging process. The biomasses were burning at the different burning phases (flaming and smoldering phase). The burning phases were classified by measuring CO and CO_2 concentrations. For the determination of the hygroscopic property of size-resolved particles, the hygroscopic tandem differential mobility analyzer (H-TDMA) was used. The fresh biomass burning particles showed the higher hygroscopic growth factor (HGF) and cloud formation potential (κ) for rice straw burning particles than pine stem burning particles. The higher hygroscopicity was observed for both particles under the smoldering phase than the flaming phase. Hygroscopic property of the aged particles will be compared with that of fresh particles.

4AC.9

Modeling the Enhanced Growth by α-Pinene Ozonolysis of Wet over Dry Ammonium Sulfate Seed Particles.

MICHAEL S. TAYLOR, Devon Haugh, Murray Johnston, *University of Delaware*

Organic compounds capable of gas-particle phase condensation or partitioning are capable of contributing significantly to particle growth in the Aitken mode size range (10-100 nm). These particles often represent the largest number fractions in the air of ambient environments. Understanding the mechanisms responsible for the growth of these particles allows for cloud condensation nuclei (CCN) to be better predicted. Biogenic volatile organic compounds (BVOCs) such as α-Pinene have been shown to produce low volatility organic compounds via gas phase oxidation reactions. These products 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. Recent work by our group has shown that growth rate is affected by the phase of the seed particle. For experiments performed at 60% RH, deliquesced ammonium sulfate seed particles grow approximately 50% faster than effloresced ammonium sulfate seed particles. For growth by α-Pinene ozonolysis, effloresced particles grow according to a condensational growth model with a condensable organic vapor (COV) yield of approximately 13% (Krasnomowitz et al., AS&T 2019). This yield is somewhat larger that the yield of nonvolatile organic compounds (NVOC) reported in the literature, and one possible explanation is that semivolatile compounds react very quickly at the particle surface with NVOC. Deliquesced seed particle growth would extend these types of reactions to the particle volume as well as the surface. Deliquesced particle growth is modeled by incorporating fast accretion reactions of semi-volatile organic compounds (SVOCs) that partition into the particle phase. By varying the molar yield and volatility of SVOC along with its accretion reaction rate constant, we identify constraints on these variables that are needed in order to explain the experimentally measured particle growth. These constraints give insight into the types of reactions that contribute to enhanced growth of wet particles.

4AC.10

Initial pH Governs Secondary Organic Aerosol Viscosity and Morphology after Uptake of Isoprene Epoxydiols (IEPOX).

ZIYING LEI, Yuzhi Chen, Yue Zhang, Madeline Cooke, Isabel Ledsky, N. Cazimir Armstrong, Nicole Olson, Zhenfa Zhang, Avram Gold, Jason Surratt, Andrew Ault, *University of Michigan*

Aerosol acidity increases secondary organic aerosol (SOA) formation by facilitating reactions that increase the amount of organic material in the condensed phase. Isoprene-derived SOA is largely formed through acid-catalyzed reactive uptake of gaseous species, such as isoprene-derived epoxydiols (IEPOX) onto acidic, sulfate-containing particles. However, the resulting physicochemical properties of mixed inorganic-organic particles after reactive uptake of IEPOX to particles with acidities covering the range of atmospheric pH values (0-5) are not well understood. This study investigated morphology, phase state, and chemical composition of individual organic-inorganic particles with different initial acidities (pH = 1, 3, and 5) after IEPOX uptake using atomic force microscopy coupled with photothermal infrared spectroscopy (AFM-PTIR) and Raman microspectroscopy. Enhanced IEPOX reactive uptake to the most acidic seed particles (pH = 1) resulted in 23% more formation of organosulfates compared to less acidic seed particles (pH 3 and 5). Distinct phase separations (i.e., core-shell morphologies) primarily occurred for initial pH values < 3. Increased aerosol acidity (lower pH) also led to more viscous organic components of SOA particles and more irregularly shaped morphologies as the organic phase transitioned to semi-solid or solid. Conversion of inorganic sulfate to organosulfates corresponded with the transition to the higher viscosity of the organic phase and more complex structures. This study highlights that aerosol acidity controls key multiphase chemical reactions and the subsequent modification of aerosol physicochemical properties, such as viscosity and morphology, which can be used to improve predictions of SOA formation, as well as subsequent climate and health impacts.

4AC.11

Effect of Solution Activity on Regioselectivity of Sulfate Addition in Acid-Catalysed Aqueous Reactions of IEPOX.

SARAH SUDA PETTERS, Tianqu Cui, Zhenfa Zhang, Avram Gold, V. Faye McNeill, Jason Surratt, Barbara Turpin, *University of North Carolina at Chapel Hill*

Atmospheric oxidation of isoprene yields large quantities of highly water-soluble isoprene epoxydiols (IEPOX) that partition into fogs, clouds, and wet aerosols. In aqueous aerosols, acid-catalyzed ring-opening of IEPOX followed by nucleophilic addition of inorganic sulfate or water forms organosulfates and 2-methyltetrols, respectively, contributing substantially to secondary organic aerosol (SOA). However, the fate of IEPOX in clouds, fogs and evaporating hydrometeors is not well understood. Here we investigate the rates, product branching ratios, and stereochemistry of organosulfates from reactions of dilute IEPOX (5 to 10 mM) under a range of sulfate concentrations (0.3 to 50 mM) and pH values (1.83-3.38) in order to better understand the fate of IEPOX in clouds and fogs. From these aqueous dark reactions of β-IEPOX isomers (*trans*- and *cis*-2-methyl-2,3-epoxybutane-1,4-diols), which are the predominant IEPOX isomers, products were identified and quantified using hydrophilic interaction liquid chromatography coupled to an electrospray ionization high-resolution quadrupole time-of-flight mass spectrometer operated in negative ion mode (HILIC/(–)ESI-HR-QTOFMS). The rate constants for the reaction of IEPOX under cloud-relevant conditions are up to one order of magnitude lower than reported in the literature for aerosol-relevant conditions due to markedly different solution activity. We found that regiochemistry and stereochemistry were affected by pH and the tertiary methyltetrol sulfate ($C_5H_{12}O_7S$; MTS) was promoted by increasing solution acidity and provide insight into a plausible mechanism for oxirane ring opening of *trans*-β-IEPOX that could prove helpful in understanding the processing of IEPOX to isomeric MTSs over the broad pH ranges observed in aerosols, fogs, and cloud droplets. The contribution of cloud and fog water reactions to IEPOX SOA may be significant in cases of lower aqueous-phase pH or during droplet evaporation. Process-level insight into the mechanistic controls on observed stereoisomers will likely be helpful in constraining the contribution of cloud and fog conditions to the breakdown of IEPOX in the atmosphere.

4AC.12

Direct Measurement of the pH of Aerosol Particles.

EMMA TACKMAN, Miriam Freedman, *The Pennsylvania State University*

The level of acidity in aqueous aerosol particles found abundantly in the atmosphere has wide ranging effects on a variety of chemical processes from reaction rates to cloud formation but remains poorly characterized. Determining the pH of aerosol particles is difficult due to their small size, so indirect measurements and thermodynamic models have been used despite shortcomings, such as imprecise modeling constraints. Here, we present a new method for directly assessing aerosol particle acidity using carbon quantum dots as a novel in situ fluorophore. Carbon dots are easy to synthesize and are sensitive to pH in the highly acidic regime relevant to ambient aerosol particles. For this study, carbon dots were synthesized in house using a commercially available microwave oven and shown to be indefinitely shelf stable. Our results support the effectiveness of using this fluorophore in previously characterized model systems and proxies for a variety of environmentally relevant aerosol particles. The pH of a series of aerosolized buffered solutions were measured to establish the method. Additionally, the pH of particles containing a complex organic mixture (COM) more representative of environmental aerosols was also determined, proving the efficacy of carbon quantum dots as pH-sensitive fluorophores. The ability to directly measure the pH of aerosol particles and populations will help to parametrize models and improve projections for other aerosol properties and their influence in the atmosphere.

4IA.1

Characterizing Ambient Droplet Aerosols on the International Space Station.

KARL CARDIN, Marit Meyer, Raúl Bayoán Cal, Mark Weislogel, *Portland State University*

In the microgravity environment of a spacecraft in low Earth orbit, aerosols can contain droplets many times larger than those observed in terrestrial environments. In this study, passive aerosol samplers (PASs) were deployed near air return registers on the International Space Station (ISS) to investigate airborne debris, including droplets present in the cabin air. The PASs utilized impaction on a carbon tape substrate to collect droplets. Multiple PAS substrates were deployed at each air return register and periodically removed from the flow one at a time to provide discrete temporal data. High resolution electron microscope images were taken of the substrates after they were returned to Earth. Analysis was performed on the circular prints of solid material left behind by droplets after the liquid evaporated to identify droplet size distributions and topological characteristics of the droplet prints. Predictions of the original droplet sizes present in the airflow were also achieved. The data from this work can inform air quality improvement measures for the ISS as well as future long-term manned space missions.

4IA.2

Aerosol Concentration Signatures on the International Space Station from a Real-time, Long Term Monitor.

MARIT MEYER, Benjamin Sumlin, *NASA Glenn Research Center*

Space is the new frontier, and currently many countries and commercial entities are pursuing exploration opportunities for humans to reside beyond Earth. The International Space Station (ISS) is a test bed for proving life support technologies that will enable safe exploration beyond Low Earth Orbit. NASA's Artemis missions will return humans to the Moon using the ISS-proven technologies. Beyond these missions, NASA's Moon2Mars exploration goals will take humans farther out in the solar system for significantly longer durations. Maintaining good air quality in spacecraft and habitats is fundamental for the success of these missions. On the ISS, the air revitalization system has been under development for the 20 years it has been inhabited by humans, and includes HEPA-level filtration, CO2 removal, oxygen generation and control of trace contaminant gases. Environmental monitoring ensures these and other processes are functioning, and for air quality, this includes gas and particulate monitoring.

The Airborne Particulate Monitor (APM), launched to the ISS in October 2020, made the first real-time aerosol measurements on ISS for the purpose of quantifying air quality. Nearly five months of continuous operation generated a large data set of particle concentrations that has been analyzed to understand trends and typical 'aerosol signatures' based on different ISS locations and total number of crew members. We present the results of this analysis, along with discussion of notable aerosol events which underscore the need for high-fidelity, long term monitoring.

4IA.3

Novel Control Strategies for Indoor Filtration.

TIANYUAN LI, Jeffrey Siegel, *University of Toronto*

Particle filtration systems are widely used indoors to reduce particle concentration and lower occupant exposure. Runtime, which is the fraction of the operation time of the systems, influences the amount of air passing through the system. While increasing the runtime can improve the removal performance of filtration systems, it also increases the energy consumption of the fans. Thus, strategies are needed to improve filtration performance while reducing runtime and conserving energy. In this work, we simulated concentrations using time-varying mass balances of residential indoor environments with stochastic emission events. The exposure reduction, a metric for filtration effectiveness, and removal efficacy, the ratio of exposure reduction to runtime, is calculated to provide a quantitative assessment on four operation strategies. These strategies are sensitive to concentration and/or presence of emission events, pulsing the filtration system regardless of concentration, and pulsing during elevated concentration periods (i.e., a hybrid strategy). The results show that the concentration strategy, which synchronizes operation with high indoor concentrations has the highest removal efficacy. It could achieve a comparable level of exposure reduction as continuous operation, but with runtimes as low as 80%. Adding emission event detection to the concentration strategy did not lead to substantial improvements. The hybrid strategy could further reduce the runtime of the concentration strategy by pulsing but at a cost of decreased exposure reduction. In homes in regions with low ambient concentration but strong indoor emission events, the concentration strategy could save approximately 100 kWh of fan energy over 3 months for efficient fans, and more than 200 kWh for conventional fans. The results show that the concentration strategy provides opportunities for households to regulate indoor concentration while conserving fan energy use.

4IA.4

Impact of Indoor Physicochemical Phenomena on Volatile Chemical Products' Emissions from Indoor Spaces.

AMIRASHKAN ASKARI, Arthur W. H. Chan, *University of Toronto*

The decrease in emissions from fossil fuel combustion sources, especially from the traffic sector, due to mitigation policies implemented during the recent decades has led to increasing relative importance from other sources. Among these emerging sources, Volatile Chemical Products (VCPs) of petrochemical origin are significant contributors to anthropogenic emissions, especially in urban regions. Further to the adverse effect of VCP emissions on ambient air quality, recent works have also provided evidence of the potential of VCP emissions to act as precursors for secondary pollutants like tropospheric ozone and secondary organic aerosol. Although a significant fraction of VCP emissions occurs within indoor spaces like residential and commercial buildings, the effects of indoor processes on their eventual emission into the ambient atmosphere are unknown. In this study, we modelled the effect of indoor gas-phase chemistry and partitioning to indoor surfaces in an unsteady-state framework to shed light on the attenuations/modifications which occur for indoor VCP emissions before they migrate outdoors. We construct a VCP emission inventory for Canada, as a typical developed country, utilizing a bottom-up approach. The differential potency of VCP emissions as pollutant precursors after being processed by indoor phenomena is also covered. The inventory estimations are constrained using building air handler samples and data provided by National Air Surveillance Program (NAPS). While more than 50% of the indoor VCP emissions are prone to gas-phase chemistry, the rate of the reactions is often negligible in comparison with the ventilation rate. Moreover, Partitioning to indoor surfaces is shown to act as a strong reservoir for some of the less volatile species which could keep the species retained within indoor surfaces for up to about 400 days before they migrate outdoors. Overall, our study highlights the importance of indoor physicochemical phenomena on VCP emissions into the atmosphere.

4IA.5

Kinetic Multilayer Modeling of Indoor Surface Chemistry: Organic Film Formation, Bleach Cleaning Chemistry and Surface Interactions.

MANABU SHIRAIWA, Pascale Lakey, *University of California, Irvine*

As part of the Modeling Consortium for Chemistry of Indoor Environments (MOCCIE), we apply kinetic multilayer models to gain fundamental and quantitative understanding of various surface processes indoors. We developed a new model to simulate the initial film formation by treating gas-phase diffusion and turbulence through a surface boundary layer and multi-layer reversible adsorption on rough surfaces, as well as subsequent film growth by resolving bulk diffusion and chemical reactions in a film. The model shows that the films should initially be patchy with the formation of pyramid-like structures on the surface. Sensitivity tests showed that highly turbulent conditions can lead to the film growing by more than a factor of two compared to low turbulence conditions. If surface films adopt an ultra-viscous state, a significant decrease in film growth is expected. The presence of chemical reactions in the film has the potential to increase the rate of film growth by nearly a factor of two. In addition, we simulated the formation and loss of species in the gas phase upon floor-bleaching as measured during the HOMEChem campaign. The model includes a boundary layer next to the bleach and reactions occurred in the aqueous bleach, in the gas phase and on aerosol particles and room surfaces. The model was able to reproduce the loss of ammonia and the formation of chloramines. We also discuss spatial and temporal scales of indoor constituents, as modulated by rates of chemical reactions, surface interactions and building ventilation.

4IA.6

Sampling of Per- and Polyfluoroalkyl Substances (PFAS) with Residential Air Filters. CLARA EICHLER, Naomi Chang, Jiaqi Zhou, Glenn Morrison, Jason Surratt, Barbara Turpin, *UNC-Chapel Hill*

Per- and polyfluoroalkyl substances (PFAS) are a diverse group of chemicals that includes over 9,000 different compounds. Because of their water- and stain-resistant and non-stick properties, PFAS are widely used in consumer products. Not surprisingly, PFAS have been found in indoor air and dust, and concentrations tend to be higher indoors than outdoors. However, the fate of PFAS in indoor environments has not been well assessed. The objective of this preliminary study was to evaluate if filters for residential heating and air conditioning (HAC) systems can be used to sample suspended particles that may contain PFAS. We deployed 6 HAC filters total in 5 single-family homes in North Carolina for 4-9 weeks, extracted the filter material, and analyzed the extracts for nine volatile PFAS using GC-MS. The HAC filter extracts were also analyzed for 34 legacy and emerging per- and polyfluoroalkyl acids (PFAAs) with an AB Sciex Triple Quad UPLC-MS/MS, and for ionic composition using a Dionex ICS-3000 and Aquion.

We found at least one volatile PFAS compound in 5 of the 6 filters. 6 out of 9 analytes were measured above their quantification limits, i.e., the fluoroalkyl sulfonamidoethanols MeFOSE and EtFOSE, the fluoroalkyl sulfonamide MeFOSA, and three fluorotelomer alcohols. The filters showed different analyte profiles for each home. One filter had been deployed for almost 9 weeks, and higher concentrations and a higher number of analytes were observed. Similar trends were observed for the PFAAs. Overall, this sampling strategy proved to be useful, but additional refinements are necessary. Over the summer, we will deploy HAC filters in additional homes for at least 8 weeks as part of a field campaign to assess PFAS partitioning and fate in indoor environments.

4IA.7

Nitrogen-Containing Emissions from Cooking: Mechanisms and Impacts on Indoor and Outdoor Air. JENNA DITTO, Jonathan Abbatt, Arthur W. H. Chan, *University of Toronto*

As emissions from the transportation sector decline due to technological advances and regulatory control, a new set of sources is emerging as important drivers of urban air quality. In particular, food cooking represents a major primary source of gas- and particle-phase organic compounds to the atmosphere, and the contribution of cooking organic aerosol to total primary organic aerosol is comparable to motor vehicles in some major North American cities. In addition to the suite of compounds emitted from heated cooking oil, which contains many mutagenic and carcinogenic hydrocarbons and oxygenates, cooking protein-rich foods can produce nitrogen-containing species across a range of structures and functional groups. Many of these compounds are particularly hazardous to human health, such as heterocyclic amines and acrylamide, and have been observed to form in food itself during high-temperature cooking processes. To evaluate the potential for inhalation exposure to these compounds, we examine the emissions of nitrogen-containing gases and particles during food cooking. Using proton transfer reaction mass spectrometry, offline sampling with gas chromatography-mass spectrometry, and a model system in the laboratory for controlled cooking simulations, we observe a range of nitrogen-containing ($C_xH_yN_{1-3}$) and nitrogen- and oxygen-containing ($C_xH_yN_{1-3}O_{1-3}$) emissions across gas and particle phases. These compounds are formed at variable rates and yields during the thermal degradation of amino acids in cooking oil, from reactions of ammonia and amino acid fragments with oil-derived oxygenates, including precursor aldehydes and carboxylic acids. We investigate these primary nitrogen-containing emissions and their fundamental formation mechanisms within cooking oil. In addition, we evaluate their propensity to react with common indoor reactive gases (e.g. ammonia, nitrous acid) to form secondary nitrogen-containing products, and their subsequent impacts on both indoor and outdoor air.

4IA.8

Measuring and Modeling the Behavior of VOCs on Indoor Wood Surfaces. ANNA ZIOLA, Paul Ziemann, *University of Colorado Boulder*

The average person spends nearly 90% of their lifetime indoors, but we know very little about the chemical and physical processes that impact volatile organic compounds (VOCs) in indoor environments. Perhaps most importantly, we do not fully understand how VOCs interact with surfaces indoors. This makes it difficult to predict and model the behavior of VOCs in rooms with a variety of surfaces, all with different properties and compositions. By measuring the interactions of VOCs with individual surfaces, data can be obtained for improving indoor models and for gaining insight into where VOCs are coming from and going. To study VOC interactions with wood surfaces specifically, we have conducted experiments in which air containing selected VOCs was flown through an uncoated or varnish-coated (umbrella term for any wood coating) wood tube, creating a chromatography-like apparatus where VOCs interact with and equilibrate with the tube surface before they are detected with an iodide chemical ionization mass spectrometer. We then calculated surface absorptive capacities and diffusion coefficients using a model to fit the VOC time profiles. An attenuated total reflectance-Fourier transform infrared spectrometer was also used to measure diffusion coefficients for VOCs in thin varnish films. These experiments have shown that the behavior of VOCs indoors relies less on the identity of the wood and more on the identity of the varnish. Shellac, one of the varnishes studied, has little interaction with carboxylic acid VOCs and is a relatively small VOC sink. Conversely, lacquer, a widely used varnish, has a much higher absorptive capacity than shellac and absorbs a relatively large fraction of the VOCs that contact the surface. The absorptive capacities and diffusion coefficients measured in these experiments can be incorporated into larger indoor air models to predict the fate and behavior of VOCs in various indoor spaces.

4IA.9

Humidity and the Uptake of a Model Organic Peroxide on Naturally Soiled Indoor Window Surfaces. MARC WEBB, Liyong Cui, Karsten Baumann, Jason Surratt, Glenn Morrison, Joanna Atkin, Barbara Turpin, *UNC-Chapel Hill*

Aqueous chemistry on wet aerosol surfaces significantly alters outdoor air composition. Likewise, aqueous chemistry on indoor material surfaces may alter indoor air composition. Surfaces play an important role in indoor air chemistry, where surface area-to-volume ratios are greater than 3 m^2/m^3, orders of magnitude greater than that of typical aqueous aerosols. Indoor material surfaces are soiled with organic and inorganic species from exposure to air pollution; soiling provides a condensed phase reservoir for partitioning of indoor gases , including water. Adsorbed water on indoor surfaces may enhance partitioning and enable aqueous surface chemistry of water-soluble organic gases (WSOGs), including organic peroxides. Here, the effect of relative humidity (RH) on the deposition velocity (v_d) and reaction probability (γ) of a model organic peroxide to naturally soiled interior window surfaces was investigated.

Isoprene hydroxy hydroperoxide (ISOPOOH) was used because of the potential importance of organic peroxides to indoor air quality and chemistry. Glass was soiled in 3 local homes for 1+ years and the surface composition measured. The uptake of ISOPOOH by clean and soiled glass was measured under 5%, 55%, and 85% RH conditions using a novel indoor surface flow reactor coupled to a chemical ionization mass spectrometer (CIMS). Under humid conditions ISOPOOH was initially substantially (78%) depleted for soiled glass; in contrast only 24% removal was observed for clean glass. Under dry conditions, there was no significant enhancement of ISOPOOH uptake to soiled glass compared to clean glass. Steady-state v_d and γ to soiled glass at 55% RH was 0.003-0.001 cm sec^{-1} and 3.3×10^{-7}-6.0×10^{-8}, respectively. The fate of the ISOPOOH and reversibility of uptake will be discussed. This work contributes parameters for indoor air quality and exposure modeling for indoor settings.

4IA.10

Moisture Influences Both Fungal Gene Expression and MVOC Emissions from Carpet and Dust. SARAH R. HAINES, Emma C. Hall, Pawel K. Misztal, Allen Goldstein, Rachel I. Adams, Karen C. Dannemiller, *The Ohio State University*

Microorganisms grow at elevated humidity levels (>80%) in carpet and dust and may release microbial volatile organic compounds (mVOCs) during this growth. Microbes in dust are also metabolically active with metabolic activity increasing with increasing humidity levels. We currently do not understand the relationship between gene expression and the release of mVOCs from microbes in dust at different moisture conditions. The goal of this work was to elucidate how gene expression relates to mVOC emissions at increasing moisture levels. A de novo metranscriptome study was performed utilizing samples of dust only and carpet with dust incubated at 50%, 85% or 95% equilibrium relative humidity for a period of 14 days. Emissions were measured in real time using a proton transfer time-of-flight mass spectrum (PTR-TOF-MS) allowing for unprecedented detection of volatile organic compounds (VOCs). A total 1,140,619,252 paired-end reads were produced from NovaSeq RNA sequencing. After quality trimming, 2,065,127 contigs with a median contig length of 517 were assembled. Results revealed differences in the emissions profile of dust only samples compared to carpet with dust. The total emissions from carpet with dust samples ranged from 8.5 – 9.0 µg/hr over each relative humidity while the dust only samples ranged from 0.22 – 3.1 µg/hr, increasing with moisture level. Across both dust and carpet with dust samples the majority of emissions belonged to the $C_xH_yH^+$ family. $C_5H_{10}H^+$ (cyclopentane or pentene) was the most abundantly emitted compound for each sample type. Ultimately, moisture influenced both fungal gene expression and mVOC emissions from carpet and dust.

4IA.11

Processes and Sources Determining the Composition of Indoor Aerosols. PETER F. DECARLO, Erin Katz, Anita Avery, Michael Waring, David Lunderberg, Allen Goldstein, Wyatt Brown, Jose-Luis Jimenez, *Johns Hopkins University*

While ambient particulate matter (PM) mass concentration remains the main metric for estimating human health impacts from PM exposure, both the location of exposure and composition remain under appreciated factors that may modulate the overall health impacts from PM. This presentation will draw upon results from several field measurement campaigns to explore compositional differences between outdoor and indoor PM and the sources and processes which modify the composition of indoor PM. Temperature and relative humidity gradients between the indoor and outdoor environment change the relative composition of outdoor sourced particles. Indoor activities such as cooking and cleaning can modify indoor aerosol composition. Finally, secondary chemistry with indoor occupants and off-gassing from material and surfaces add additional material and specific chemical species and classes to indoor aerosols. Since the majority of our time is spent in the indoor environment, processes described above play an important role in better characterizing human exposure to particulate matter.

4IA.12

Measurement of Aerosol Volatility Using a Modified Piezoelectric Instrument. LANCE WALLACE, Wayne Ott, *Stanford University*

Collection of an aerosol on a filter and then weighing the filter is often called the "gold standard" for determining the mass of the collected aerosol. Yet if the aerosol is volatile, a portion will evaporate from the filter during collection. For example, an important component of PM2.5, particularly in the West, is ammonium nitrate, which can account for a substantial fraction of the mass. A more recently popular example of a volatile aerosol is the secondhand aerosol produced by vaping electronic cigarettes and, possibly, by vaping marijuana liquids[1]. The cited reference employed 40-year-old Piezobalances (Kanomax, Japan) that had been modified to report and log the frequency differences as well as mass concentrations in each time step. When the frequency difference turns negative, it indicates evaporation from the crystal. However, the standard Piezobalance shows only concentrations and thus cannot measure the loss due to evaporation. However, in response to a letter from a number of scientists asking Kanomax to make available some instruments modified to report frequency differences, it has just been learned (May 2021) that Kanomax will make such modifications upon request of buyers. This presentation will explain how to use the newly modified instruments to measure volatility of selected aerosols.

[1] Wallace, L.A., Ott, W.R., Zhao, T., Cheng, K-C, and Hildemann, L.M. 2021 Method for estimating the volatility of aerosols using the Piezobalance: examples from vaping e-cigarette and marijuana liquids. Atmospheric Environment Volume 253, 15 May 2021, 118379.
https://doi.org/10.1016/j.atmosenv.2021.118379

4IM.1

In-Silico Investigation of Electron Ionization Mass Spectra of Nitro-Heterocyclic Chromophores in Brown Carbon Aerosols. MEGAN WOODS, Kunpeng Chen, Nilofar Raeofy, Roya Bahreini, Ying-Hsuan Lin, *University of California, Riverside*

Brown Carbon (BrC) aerosol's ability to absorb solar radiation has emerged as an uncertain factor in climate forcing. Heterocycles are abundant components in biomass burning emissions; however, the optical properties of their resultant secondary organic aerosol remain unclear. These uncertainties stem from an incomplete characterization of BrC chromophores. Mass spectrometry-based analytical measurements have been widely used to speciate BrC aerosol constituents. Nevertheless, due to the large variety and chemical complexity of BrC aerosols, there is a lack of authentic standards readily available to aid in the identification of these compounds. Utilizing Quantum Chemical Electron Ionization Mass Spectra (QCEIMS) to simulate a theoretical EI mass spectrum may facilitate overcoming this barrier. In this study, we examined the performance of varying Density Functional Theory (DFT) computational methods (e.g., PBE and B97D) as well as the new standalone XTB-2 method in QCIEMS to determine a method of high accuracy and computational efficiency. We assessed the performance of these computational methods on nitro-heterocyclic compounds, including 2-nitrofuran, 2-nitrothiophene, and 2-nitropyrrole. In preliminary work, the accuracy of the computational chemistry functional methods was evaluated using Stein/Scott matching method to compare the theoretical spectra to National Institute of Standards and Technology (NIST) EI standards. The gradual gradient approximation (GGA) DFT methods PBE, B97D, and the XTB-2 method on 2-nitrofuran showed matching scores of 679, 591, and 681, respectively, while their required computational times were 192, 36, and 2 hours, respectively. Our results indicate that XTB-2 method may be used to speciate molecular structures of BrC chromophores when authentic standards are not readily available. Together with experimental characterization of BrC constituents obtained from aerosol mass spectrometry (AMS), this technique may be used in conjunction with positive matrix factorization (PMF) to develop comprehensive source profiles of complex aerosols.

4IM.2

Development of a Higher Mass Resolution Aerosol Chemical Speciation Monitor.

PHILIP CROTEAU, Benjamin A. Nault, Leah Williams, Manjula Canagaratna, Harald Stark, Donna Sueper, John Jayne, Douglas Worsnop, *Aerodyne Research, Inc.*

Over the past ten years, the aerosol chemical speciation monitor (ACSM) has become a valuable tool for understanding aerosol chemistry by enabling measurements of long-term trends in particle composition with high temporal resolution. However, the low mass resolution of the ACSM detector limits the chemical specificity of the measured mass spectra when compared with, for example, the high-resolution time-of-flight aerosol mass spectrometer (HTOF-AMS). Specifically, the detection limit of ammonium with the standard unit mass resolution ACSM is much higher than with HTOF-AMS because its largest signals, NH_2^+ at m/z 16 and NH_3^+ at m/z 17, are measured against the much larger isobaric signals of O^+ and OH^+ from oxygen and water. Furthermore, ACSM organic aerosol chemical composition measurements are limited by their inability to directly distinguish oxygen-bearing organic fragments from hydrocarbons, such as $C_2H_3O^+$ and $C_3H_7^+$ at m/z 43. Here we present instrumental details and data from a new version of the ACSM, the TOF-ACSM X, designed to mitigate these limitations. The TOF-ACSM X detector is a mass spectrometer designed to be robust and capable of long-term, unattended operation, like the standard ACSM, but to also provide enough mass resolution to dramatically improve the quantification of ammonium and to allow for more accurate quantification of the elemental ratios O:C and H:C in the organic aerosol.

4IM.4

Detailed Characterization of Secondary Organic Aerosol Composition Using Multiple Mass Spectrometric Techniques.

ERIK HELSTROM, Abigail Koss, Jordan Krechmer, Manjula Canagaratna, Frank Keutsch, Alexander Zaytsev, Jesse Kroll, *MIT*

Chemical processing of gas-phase organic molecules in the atmosphere can lead to the formation of secondary organic aerosol (SOA). Because thousands of species can be involved in the chemical processing of organic carbon in both the gas and particle phase, tracking the evolving properties of SOA presents a formidable analytical challenge. Real-time chemical characterization of aerosol-phase mixtures can be achieved with a variety of mass spectrometric instruments, but there are important limitations on the capabilities of each individual measurement. “Hard” ionization techniques like Aerosol Mass Spectrometry (AMS) are suitable for the measurement of total particle carbon, but they are chemically nonspecific. By contrast, chemical ionization mass spectrometers (CIMS) can identify individual species but are more selective. Coupled with inlet schemes for phase-separated sampling, these CIMS allow for highly resolved measurements, but only of a subset of the total mixture. Any analytic assessment of the total carbon behavior from a single instrument therefore may be biased by omission of undetected species. In order to more comprehensively characterize SOA composition and behavior, we consider measurements of chamber oxidation experiments of various organic compounds taken by four mass spectrometers: AMS, Thermal Desorption-Proton Transfer Reaction-Mass Spectrometer (TD-PTR-MS), Thermal Desorption-Ammonium-CIMS (TD-NH4-CIMS), and Iodide-CIMS with a Filter Inlet for Gases and Aerosols (FIGAERO-I-CIMS). Carbon number, oxidation state, volatility, and nitrogen content are considered on the individual species level and for the total measured product distribution. These metrics allow for comparison between instruments, as a function of precursor identity and oxidant exposure. Overlaps between measurements are used to identify biases for different instruments and to construct a multi-instrument synthesis of measurements, enabling a comprehensive and quantitative measurement of organic aerosol composition. These measurements can then be compared with the composition of gas phase products and used for updated descriptions of organic carbon evolution and SOA formation.

4IM.5

Non-Targeted Screening Approach for Biomass Combustion Organic Aerosol Composition. THUSITHA DIVISEKARA, Simeon Schum, Lynn Mazzoleni, *Michigan Technological University*

Biomass combustion contributes a large amount of aerosol particles to the atmosphere impacting the climate system and human health. Identification of the molecular composition of biomass burning organic aerosol is challenging because of its complex nature. Ultrahigh resolution mass spectrometry (UHRMS) is often used for organic aerosol analysis, but direct infusion does not provide structural or quantitative information. Traditionally, liquid chromatography (LC) coupled with mass spectrometry uses targeted screening methods, which can limit the analysis of aerosol to preconceived compositions. Non-Targeted Screening (NTS) methods provide a comprehensive analysis, but instrument and data analysis methods are challenging due to the extreme complexity of natural samples. In this work, we use LC and UHRMS to analyze commercially available liquid smoke as a surrogate for biomass burning aerosol. Non-targeted chromatographic data was studied using MZMine2.53 and the extracted analytes were identified using MFAssignR software. Over 1300 individual molecular formulas corresponding to 5241 molecular species including structural isomers were successfully assigned. Of these, 1153 molecular formulas were common between direct infusion and LC/UHRMS analysis for the same liquid smoke sample. The common formulas accounted for 99% of the total peak area in the LC/UHRMS identified species and 97% of the total abundance of the direct infusion UHRMS identified species. The results demonstrate a significant advance in our ability to obtain structural and quantitative information about the molecular level composition of biomass burning aerosol.

4IM.6

Aerosol Mass Spectrometer Quantification of Cooking Organic Aerosol Indoors and Implications for Outdoor Reduced Aerosol. Erin Katz, Hongyu Guo, Pedro Campuzano-Jost, Douglas Day, Wyatt Brown, Erin K. Boedicker, Matson A. Pothier, David Lunderberg, Sameer Patel, Kanan Patel, Patrick Hayes, Anita Avery, Lea Hildebrandt Ruiz, Allen Goldstein, Marina Vance, Delphine K. Farmer, Jose-Luis Jimenez, PETER F. DECARLO, *Johns Hopkins University*

The Aerodyne aerosol mass spectrometer (AMS) is used extensively to study the composition of non-refractory submicron aerosol composition during atmospheric field studies. During two recent studies of indoor environments, HOMEChem and ATHLETIC, the default ambient organic aerosol AMS quantification parameters resulted in a large discrepancy with co-located instruments while sampling cooking organic aerosol (COA). Instruments agreed within uncertainty estimates during all other sampling periods. Assuming a collection efficiency (CE) of unity, adjustments to the AMS relative ionization efficiency (RIE) were required to reach agreement with co-located instruments. The range of RIECOA observed (ATHLETIC: RIE_{COA}=4.26-4.96, HOMEChem: RIE_{COA}=4.70-6.50) was consistent with RIE measured in the laboratory for cooking-specific molecules. These results agree with prior AMS studies which have indicated that more oxidized outdoor ambient organic aerosol has a relatively constant RIE of 1.4 ± 0.3 while more reduced organics have higher RIE. The applicability of a higher RIE was considered for two ambient datasets, and agreement between the AMS and co-located instruments improved when an increased response factor (RIE CE) × was applied to positive matrix factorization-derived primary organic aerosol (POA). Based on the observations presented here and the literature, we recommend AMS users consider applying RIE_{COA}=4.2 to source and indoor studies of COA and evaluate a higher POA response factor of the order of ~1.5 in outdoor studies at urban background sites, and ~2 at sites impacted by fresh sources. This study aims to improve AMS quantification methodology for reduced POA and highlights the importance of careful intercomparisons in field studies.

4IM.7

Potential Underestimation of Particulate Organic Nitrate Concentration by an Aerosol Mass Spectrometer. MASAYUKI TAKEUCHI, Yuchen Wang, Benjamin A. Nault, Manjula Canagaratna, Nga Lee Ng, *Georgia Institute of Technology*

Ambient measurements across the globe to date indicate the ubiquitous presence and substantial contribution of particulate organic nitrate (pON) to sub-micron organic aerosol. Accurate quantification of gas- and particle-phase ON is crucial to understand its role in secondary organic aerosol (SOA) formation and NO_x cycling. Yet, a limited number of techniques is available for ON quantification and instrument inter-comparison efforts are scarce. An Aerodyne aerosol mass spectrometer (AMS) is widely used for pON measurements. In this study, we examined the response of the AMS towards aerosol species with hydroxyl nitrate moieties using authentic standards. Four hydroxyl nitrates derived from isoprene, α-pinene, β-pinene, and limonene were investigated. The methanol solution of each hydroxyl nitrate was atomized, size-selected at 250-400 nm via a differential mobility analyzer, and introduced into the AMS and a condensation particle counter (CPC). The measured NO_3:Org molar ratio is substantially lower (0.3) than the expected ratio of 1 based on the molecular structure of the standards. The mass-based comparison with CPC suggests that the NO_3 measured by the AMS (collection efficiency corrected) is lower than CPC-measured NO_3, with a slope of 0.44-0.6 depending on the precursor compounds (isoprene vs. different monoterpenes). In other words, AMS underestimates pON-derived NO_3 concentrations by approximately a factor of two. We hypothesize that relative ionization efficiency of lab-generated organic hydroxyl nitrate species differs from that of inorganic nitrate in the AMS. As pON quantification from AMS relies proportionally on the NO_3 measurements, this study provides new insights for a more accurate pON quantification.

4IM.8

Optimizing a Pressure-controlled Inlet (PCI) Coupled with a PM2.5 Lens for Aircraft Measurements with the Aerodyne Aerosol Mass Spectrometer (AMS) in the Lower Stratosphere. DONGWOOK KIM, Pedro Campuzano-Jost, Hongyu Guo, Da Yang, Mark Kanaparthi, Suresh Dhaniyala, Leah Williams, John Jayne, Douglas Worsnop, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

Aerosols in the upper troposphere and lower stratosphere (UTLS) are crucial to understanding radiative forcing, ice cloud formation, and ozone chemistry. In-situ aircraft measurements with fast chemical composition sensors are essential to further our understanding of the underlying processes. Mass spectrometers such as the Aerodyne Aerosol Mass Spectrometer (AMS) and several single particle mass spectrometers have been used for these measurements. Such instruments typically use an aerodynamic lens as an inlet that collimates aerosols into a small detection volume over a wide range of particle sizes. However, such lenses depend on a constant upstream pressure to work consistently, and airborne interfaces that provide that (pressure-controlled inlets –PCI-) have historically performed less well at high altitudes. In this study, we are developing and testing a new PCI design coupled with two types of recently developed $PM_{2.5}$ aerodynamic lenses towards the goal of sampling PM_1 aerosols up to ~16 km altitude. We use state-of-the-art fluid dynamic models to inform development and testing. We characterize the transmission efficiency (TE) as a function of particle size over the range of pressures relevant for airborne sampling. As part of this project, a new lens alignment tool and a new particle beam imaging device, based on the Aerodyne aerosol Beam Width Probe (BWP) have been developed and tested. We show the current performance of the new PCI combined with the two different $PM_{2.5}$ lenses and discuss potential improvements.

4IM.9

A New Method to Quantify Particulate Sodium and Potassium Salts (Sulfate, Nitrate, and Chloride) by Thermal Desorption Aerosol Mass Spectrometry.

YUYA KOBAYASHI, Nobuyuki Takegawa, *Tokyo Metropolitan University*

Aerosol particles emitted from sea spray and biomass burning have significant contributions to the global budget of aerosols. The reaction of sea salt (or biomass burning) particles with sulfuric acid (H_2SO_4) and nitric acid (HNO_3) leads to the displacement of chloride relative to sodium (or potassium). We have recently developed a new particle mass spectrometer to quantify non-refractory and refractory sulfate aerosols (referred to as the refractory aerosol thermal desorption mass spectrometer: rTDMS). The combination of a graphite particle collector and a carbon dioxide laser enables high desorption temperature (up to 1200 K). Ion signals originating from evolved gas molecules are detected by a quadrupole mass spectrometer. Here we propose a new method to quantify the mass concentrations of sodium chloride (NaCl: SC), sodium sulfate (Na_2SO_4: SS), sodium nitrate ($NaNO_3$: SN), potassium chloride (KCl: PC), potassium sulfate (K_2SO_4: PS), and potassium nitrate (KNO_3: PN) particles by using the rTDMS. Laboratory experiments were performed to test the sensitivities of the rTDMS to various types of particles. We measured ion signals originating from single-component particles for each compound, and found a good linearity ($r^2 > 0.8$) between the major ion signals and mass loadings. We also measured ion signals originating from internally mixed SC/SS/SN (or PC/PS/PN) particles, and found that the temporal profiles of the ion signals at m/z 23 (or 39) were characterized by three sequential peaks associated with the evolution of the desorption temperature. We tested potential interferences in the quantification of sea salt particles under real-world conditions by artificially generating “modified” sea salt particles from the mixture of diluted seawater and SS/SN solution. Based on these experimental results, the applicability of the rTDMS to ambient measurements of sea salt and biomass burning particles is discussed.

4IM.11

Characterization of Organic Aerosol Relative Ionization Efficiency for the Aerosol Mass Spectrometer and Aerosol Chemical Speciation Monitor.

BENJAMIN A. NAULT, Philip Croteau, Leah Williams, Manjula Canagaratna, *Aerodyne Research, Inc.*

The Aerosol Mass Spectrometer (AMS) and the Aerosol Chemical Speciation Monitor (ACSM) are widely used to measure the chemical composition and mass concentration of submicron, non-refractory aerosol particles. An important component of the non-refractory aerosol is organic aerosol (OA). Unlike non-refractory inorganic aerosol, which can easily be calibrated, OA is composed of 1000s of compounds. The response of the AMS/ACSM to non-NH4NO3 particle mass is determined with species-dependent relative ionization efficiencies (RIE) and a primary ionization efficiency that is obtained from calibrations with an instrument standard (NH4NO3). Although a value of 1.4 has been found to explain the ambient OA observed across various campaigns, recent laboratory and ambient measurements have suggested the RIE of OA may have a dependence on OA oxidation state (OSc), with more reduced OA having higher RIE values than more oxidized OA.

Here, we develop a simple method for calibrating OA_RIE across the range of OSc relevant for ambient OA measurements. We use laboratory measurements of atomized OA surrogates to characterize the OA_RIE for both the AMS/ACSM. These standards have been sampled in a variety of solvents and mixtures to evaluate potential matrix effects and to create a standard procedure for AMS/ACSM users to calibrate their instruments. We identify several binary mixtures of alcohols and NH4NO3 that can be used to produce consistent OA_RIE measurements for organics within the OSc range of –1.5 to 0.5. High OA_RIE values that are observed for laboratory OA species in the OSc range of –2.5 to –1.5 are compared with those calculated for realistic, reduced OA species extracted from ambient filters collected at urban sites and from emission sources. The use of ambient filters allows for deconvolution of potential species-dependent lens transmission and RIE effects in on-line, ambient AMS measurements.

4IM.12

A Searchable Database and Mass Spectral Comparison Tool for Aerosol Mass Spectrometer (AMS). SOHYEON JEON, Michael Walker, Donna Sueper, Anne Handschy, Douglas Day, Jose-Luis Jimenez, Brent Williams, *Washington University in St. Louis*

The aerosol mass spectrometer (AMS) is one of the most widely applied tools for analyzing the bulk composition of atmospheric particles. AMS observations from field and laboratory studies have generally been reported in text form in peer-reviewed literature. An AMS-users mass spectral database has been created and maintained on an open-access website, but with growing numbers of datasets from around the globe and higher mass resolution spectra, the database needs revisions to meet new demands and applications. One major limitation of the web-based database is the inability to automatically search the database and compare previous mass spectra with the researcher’s own data. In this study, a searchable database tool for the AMS spectral dataset was built to improve the efficiency of the data analysis process using Igor Pro, consistent with existing AMS software. The database incorporates the published mass spectra and sample information from source-specific ambient, laboratory, and factor analysis-derived data uploaded on the website. It compares the target mass spectrum with the existing mass spectra in the database, calculating cosine similarity, and provides a range of mass spectral comparison plots. The aim is to help AMS users efficiently analyze their own data for possible source or atmospheric processing contributions in comparison to previous studies. Furthermore, users are able to submit their data using an export panel to upload their data to further expand the database. The AMS database will be regularly updated and posted on the website including the newly submitted mass spectra.

4SI.1

Evaluating the Decay of SARS-CoV-2 Aerosols: An Overview of Methods, Results, and Remaining Knowledge Gaps. MICHAEL SCHUIT, Paul Dabisch, *BNBI / DHS NBACC*

Aerosol transmission is thought to contribute to the spread of SARS-CoV-2, although the potential for aerosol transmission to occur in specific scenarios is dependent on many factors, including the sensitivity of the virus to ambient environmental conditions. Over the course of the COVID-19 pandemic, studies from several institutions have reported data on the effect of environmental conditions, particle composition, and other parameters on the stability of SARS-CoV-2 in aerosols. The results of these studies have provided valuable insights into the potential for SARS-CoV-2 transmission to occur via the aerosol route. Here we present an overview of the existing data on SARS-CoV-2 aerosol decay and the approaches that have been used to generate those data, with a particular focus on the studies that have been performed by our laboratory. A summary of remaining key questions associated with the survival of SARS-CoV-2 in aerosols will also be discussed.

4SI.2

Medium Scale Wind Tunnel Testing of Aerosolized Coronavirus Collection and Inactivation in Recirculating Air Purification Systems. YUECHEN QIAO, My Yang, Ian Marabella, Devin McGee, Bernard Olson, Montserrat Torremorell, Christopher J. Hogan, *University of Minnesota*

A number of recirculating air purification technologies are available for consumers, which are now marketed towards effectively reducing concentrations of virus-carrying particles indoors. These products can incorporate a wide variety of control technologies, including but not limited to fibrous filters and UV sources. However, the majority of such technologies remain untested not only in their ability to collect particles, but to collect and inactivate airborne viruses. We have developed a method to directly evaluate the single-pass efficiency of the consumer available recirculating air purification technologies marketed for removal of infectious aerosol airborne viruses. Specifically, inspired by the ASHRAE 52.2 testing protocol, we have designed wind tunnel which can operated from 283 L min^{-1} to 2406 L min^{-1}, and by sealing recirculating air purifiers within it, upstream and downstream sampled virus concentration measurements yield single-pass removal efficiency and single pass log-reduction. To date we have tested several technologies with three aerosolized viruses: porcine respiratory coronavirus, bovine coronavirus, and influenza (H1N1). Upstream and downstream sampling of virus-laden aerosols in the wind tunnel enables log reduction in viral and particle concentration via fluorimetry (detected fluoroscien, spiked into nebulized viral suspensions), virus titration, and RT-qPCR measurements; comparison of titration and RT-qPCR results enables inference of inactivation based log reduction. To date, virus aerosol capture and inactivation performance has been determined for three air purification technologies with this wind tunnel: (1). a UV-C ducted system which is designed purely for virus inactivation; (2) a recirculating fibrous filter system containing a photoelectrochemical oxidation (PECO) layer, and (3) a combined electrostatic precipitator (ESP) and HEPA filter system. This presentation will discuss design and operation of the wind tunnel for such tests, as well as results to date for virus inactivation and removal for the aforementioned systems.

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4SI.3

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 chamber. An air-jet nebulizer was used to disseminate known numbers of BCoV particles. Particle tracking velocimetry, PTV, 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) at 100 L/min with the MD8 reference sampler at 50 L/min and quantitated by qPCR. BCoV samples were tested before aerosolizing in the humidity chamber and again after the aerosol samples were collected using biolayer interferometry to determine the environmental effects on association and dissociation of the virus to surfaces. The study shows that impaction-based collection using gelatin filters results in virus aerosol numbers that are a magnitude higher compared to impingement-based sampling. Similarly, high numbers of virus aerosols were collected from the chamber surfaces. Kinetics studies with interferometry show a strong attachment of the coronavirus to hydrophobic surfaces, exhibiting increasing association at low temperatures and in the presence of hydrophobic compounds. PTV analysis of the aerosols shows that environmental parameters affect virus aerosolization and resuspension and could play an important role in COVID-19 transmission.

4SI.4

Effects of Ventilation Strategy and Social Distancing on Inhalation Exposure to Airborne Respiratory Aerosols.

GEN PEI, Mary Taylor, Donghyun Rim, *Penn State University*

Airborne disease transmission via respiratory aerosols is one of the major routes of the spread of the infectious diseases. Ventilation and social distancing are two widely recognized control strategies to reduce the airborne infection risk in indoor environments. However, little information is available on how inhalation exposure to infectious aerosols varies with ventilation strategy and social distance. The objective of this study is to provide a better understanding of the efficacy of ventilation strategy and social distancing in control of inhalation exposure to respiratory aerosols. This study employed the Computational Fluid Dynamics simulations of the aerosol transport in the ventilated rooms and performed the infection risk assessment. The study results show that indoor airflow patterns associated with ventilation strategy have notable impacts on the concentration of respiratory aerosols in the human breathing zone. In the buoyancy-driven flow regime (that can be found in many residential buildings and naturally-ventilated rooms), the exhaled aerosols due to talking of an infector can penetrate into the other occupant's breathing zone within 1 min, which leads to elevated human exposure to the aerosols. In such cases, a 2 m (6 ft) social distance between occupants is not sufficient to effectively reduce the infection risk. Our results also reveal that the virus transmission risk is highly dependent on the aerosol emission mode (e.g., talking and breathing) and initial exhaled airspeed.

4SI.5

Comparison of CFD Model and One-Compartment Materials Balance Model for Predicting 8-Hr Exposure to Pathogen-Laden Expiratory Droplets in a Two-Person Office.

MAHENDER SINGH RAWAT, Sohaib Obeid, Paul White, Jacky Rosati Rowe, Goodarz Ahmadi, Andrea Ferro, *Clarkson University*

In this study, we estimate predicted levels of 8-hr exposure to pathogen-laden expiratory droplets within a representative two-person workspace. The scenario modeled included one asymptomatic infected individual present in the simulated workspace. Inhalation exposure was estimated at the adjacent office workstation, which is physically separated by a cubical divider. The pathogen release is represented by the quanta emission rate, where one quanta is the "dose of airborne droplet nuclei required to cause infection in 63% of susceptible persons", using SARS-CoV-2 as an example (Buonanno et al. 2020). The quanta emission rate was divided into several particle sizes based on size distributions found in the scientific literature.

The computational fluid dynamic (CFD) approach with the use of the three–equation (k-kl-ω) turbulence model of Walters and Cokljat (2008) was used in the simulations. The infected droplet concentration in the office space was evaluated with a user-define-function (UDF) accounting for the turbulent diffusion and gravitational sedimentation. Size-resolved deposition rates for the materials balance modeling were obtained from the indoor aerosol literature.

For the same baseline scenario, the average concentration of 1-micron particles predicted by the CFD model and the materials balance model is approximately the same. Both models estimate 0.35 quanta for an 8-hr emission and intake. The CFD and materials balance model results diverge for the larger particle sizes. For the small two-person office, both increases in the ventilation rate and face coverings worn by the infected and susceptible individuals reduced 8-hr exposure estimates dramatically. Because many exposure models are based on the materials balance modeling approach for which instantaneous mixing is a basic assumption, a comparison with the CFD modeling approach quantifies the result of this assumption for time-averaged exposure estimates.

This document has been reviewed in accordance with U.S. Environmental Protection Agency policy and approved for publication.

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4SI.6

Synergies Between Indoor and Outdoor Air Quality Monitoring Tools in a Home-Working Environment.

Stefano Natali, MIHAI CHIRUTA, *AerosolWorks LLC, Madison, Wisconsin, USA*

In the past year the typical office workspace had become unusable due the poor air quality associated with the airborne transmission nature of the virus responsible for the Coronavirus disease 2019 (COVID-19). Many businesses using office spaces took measures trying to limit the spreading of COVID-19. One of these measures, where it was possible, was to close the office spaces and allow the personnel to work from home. In this context the transmission of COVID-19 was reduced being limited to the household environment. With such a massive workforce migration from a controlled environment to individual households' workspace arise the question of workspace at home indoor air quality.

At the same tine, outdoor air quality monitoring tools have significantly improved thanks to new satellite technologies, numerical modelling and synergies of these two sources with ground measurements. The result are reliable assessment and forecast services for urban and countryside areas.

In this paper we are going to monitor outdoor and indoor air quality parameters using the newly developed “my air” integrated environmental monitoring system for indoor analysis, and the Copernicus Sentinel-5P and the Copernicus Atmospheric monitoring Service (CAMS) for outdoor atmospheric and air quality conditions. The parameters that we will monitor are: barometric pressure, temperature, relative humidity, CO2 concentration, total volatile organic compounds concentration, and particulate matter concentration in four channels PM 1, PM2.5, PM 4, PM10. At least one urban test site (Vienna, Austria) will be taken into account. This study will contribute to the upcoming request of home-based workspaces with good indoor and outdoor air quality conditions.

4SI.7

Feasibility of a High-Volume Filter Sampler for Detecting SARS-Cov-2 RNA in COVID-19 Patient Rooms.

KAMALJEET KAUR, Amanda Wilson, Rachael Jones, Kerry Kelly, *University of Utah*

The presence of aerosolized virus particles in COVID-19 positive patients’ rooms are a serious issue in healthcare as it places healthcare providers at risk of possible infection. To better understand this risk, researchers have been collecting aerosol samples in high-risk areas, and many different methodologies, with differing uncertainties regarding the feasibility and reliability, have been implemented. This study evaluated the feasibility of using a high-volume filter sampler for detecting SARS-Cov-2 in a medical intensive care unit (MICU), and in a COVID-19 ward, specifically in patients’ rooms and the nurse’s station. The high-volume sampler collects air at a flow rate of 200 LPM through a filter, which later was extracted in an elution buffer, followed by multi-plex nested polymerase chain reaction (PCR) to detect for SARS-CoV-2-RNA. The instrument was compared to the BioSpot-VIVAS, known for high efficiency in the collection of virus-containing bioaerosols. One of 28 (high-volume filter sampler) and zero out of 6 (BioSpot-VIVAS) samples were positive for SARS-CoV-2. The high-volume filter sampler was more portable and less intrusive in healthcare environments than the BioSpot-VIVAS. However, limits of detection and virus recovery efficiencies remain unknown. This study will inform future work to evaluate the reliability of these types of instruments and inform best practices for their use in healthcare environments for SARS-CoV-2 air sampling.

4SI.8

Quantifying SARS-CoV-2 Infectious Particulate Exposure Risk, Mixing, and Removal Using DNA-Tagged and Real-Time Fluorescent PSL Microsphere Tracers in Wide-Bodied Boeing 777 and 767 Airframes. SEAN KINAHAN, David Silcott, Blake Silcott, Ryan Silcott, Peter Silcott, Braden Silcott, Steven Distelhorst, Vicki Herrera, Danielle Rivera, Kevin Crown, Gabriel Lucero, Joshua Santarpia, *National Strategic Research Institute*

Airplane travel provides a unique potential for exposure to infectious aerosols because of long flight times and densely packed seating. In this study fluorescent (one micron) and DNA-tagged (three micron) PSL tracer beads were used to mimic the spread and removal of small aerosols in Boeing 767 and 777 airframes. Tracer particles were released from a medical nebulizer mounted in a mannequin mouth to simulate a single infected person seated during flight. Releases occurred in multiple sections of the planes and from multiple seats during ground and in-flight testing. A combination of Sartorius MD-8 Airport collectors for the DNA-tagged tracer and real-time light-induced fluorescence (LIF) Instantaneous Biological Analyzer and Collector (IBAC) sensors placed in nearby seats from the simulated infected individual quantified the number of particles reaching each breathing zone of the simulated non-infected individuals.

In-flight, for both the 767 and 777 airframes, the minimum observed concentration of one micron aerosols from the infectious individual to the breathing zone of a non-infected individuals seated immediately adjacent was reduced by 99.54% during all testing. For all other proximate seats (two forward and aft, two to the side, and the diagonals), the average reduction of one-micron aerosols were 99.98±0.0027% (n=177 seats) and 99.97±0.0086 (n=152 seats) in the 767 and 777, respectively. High reduction rates are attributed to the 30 air-change-per-hour exchange rates and limited longitudinal air movement integral to the aircraft design.

The results of the present study support the existing epidemiological data that large-scale transmission events during flight are improbable. Notably, the present study only investigates small particles to simulate infectious aerosols. Other factors, such as the amount of SARS-CoV-2 shedding from an individual, viral fate in the air, infectious dose via the aerosol route, and potential non-aerosol (droplet or fomite) transmission are important when assessing the overall transmission risk.

4SI.9

Real-Time Space-Resolved Monitoring of Aerosol Distribution in Operating Rooms and Intensive Care Units. KAITLYN GLENN, Jiayang He, Robert Rochlin, Abhyjot Pandher, Ching-Hsuan Huang, Joelle Segovia, Bailey Deck, Selina Teng, James Hecker, Igor Novosselov, *University of Washington*

Many infection diseases, including Covid-19, can spread by aerosols. In hospital environments such as operating rooms (ORs) and Intensive Care Units (ICUs), it is critical to assess the persistence of potentially infectious aerosols to minimize their effect on patients and staff. Medical facilities do not assess the fate of aerosols generated by an infected person or particles generated during medical procedures, as both time and space resolution measurement of aerosol concentration is required. We deploy a monitoring network of 16-20 low-cost particle sensors per room in four ORs and four ICUs to map the movement and size of particles with a time resolution of ten seconds. Monitors are placed around the bed and room at various heights and distances between 2-6 feet apart and outside the room at a nursing station to record the concentration passing through each point. Mimicking aerosol generation by a patient, we nebulize saline solution to create NaCl particles that act as tracers for potentially infectious aerosols. We could draw several conclusions from the experiments performed at the University of Washington Medical Center. (i) Operating rooms are very effective at exchanging air and may require less than a third of the time that is currently recommended by the guidelines for infectious disease control. Typically, the aerosol concentration returns to the baseline within 5 minutes after aerosolization is terminated. (ii) Often, medical equipment blocks the air vents, which contributes to reduced airflow and increase exfiltration of potentially infectious aerosol from the OR into the hallway. (iii) Negative pressure ICUs are more effective at removing the aerosol particles and require up to one-third less time to clear the aerosol loading than positive pressure ICUs. The sensor network approach can be used to optimize the HVAC system and to understand the spread of infectious diseases in hospitals.

4SI.10

Respirator and Face Mask Particle Filtration Efficiency: Experimental Comparison of Test Methods. JOEL CORBIN, Gregory Smallwood, Ian Leroux, Jalal Norooz Oliaee, Fengshan Liu, Richard Green, Nathan F. Murnaghan, Timothy Sipkens, Triantafillos Koukoulas, Prem Lobo, *National Research Council Canada*

Respirators, medical masks, and face coverings all filter airborne particles using similar physical principles. Measurements of their filtration efficiency must also be made using comparable test methods. Current standardized test methods address this need by specifying environmental conditions, flow rate through the filter media (face velocity), key aerosol-particle properties (mean size, size variability, electric charge, density, and shape), and measurement techniques. However, these specifications vary between existing measurement test methods such as the NIOSH TEB-APR-STP-0059 under US 42 CFR 84 (for N95 respirators), ASTM F2299/F2100 (for medical face masks) and their international analogues. To quantify and understand the effects of each of the differences listed above, we have performed systematic experiments using a custom-built measurement system and combined the results with theoretical calculations and physical interpretations. The filtration efficiency is most sensitive to changes in face velocity and particle charge. For example, a material may filter charged and neutral particles with 99.5 % and 68 % filtration efficiency, respectively. Separately, the filtration efficiency may drop from 92% to 75% for face velocities representing adult breathing rates at rest and during exercise, respectively. Relative to the NIOSH method, users of the ASTM F2299 method have normally used non-neutralized (highly charged) aerosols at lower face velocities, although a strict reading of the latter method allows for higher face velocities and includes a recommendation for neutralization. On the other hand, the performance of some respirators was found to increase or decrease with environmental conditioning under the NIOSH method, allowing for potential false positives as well as false negatives in respirator testing. We discuss the application of our results to FFP2, KN95, P2, Korea 1st Class, and DS2 respirators, as well as barrier face coverings in the context of the COVID-19 pandemic.

4SI.11

Effect of Valved and Unvalved N95 Respirators and Face Coverings on Exhaled Particles. ANDREW VINER, Christine McCool, David Buckley, Nicole McCullough, *3M*

Face coverings have been recommended by the U.S. Centers for Disease Control and Prevention for source control to help reduce the spread of COVID-19, the disease caused by the SARS-CoV-2 virus. NIOSH-approved respirators, which decrease wearers' exposure to potentially infectious aerosols and droplets when properly selected and worn, also provide source control; however, some respirators include exhalation valves to help exhaust exhaled air from inside the respirator and increase user comfort. The fraction of exhaled particles that penetrate through filter media, exhalation valves, and escape around the perimeter of a respirator or face covering can be defined as total outward leakage. Here we present total outward leakage measurements from valved N95 respirators, unvalved N95 respirators, and face coverings worn by human test subjects over a particle size range of 0.3-20 µm. Additionally, we present outbound particle penetration data through respirator exhalation valves for particles larger than 0.3 µm. These data provide insight into the effectiveness of face coverings and respirators as a source control for exhaled particles.

4SI.12

Assessing the Effectiveness of Facemask Filter Materials Using DEHS Aerosol and the ELPI+. BORIS GALVIS, Nestor Rojas, David Sierra, Carlos Sanchez, Bernal Camilo, Andres Monroy, *Gesoltec s.a.s*

The Sars-CoV-2 pandemic sprang new businesses to manufacture protective coverings using common fabrics such as cotton and polyester, certified surgical masks, and respirators. As the scientific knowledge of the virus grew, namely its size, its main means of transmission through droplets spread originating in the respiratory tract and the distance it is propelled when we breathe, talk, cough, or sneeze, awareness of social distance and the importance of wearing masks grew.

In this work we assessed the filter material performance of facemasks found commercially in Bogota, Colombia. By challenging the material with Di-Ethyl-Hexyl-Sebacat (DEHS), an aerosol with a known size distribution, nebulized with a Topas' generator and analyzed with the help of the Electrical Low-Pressure Impactor (ELPI+). We were able to determine the filtration efficiency and the most penetrating particle size of the sample materials. We found that the overall protective performance of a cotton/polyester fibers is between 10% and 12% of filtration, the material of a certified surgical mask offers up to 53% of filtration, and the material used in a certified respirator filters between 93% and 94% of particles ranging from1 00 nm to 1 micron. The woven cloth seems to filter only large droplets (>1 micron) but offer no protection against smaller droplets (<1 micron). To prevent the spread of the virus, surgical masks offer adequate protection, and certified respirators give the best protection.

4ST.1

Communication of Real-Time Air Quality by Blending Model, Regulatory Monitor, and Low-Cost Sensor Data. Nico Schulte, Xiang Li, Jo Kay Ghosh, Philip Fine, SCOTT A. EPSTEIN, *South Coast Air Quality Management District*

With the proliferation of low-cost sensors, the public has become increasingly interested in the air quality conditions in their neighborhood. Understanding air quality levels is particularly important in the greater Los Angeles area, a region with 17 million people that typically records the worst air quality in the United States. Low-cost sensor data can be a powerful tool to understand local scale air quality, especially in areas far from regulatory monitors. However, sensor data is commonly misinterpreted, as the accuracy, siting, pollutants measured, and any necessary calibrations are not typically considered by the public. To provide more granular air quality information to the public, the South Coast Air Quality Management District (South Coast AQMD) developed a real-time air quality index (AQI) map that blends data from a chemical transport model, regulatory monitoring data that we collect, and calibrated/quality controlled low-cost PM2.5 sensor data. Each data source is weighted by its relative uncertainty to provide AQI values calculated with PM2.5, PM10, O3, NO2, and CO concentrations at 5 km resolution throughout the jurisdiction. These AQI values are more accurate than values calculated with previous methods, especially during wildfires, and the map also helps to avoid public misinterpretation of sensor data. This interactive real-time AQI map and corresponding plain-language recommendations for how to minimize exposure during periods of poor air quality are currently available on the South Coast AQMD website and the South Coast AQMD mobile app.

4ST.2

Air Partners: Community-Driven Air Monitoring, Mitigation, and Collaborative Governance in Boston, MA.

SCOTT HERSEY, Allison Busa, Abigail Fry, Maia Materman, Megan Ku, Miranda McMillen, Francelis Morillo Suarez, Eben Cross, David Hagan, *Franklin W. Olin College of Engineering*

Air Partners is a community-engaged research group based at Olin College of Engineering that has a mission of supporting local community partners in improving the environmental and racial injustice aspects of air pollution. Air Partners seeks to not only understand the dynamics of air pollution in Environmental Justice (EJ) communities, but also to supplement that understanding with engineering and design to make tangible steps toward greater air justice with a range of stakeholders. We employ a framework of multi-stakeholder planning and execution to identify needs and opportunities, propose work, secure funding, conduct research and pilot work, and communicate results in an understandable way to a variety of audiences. Research outputs are primarily designed to support community-based capacity building, advocacy and collaborative governance to promote air health in the near-source environmental justice communities in Boston, MA, and academic publications are strategically pursued to establish the credibility of our results.

While much of the work of Air Partners is oriented toward community-initiated direct intervention for air monitoring and mitigation, we have also established strong relationships with elected officials at the city, state, and federal levels to directly influence and co-author air quality legislation, aiming to shorten the lag time associated with translating scientific insights into policy. Our paradigm is both community-driven and closely aligned with Olin's mission of practicing people-centered engineering while developing students, and incorporates community-based development, social entrepreneurship, environmental policy, and evidence-driven air quality science and engineering to improve air quality in at-risk communities.

Here we present a case study of our work, describing the process of identifying opportunities, collecting data with a range of low-cost and reference instrumentation, and translating results into actionable insights for community stakeholders.

4ST.3

An Educational Toolkit to Ensure the Successful Operation and Use of Air Quality Sensors by the Public.

ASHLEY COLLIER-OXANDALE, Vasileios Papapostolou, Brandon Feenstra, Berj Der Boghossian, Andrea Polidori, *South Coast Air Quality Management District*

Through the use of air quality sensors, public participation in aerosol research can increase knowledge and awareness of air quality issues and lead to the collection of data that informs actions reducing emissions and exposure. While there has been much research into the performance and capabilities of sensors, there has been less focus on the technology's effectiveness for users. However, issues such as how easy it is to install a sensor are essential as they can directly impact data quality. Under a US EPA funded Science To Achieve Results Grant, titled "Engage, Educate and Empower California Communities on the Use and Applications of Low-Cost Air Monitoring Sensors", the South Coast Air Quality Management District enabled the deployment of nearly 400 sensor units in 14 different communities. Throughout the project, discussions, surveys, and products created by the communities offered the opportunity to gather feedback from the participating communities through an extensive series of community meetings and public workshops about air quality, sensors, and data that collectively informed the development of an Educational Toolkit. The key component of this Toolkit is a comprehensive Guidebook consisting of an introduction to air quality and monitoring, advice for planning a project (including sensor selection), guidance on implementing a project (including sensor siting, procedures for monitoring data quality, and data analysis), and next steps to consider following the completion of a project. Other Toolkit resources include data processing, analysis, and visualization tools, short training videos, surveys, questionnaires, infographics, and sensor installation guides. This Toolkit is intended to help ensure the appropriate use of sensors in community-based air quality projects. Our presentation will highlight key lessons learned regarding communication, provide an overview of the resources in this publicly available Toolkit, and describe how these resources could be leveraged to support public participation in aerosol research.

4ST.4

Environmental Justice Analysis for Six Future Energy Scenarios in California. YITING 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.

The study focused on six future energy scenarios in California, including: (1) a Business as Usual (BAU) scenario; (2) a climate-friendly strict GHG reduction scenario - GHGAi; (3) a loose GHG reduction scenario – 2030CAP; (4) a scenario that focus on the effect of carbon capture sequestration technology (CCS); (5) a scenario that focus on natural gas usage in residential and commercial buildings – NGB and (6) a scenario that focus on natural gas combustion for electricity generation – NGT. Future year 2050 air quality simulations of six scenarios were carried out for 32 randomly-selected weeks between 2046-2055 (to account for effects of medium-term meteorological cycles such as ENSO) by using UCD-CIT chemical transport model. Nine source types were also tracked in air quality simulations. (1) Population exposure to PM2.5, PM0.1 total mass, primary/secondary PM and (2) Source composition of six scenario were then estimated for different socio-economic classes under the six scenarios. The results from this study identify the future EJ analysis under six energy scenarios in California, and compare the benefits of six future energy scenarios across socio-economic classes.

4ST.5

The NASA Multi-Angle Imager for Aerosols (MAIA): Enhancing Societal Impact through Early Community Engagement. ABIGAIL NASTAN, David Diner, *Jet Propulsion Laboratory, Pasadena, CA*

The NASA Multi-Angle Imager for Aerosols (MAIA) investigation seeks to extend our current understanding of the impact of the amount and composition of outdoor, airborne fine particulate matter on adverse health outcomes. The MAIA satellite instrument, in development at the Jet Propulsion Laboratory and currently planned for launch in late 2022, will collect multiangular, multispectral, and polarimetric measurements of scattered sunlight over a set of globally distributed targets. Retrieved aerosol properties will be combined with ground-based air quality monitor data and chemical transport model results to produce 1-km gridded data products of daily-averaged PM10 and PM2.5 mass, and the fractional abundances of sulfate, nitrate, organic carbon, elemental carbon, and dust making up PM2.5 mixtures. Epidemiologists on the MAIA Science Team will use these data to conduct studies on health outcomes in MAIA's Primary Target Areas. Observations will also be collected over a wider set of Secondary Target Areas. The MAIA team anticipates these data to be of value to epidemiologists, environmental health researchers, air quality agencies, environmental justice advocates, aerosol and climate researchers, and others.

MAIA's data products will be publicly available from NASA's Atmospheric Science Data Center (ASDC), free of charge. With the objective of optimizing the MAIA data for our various user communities, the MAIA project and the NASA Applied Sciences Program partner on a MAIA Early Adopters Program, which invites potential users to give feedback on the planned products and provides resources to users pre-launch to assist them in incorporating the products into their workflows. This presentation will highlight the contributions of the MAIA Early Adopter community, which includes 172 members as of this writing, to improvements in the investigation and data product design. These improvements underscore the importance of establishing an open and collaborative relationship between data providers and data users throughout the lifetime of a project, especially early in development.

4ST.6

Global Climate, Environmental, and Health Benefits of Replacing Traditional Solid Fuels with Liquified Petroleum Gas. EMILY FLOESS, Rob Bailis, Elisa Puzzolo, Dan Pope, Andrew Grieshop, *North Carolina State University*

2.8 billion people in low- and middle-income countries (LMICs) globally cook and heat using solid fuels (e.g. wood, charcoal, agricultural residues) , resulting in 2.6 million deaths annually from illnesses related to poor household air quality. Additionally, cooking and heating on solid fuels is a major contributor to climate forcing pollutants. Climate and health impacts are driven by non-renewable biomass use/short-lived species (including aerosols) and particulate matter (PM) exposures, respectively. Liquified Petroleum Gas (LPG) is a potential clean alternative to traditional solid fuels, and has been promoted widely. However, the climate, environmental, and health benefits or impacts of widespread LPG adoption across diverse LMIC settings has not been comprehensively studied. In this scoping analysis, we compare the impacts of current residential fuel choices to scenarios with full or partial replacement of traditional stoves with LPG. We conduct a high-level analysis for all LMICs and conduct more in-depth analysis for four priority countries: Kenya, Rwanda, Nigeria, and Haiti. Priority country analyses focus on differences between urban, peri-urban, and rural areas and regional differences in LPG adoption. Transition scenarios in the global analysis are based on those developed in the World Energy Outlook. We calculate climate benefits via the Global Warming and Global Temperature Potential metrics, including short lived climate forcers and upstream impacts of fuel processing and distribution. We calculate health benefits via estimated reductions in Disability Adjusted Life Years (DALYs) using national- and sub-national-level PM exposure estimates under baseline and LPG-adoption scenarios. The results from this study will be used to quantify the impacts of LPG replacement, and help to communicate and inform policy decisions regarding household energy.

4ST.8

Communication of PM2.5 Air Sensor Performance Evaluations in the Field Using EPA's Recommended Performance Metrics and Target Values. SAMUEL FREDERICK, Rachelle Duvall, Karoline Barkjohn, Cortina Johnson, Andrea Clements, *U.S. EPA Office of Research and Development*

Air quality monitoring has undergone a paradigm shift due to an increase in the number of commercially available air sensors. Numerous studies have implemented sensors for non-regulatory supplemental and informational monitoring applications (NSIM) such as educational programs, community hotspot detection, and city-wide network deployments. These applications may result in the collection of actionable data and development of insightful practices for reducing exposure, however, the quality of sensor data is highly variable. Consistent protocols for evaluating air sensor performance are essential to quantifying sensor accuracy, precision, and bias. In February 2021, the U.S. Environmental Protection Agency (EPA) released recommended performance testing protocols, metrics, and target values for evaluating fine particulate matter ($PM_{2.5}$) air sensors for use in ambient, outdoor, fixed site NSIM applications. The report recommends base testing of sensors at an ambient, outdoor monitoring site and presenting results in a standardized reporting template. This template complements the goals of the report by proposing a common framework for displaying sensor performance evaluation results. Using data from previous $PM_{2.5}$ sensor field evaluations conducted by EPA at a site in Research Triangle Park, NC, the performance metrics were calculated and compared to EPA's recommended performance targets for base testing. Findings were presented via the reporting template. EPA's recommendations for testing and communicating sensor performance results seek to ensure all users are equipped with the knowledge to select $PM_{2.5}$ sensors best suited for their applications.

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. Testing results do not constitute certification or endorsement by EPA.

4ST.9

Sensor Data Cleaning and Correction: Application on the AirNow Fire and Smoke Map. KAROLINE BARKJOHN, Amara Holder, Andrea Clements, Samuel Frederick, Ron Evans, *US Environmental Protection Agency*

As smoke from wildfires becomes a larger public health concern, residents of smoke impacted communities frequently use lower-cost air sensors to provide more localized air quality data. However, it can be challenging for the public to understand data accuracy, the impact of averaging time, and ultimately which source to trust and how to interpret the data to protect health. In 2020, the United States Environmental Protection Agency (US EPA) and the US Forest Service began the sensor data pilot showing sensor data alongside permanent and temporary monitors on the AirNow Fire and Smoke map (fire.airnow.gov). Data cleaning methods and a correction equation were applied to PurpleAir sensor fine particulate matter ($PM_{2.5}$) data to make it more comparable to AirNow monitors thus reducing data accuracy concerns and streamlining several discrete data sources to help users view and interpret data. The original correction equation was evaluated under typical US ambient conditions and smoke impacted conditions with $PM_{2.5}$ concentrations up to 250 $\mu g\ m^{-3}$. However, smoke conditions were extreme during 2020 wildfires with some sites seeing $PM_{2.5}$ concentrations over 1,000 $\mu g\ m^{-3}$ with sensors underestimating concentrations above 250 $\mu g\ m^{-3}$. A collocated dataset collected during the 2020 wildfire season was used to extend the correction equation into the higher concentration regime. Since US EPA primarily communicates air quality data using the Air Quality Index (AQI), a piecewise correction equation was selected to reduce the error at each AQI category break point. This correction enables PurpleAir $PM_{2.5}$ data to be used with greater confidence and will provide the public with more spatially resolved data on the Fire and Smoke map.

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4ST.10

Using Modeled Respiratory Aerosol and Measured CO2 to Inform COVID-19 Risk Prevention on a University Campus. J. ALEX HUFFMAN, Nora Carmody, *University of Denver*

Due to the COVID-19 pandemic, colleges struggled to offer in-person learning opportunities and faced even deeper challenges with experiential learning opportunities, i.e. ensemble music performance. Navigating the options to reduce risk was bewildering for most organizations, and limited budgets forced tough choices between interventions. To help quantify risk and provide a framework by which decisions could be made, I utilized available aerosol modeling tools to inform university administrators about preventative steps that would provide the greatest reduction of COVID infection risk.

The Wells-Riley box model for infectious aerosol transmission has been utilized for many decades as a basic tool to estimate relative risk. I built the model onto the Igor Pro platform and added functionality with respect to CO_2 concentrations and wait times after room use. By analyzing a variety of room types on the University of Denver (DU) campus (including music performance and practice, lecture classrooms, and gym spaces) I was able to individually investigate intervention parameters such as room occupancy loads, duration and wait times of classes, effect of added ventilation and in-room HEPA filtration. By analyzing the relative infection risk by varying key parameters, we were able to focus on strategies that would have the most impact on reducing risk, without wasting resources that were unlikely to reduce respiratory aerosol burden and risk.

In parallel, twelve CO_2 sensors deployed in rooms on the campus provided real-time feedback to reveal when ventilation rates or schedules were insufficient for given spaces. Comparing measured CO_2 values, used as a proxy for respiratory aerosol output, to the modeled results also helped test model input assumptions. Results of aerosol modeling and CO_2 measurement results will be shown, focusing on lessons learned about how available tools can be leveraged for best use of available intervention resources.

4ST.11

Disparities in Air Quality Downscaler Model Uncertainty across Socioeconomic and Demographic Indicators in North Carolina. SHAN ZHOU, Robert Griffin, Alexander Bui, Mercedes Bravo, Claire Osgood, Marie Lynn Miranda, *Rice University*

An increasing number of studies uses output from the EPA's Fused Air Quality Surface Downscaler ("downscaler"), which provides spatial predictions of daily ozone and PM2.5 concentrations at the census tract level, to study the health and societal impacts of exposure to air pollution. It has been shown that lower socioeconomic status (SES) and higher proportion minority populations typically are exposed to higher levels of fine particulate matter ($PM_{2.5}$) and lower levels of ozone (O_3). However, the uncertainty of the downscaler estimates remains poorly characterized, and it is not known if all subpopulations are benefiting equally from reliable predictions. We examined the predictions and standard deviations of daily concentrations of $PM_{2.5}$ and O_3 between 2002 and 2016 at the 2010 census tract centroids across North Carolina in association with SES, the racial isolation of non-Hispanic blacks, educational isolation of non-college educated individuals, and the Neighborhood Deprivation Index. Results showed that there were socioeconomic and demographic disparities in surface concentrations of O_3 and $PM_{2.5}$. The reliability of air quality predictions also showed socio-demographic inequality; more disadvantaged neighborhoods with lower SES suffered from less reliable predictions. Overall, $PM_{2.5}$ and O_3 levels decreased between 2002 and 2016; the uncertainty of O_3 predictions also has decreased since 2002. However, the uncertainties associated with predicted $PM_{2.5}$ concentrations have increased since 2009. Substantial spatial variability was observed in these temporal changes; the disadvantaged, lower SES, and higher proportion minority population experienced greater improvements in air quality and O3 prediction reliability. Although PM2.5 uncertainty increased over the years, these populations experienced a less significant absolute increase.

5AC.1

Chemical Composition and Mass Yield of Secondary Organic Aerosol Generated from the Oxidation of Biogenic and Anthropogenic Precursors by Hydroxyl Radicals, Chlorine Atoms, and Bromine Atoms.

ANDREW LAMBE, Anita Avery, Harald Stark, Jordan Krechmer, Francesca Majluf, Manjula Canagaratna, Catherine Masoud, Nirvan Bhattacharyya, Mrinali Modi, Lea Hildebrandt Ruiz, William Brune, *Aerodyne Research, Inc.*

The role of hydroxyl radicals (OH) as a daytime oxidant is well established on a global scale. In specific regions such as the marine boundary layer and polluted coastal cities, other daytime oxidants such as chlorine atoms (Cl) and even bromine atoms (Br) may compete with OH for the oxidation of volatile organic compounds. However, the number of chamber studies investigating halogen-initiated secondary organic aerosol (SOA) formation is extremely limited compared to the number of studies for OH, resulting in larger uncertainties in their oxidation mechanisms. To address these knowledge gaps, we characterized the chemical composition and yield of laboratory SOA generated in an oxidation flow reactor (OFR) from the OH and Cl oxidation of toluene and *n*-dodecane, and the OH, Cl, and Br oxidation of isoprene and α-pinene. In the OFR, precursors were oxidized using OH (5×10^{8} to 2×10^{10} cm^{-3}), Cl (5×10^{7} to 2×10^{9} cm^{-3}), or Br (3×10^{9} to 3×10^{10} cm^{-3}) over exposure times of approximately 2 min. SOA mass spectra and yields obtained in the OFR studies were comparable to those obtained from OH and Cl oxidation of the same precursors in environmental chamber studies. Results suggest that specific precursor classes such as alkane, aromatic, and terpenoid SOA precursors are characterized by distinct OH- and halogen-initiated SOA yields.

5AC.2

Changes in Mass Yield, Volatility Distribution, and Chemical Composition of Secondary Organic Aerosol Formed From Simultaneous and Sequential Oxidation of α-Pinene and Limonene by Nitrate Radicals.

MASAYUKI TAKEUCHI, Thomas Berkemeier, Gamze Eris, Nga Lee Ng, *Georgia Institute of Technology*

Traditional approaches to study secondary organic aerosol (SOA) in laboratory studies often focus on the oxidation of one single volatile organic compound (VOC) at a time, whereas chemical transport models also treat SOA formation explicitly from each precursor VOC assuming linear additivity. However, it has been shown recently that SOA formation in multi-VOC systems cannot be explained by linear combination of each species involved. Specifically, McFiggans et al. (2019) observed a reduced SOA mass yield of α-pinene+OH in the presence of isoprene. In this study, we focused on the following research questions:

(1) What multi-VOC effects can be observed for nitrate radical oxidation?
(2) Do multi-VOC effects differ between simultaneous and sequential VOC oxidation of two precursors?

Here, we performed four chamber experiments: nitrate radical oxidation of α-pinene, limonene, α-pinene and limonene simultaneously, and limonene followed by α-pinene oxidation. Oxidation products were measured by a filter inlet for gases and aerosols coupled to a chemical ionization mass spectrometer (FIGAERO-CIMS), an aerosol mass spectrometer, and a scanning mobility particle sizer. We found that SOA mass yield from limonene oxidation reduced almost by half when oxidized simultaneously, but not during sequential oxidation. On the other hand, SOA mass yield of α-pinene showed little difference regardless of the presence of limonene. The reduced SOA mass yield in the simultaneous oxidation experiment is attributed to the inhibited formation of low-volatility limonene oxidation products, evident by the lack of signal at a high desorption temperature in the FIGAERO-CIMS thermogram. This likely arises from altered gas-phase chemistry between α-pinene and limonene oxidation products. Without considering this multi-VOC effect, the modelled SOA mass concentration via nitrate radical oxidation of biogenic VOCs in the southeastern U.S. could be overestimated by ~40%.

5AC.3

Comprehensive Measurements of Organic Carbon over Long Oxidation Timescales. LESLY FRANCO DELOYA, Jesse Kroll, *MIT*

Nonmethane organic carbon makes up a large fraction of reactive species in the atmosphere, yet most studies have only examined early generation oxidation products. Understanding the multigenerational chemical evolution of gas-phase mechanisms can help in better understanding the dynamic partitioning between the gas- and particle-phase of organic carbon, especially on multiday to multiweek scales. By using OH concentrations thousands of times higher than that of the atmosphere, we can simulate longer timescales of atmospheric aging and measure the multigenerational evolution of both gas- and particle-phase oxidation products. The OH oxidation of α-pinene under low NOx conditions is used as a model system. Gas-phase measurements were made using a PTR3 in H3O+ and NH4+ mode, and particle-phase measurements were made using an AMS and SMPS, enabling reasonably comprehensive measurements of the entire reaction product mixture. The gas-phase results are compared to predictions by the Master Chemical Mechanism (MCM), and discrepancies between models and observations are examined. Such comparisons provide an important test of our understanding of the lifecycle of reactive organic carbon in the atmosphere.

5AC.4

Vapor-phase Chemical Speciation and Condensation of Cerium Oxide. KATE RODRIGUEZ, Batikan Koroglu, Zurong Dai, Kim Knight, *LLNL*

We track the vapor-phase synthesis of cerium oxide nanoparticles created in a plasma flow reactor, starting with early-stage oxidation of the gaseous metal atoms and subsequent homogeneous nucleation and continuing to later-stage particulate condensation and eventual agglomeration. Incipient chemical speciation and consequent product formation are investigated as a function of both temperature and oxygen fugacity. In situ optical emission spectroscopy is used to detect the presence of atomic, ionic, and molecular species and measure their relative variations with temperature and oxygen content. Condensed cerium oxide nanoparticles are also collected and analyzed ex situ via transmission electron microscopy and X-ray scattering techniques to determine their elemental composition, crystal structure, and size distribution. We find that the relative rate of gas-phase oxidation of cerium is highly dependent on both the temperature and local redox conditions within the flow reactor, while the size and morphology of the condensed nanoparticles depends predominantly on temperature, forming the same crystal type with the same size distribution regardless of oxygen availability. In this way, we show that the processes that underpin the vapor-phase chemical speciation and subsequent gas-phase evolution of cerium oxide are highly dependent on the local environment.

5AC.5

Influence of Salt Identity on the Size Dependent Morphology of Aerosol Particles.

MIRIAM FREEDMAN, Emily-Jean Ott, *Penn State University*

Heterogeneous and multiphase chemistry are impacted by particle morphology. The internal structure of a particle depends on phase transitions and can change based on particle size. We have previously found that aerosol particles that undergo liquid-liquid phase separation have a size-dependent morphology, where the transition to two phases is inhibited in small particles. In this work, we investigate the influence of the identity of the salt on the size dependence. The ions NH_4^+, Na^+, SO_4^{2-}, HSO_4^-, and Cl^- were investigated along with the two organic compounds, 2,5-hexanediol and diethylmalonic acid. A strong dependence of the size dependence on the cations is found with no dependence on the anion. We explain our results in terms of the hardness of the cation, where the harder cation (Na^+) results in phase separation down to smaller sizes while the softer cation (NH_4^+) leads to an inhibition of phase separation at larger sizes. Our results have implications for understanding the differences between the morphology of sea spray and continental aerosol, which will impact the heterogeneous and multiphase morphology of these species.

5AC.6

Molecular Investigation of the Multi-Phase Photochemistry of Fe-citrate Aerosol Proxies.

CHRISTOPHER WEST, Jackson Ryan, Felipe Rivera-Adorno, Ana Morales, Jay Tomlin, Anusha P.S. Hettiyadura, Maria Misovich, Andrew Darmody, Peng Lin, Brittany Linn, Alexander Laskin, *Purdue University*

Soluble Fe(III) on Earth is ubiquitously present in terrestrial, oceanic, and surface waters, mineral-rich soil, vegetative crops, plants, and atmospheric particulate matter. Upon dissolution of Fe3+ from wind-blown dust or atmospheric cloud water, organic carboxylic acids efficiently chelate dissolved Fe3+ to form photo-catalytically active Fe(III)-carboxylate complexes that catalyze a range of radical-induced chemical reactions in these complex aerosol/aquatic systems. The chemical composition and atmospheric transformations of these mixtures are ambiguous, making it challenging to estimate their resulting impact on the aqueous-phase chemistry of atmospheric aerosols. This work presents a systematic investigation of the molecular composition and the extent of aqueous photochemical processing of Fe(III)-citrate complexes as laboratory proxies of atmospheric water. We monitored the overall extent of the reaction and determine its effects on the light absorption by the bulk material. Water-soluble chemical constituents from each of the photoreacted mixtures were separated and characterized using liquid chromatography, photodiode array, and electrospray ionization high-resolution mass spectrometry platform. In addition, colloidal material formed in the photoreacted samples was aerosolized and probed by the soft X-ray spectro-microscopy. The aqueous-suspended colloidal material was also probed using dynamic light scattering methods. We demonstrate for the first time a high-level optical and molecular description of the water-soluble components (i.e. FeIII/II-organic complexes, oligomers, and organic acid products) along with chemical imaging of 'pyrolytic-like' solid carbonaceous colloids formed during the photolysis reactions.

5AC.7

The Role of Ammonia in Atmospheric New Particle Formation and Aerosol Number Abundance at the Southern Great Plains Site. ARSHAD NAIR, Fangqun Yu, Gan Luo, *The State University of New York at Albany*

New particle formation (NPF) and subsequent growth to cloud condensation nuclei (CCN) can contribute upwards of 50% of the global CCN budget. It is also a significant source of ultrafine aerosols with health implications. Ammonia (NH_3) can play a significant role in determining NPF rates by its stabilizing effect on neutral and charged clusters. Understanding these processes are vital for air quality and climate. Here, we examine the role of NH_3 in NPF and consequent effects on aerosol properties (number concentrations and their size distributions) during springtime 2018–2019 at the U.S. Department of Energy's (DOE) ARM Southern Great Plains (SGP) Central Facility located in Lamont, Oklahoma (36°36′18′′ N, 97°29′6′′ W; 318 m). We use the GEOS-Chem global 3-D atmospheric chemistry and transport model coupled with the size-resolved, multi-type, multi-component Advanced Particle Microphysics (APM) Model that incorporates the recently developed H_2SO_4–H_2O–NH_3 Ternary Ion-mediated Nucleation (TIMN) scheme, constrained with thermodynamic data from quantum-chemical calculations and Cosmics Leaving OUtdoor Droplets (CLOUD) measurements. For comparison with model simulations, we use the SGP observations of particle number size distributions (3–500 nm; TSI Model 3936 scanning mobility particle sizer (SMPS) and nanoSMPS), CN10 (condensation nuclei > 10 nm; TSI Model 3772 Condensation Particle Counter), CCN0.4 (CCN at 0.4% supersaturation; Droplet Measurement Technologies CCN-200), and aerosol composition speciation (SO_4, NO_3, NH_4, Organics; Aerodyne ACSM). Inclusion of the effect of NH_3 captures the occurrence of strong NPF and growth events and the magnitude and temporal variations of observed particle number concentrations. Simulated CN10 and CCN0.4 show improved agreement with observations (over a range of 4 orders of magnitude) with mean fractional bias reducing from -1.2 to -0.03 and -0.6 to -0.1, respectively. With the additional aid of submicron aerosol composition measurements and simulations, the role of NH_3 in NPF and growth to potential cloud-forming particles is examined.

5AC.8

Regional and Nearfield Per- and Polyfluoroalkyl Substances (PFASs) in Ambient Fine Aerosol (PM2.5) in North Carolina, USA. Jiaqi Zhou, Karsten Baumann, Ralph Mead, Stephen Skrabal, Robert Kieber, Gene Avery, Megumi Shimizu, Mei Sun, Samuel Vance, Wanda Bodnar, Zhenfa Zhang, Leonard Collins, Jason Surratt, BARBARA TURPIN, *UNC-Chapel Hill*

Per- and polyfluoroalkyl substances (PFASs), being environmentally persistent, are ubiquitous and have been found globally in groundwater, surface water, crops and wildlife. However, PFASs in air remain poorly understood, especially in the United States (US). Given the existence of a fluoropolymer and specialty chemical manufacturing plant (Chemours) and large military bases, as well as more typical sources of environmental PFAS contamination (e.g., fluorinated fire-fighting foam use, urban waste streams), North Carolina (NC) is a good place to study PFAS. This study measured statewide seasonal PFAS concentrations in ambient fine aerosols ($PM_{2.5}$) in a one-year field campaign at five NC locations (Fayetteville, Charlotte, Research Triangle Park, Wilmington, and Greenville), and measured nearfield weekly PFAS concentrations in fine aerosols ($PM_{2.5}$) in a six-month field campaign at two locations close to the Chemours facility in Fayetteville, NC (northeast and southwest, within a few miles). Quartz fiber filter samples were collected and analyzed for 34 targeted PFASs by LC-MS/MS on an AB SCIEX Triple Quad™ 6500 mass spectrometer system. With the exception of perfluoro-n-octanoic acid (PFOA) and perfluoro-1-octanesulfonate (PFOS), statewide ambient quarterly concentrations of all targeted species were <1 pg/m^3. All concentrations >1 pg/m^3 occurred during Jul.-Sept. Notably, $PM_{2.5}$ has a short atmospheric lifetime (<2 weeks), and thus, the presence of PFOS in these samples raises questions about their sources, since PFOS production was phased out in US ~20 years ago. Twenty-two PFASs were detected in nearfield samples, with ten PFASs above 1 pg/m^3. Upwind and downwind nearfield PFAS concentrations and potential sources/formation mechanisms will be discussed. To our knowledge, this is the first US study to provide insights into regional and nearfield ($PM_{2.5}$) PFAS concentrations.

5AC.9

First Insights into Chemical Pathways of New Particle Formation over Siberia, Russia. OLGA GARMASH, Ekaterina Ezhova, Mikhail Arshinov, Denis Davydov, Anastasiia Demakova, Meri Räty, Federico Bianchi, Tuukka Petäjä, Boris Belan, Markku Kulmala, *University of Helsinki*

New particle formation (NPF) is an important atmospheric phenomenon that can affect the concentration of cloud condensation nuclei and potentially contribute to haze in urban areas. NPF has been observed in many locations around the world, from remote Polar Regions to megacities, with varying chemical and physical characteristics. Though forests are a large source of volatile organic compounds (VOCs) that can efficiently form secondary aerosol in the atmosphere, some forests, such as in Amazon and Siberia, were reported to have very infrequent NPF. In order to confirm low NPF frequency in Siberia and elucidate the possible reasons, we conducted measurements at Fonovaya station, located about 60 km from the city of Tomsk in Western Siberia, Russia. In this study, we focus on March-May 2020, when in addition to aerosol size distribution instruments, we deployed atmospheric pressure interface time-of-flight mass spectrometer (APi-TOF). APi-TOF was configured to measure the composition of natural negatively charged ions and clusters. We detected a large number of NPF events in comparison to previous years, especially in March, when it was close to 50%. We observed the change from cold to warm season around mid-April and simultaneously polluted southern air masses changed to somewhat cleaner air from the north. Changing meteorological conditions and potential increase in biogenic activity during very warm May affected the chemistry of the clusters initiating NPF events. In addition to pointing at vapours initiating the formation of molecular clusters, APi-TOF also provided us with the first insight into the origin of highly oxygenated organic molecules over Siberian forest. Our result help to construct our understanding of chemical processes connected to secondary aerosol formation in Western Siberia.

5AC.10

Partitioning of Ambient Organic Gases to Inorganic Salt Solutions: Influence of Salt Identity, Ionic Strength, and pH. VIKRAM PRATAP, Annmarie Carlton, Amy Christiansen, Christopher Hennigan, *University of Maryland, Baltimore County*

Inorganic salts can enhance (“salting-in”) or inhibit (“salting-out”) the partitioning of organic gases to aqueous solutions relative to that in pure water. These phenomena may affect the composition and abundance of secondary organic aerosol (SOA), though their importance in the atmosphere is largely unconstrained at present. In this work, we quantify the effects of salt identity, salt concentration (ionic strength), and solution pH on the partitioning of atmospheric water-soluble organic gases ($WSOC_g$) at a site in the eastern United States. Experiments were conducted in a custom-made dual mist chamber setup where simultaneous measurements were conducted in two mist chambers – one filled with deionized water and other with the salt solution. This enabled a direct comparison of dissolved $WSOC_g$ in either chamber to estimate the salting effect of a salt. The experimental pH (pH = 1 – 6) and ionic strengths (10^{-3} – 10^{1} mol kg^{-1}) span a wide range of conditions found in atmospheric particles, clouds, and fog droplets. Chloride salts (NaCl, NH_4Cl, and KCl) exhibit a strong salting-out effect at all ionic strengths > 0.005 mol kg^{-1} and pH = 1.8 – 6. Conversely, sulfate salts (Na_2SO_4, $(NH_4)_2SO_4$, and K_2SO_4) induce both salting-in and salting-out behaviors, depending on ionic strength and pH. These results suggest that monovalent cations have a minimal effect on the partitioning behavior of ambient organic gases, while both ionic strength and pH exert important influences on the distribution of organics in the atmosphere.

5AC.11

Organosulfates Are Primarily Deprotonated at Atmospheric Aerosol Acidities: pH-Dependent Protonation State via Raman and Infrared Spectroscopy.

ALISON FANKHAUSER, Ziying Lei, Kimberly Daley, Yao Xiao, Zhenfa Zhang, Avram Gold, Bruce Ault, Jason Surratt, Andrew Ault, *University of Michigan*

Secondary organic aerosol (SOA) is a significant component of atmospheric fine particulate matter ($PM_{2.5}$) globally that can form through multiphase chemistry of oxidized volatile organic compounds (VOC) leading to lower-volatility particulate species. Condensed phase reactions of certain SOA constituents with inorganic sulfate derived from SO_2 oxidation will lead to the formation of organosulfates, which can account for up to 10 – 15% of the organic mass within $PM_{2.5}$. Despite the ubiquitous presence of atmospheric fine particulate organosulfates, our fundamental understanding of the molecular structure of organosulfates is limited, including for 2-methyltetrol organosulfates (2-MTSs), which are typically the single most abundant organosulfates measured in $PM_{2.5}$, formed from isoprene oxidation products. As atmospheric aerosol pH varies widely (0 – 6), it is important to know whether organosulfates exist primarily in their protonated ($ROSO_3H$) or deprotonated ($ROSO_3^-$) forms. In this study, vibrational modes of synthetically-pure 2-MTSs were spectroscopically probed using Raman and infrared (IR) spectroscopies, supported by density functional theory (DFT) of the protonated and deprotonated structures. Vibrational bands at 1035 and 1059 cm^{-1} were seen in both the IR and Raman spectra, and were associated with the $ROSO_3^-$ anion by comparison to DFT calculations. Analysis of Raman spectra across a range of acidities (pH = 0 – 10) shows that 2-MTSs are deprotonated ($ROSO_3^-$) at those pH values. Additional DFT calculations for organosulfates derived from isoprene, α-pinene, β-caryophyllene, and toluene suggest that most organosulfates exist in their deprotonated form ($ROSO_3^-$) in atmospheric particles. These charged species may have significant implications for our understanding of aerosol acidity and should be considered in thermodynamic model calculations.

5AC.12

Stratification, Solvent-modulated Effects, and Simulations of Solvation in Secondary Organic Aerosol Mimicking Solutions.

Emmaline Longnecker, Rebecca Miller, Lucy Metz, Asli Ali, Laura Bickart, Michelle Chen, Maya Morales, Habso Omane, 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 solutions 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. Results from our ongoing computational work exploring the link(s) between intra-solution bonding relationships and bulk organization and stratification will also be presented.

5HA.1

Physicochemical and Toxicological Characterization of Electronic Nicotine Delivery Systems.

ROBY GREENWALD, Christa Wright, Aika Davis, Qian Zhang, Ji Soo Jeon, *Georgia State University*

We evaluated the physicochemical and toxicological properties of emissions from a variety of electronic nicotine delivery systems (ENDS). We employed a puff generating system capable of operating pod and tank devices that was placed inside a 6m3 exposure chamber operating at an air exchange rate of 3 ACH. To examine the hypothesis that aged heating coils shed more toxic metal particles than new coils, we tested devices at multiple age states including new (the first 25-50 puffs for a coil), broken-in (puffs 101-125) and aged (puffs 201-250). For tank devices, we performed experiments at both the low- and high-end of the recommended power range for each type of coil, and for pod devices, we supplied power equivalent to a fully charged battery (although this power setting was always lower than all tank devices). We used a neutral flavor of liquid and generated puffs 3.5s in duration and 50mL in volume. ENDS emissions were diluted in a 1L buffer chamber by a clean dilution flow of 1-3 LPM. We collected samples for toxicological evaluation using 20-30m condensation tubes with a sample flow of 1 LPM. The remaining buffer chamber flow was vented into the exposure chamber, and we measured fine- and ultrafine-mode particle concentration and size distribution in exposure chamber air to simulate second-hand exposure characteristics. The total mass of particles emitted per puff was higher for high-power experiments, but the size distribution for low-power experiments consisted of larger particles. Consequently, the collection efficiency of the condensation tubes was higher for low-power experiments. Human airway epithelial cells exposed to ENDS emissions exhibited increased oxidative stress, increased single stranded DNA damage, and reduced cellular viability. For oxidative stress measures, there were modestly higher results for aged devices, but for DNA damage and cellular viability, results were significantly more pronounced for aged devices.

5HA.2

Development of a Ventilated Artificial Lung Model for Characterizing the Physicochemical Properties of Inhaled E-cigarette Aerosols.

LIQIAO LI, Haoxuan Chen, Airi Harui, Michael D. Roth, Yifang Zhu, *University of California, Los Angeles*

E-cigarettes (e-cigs), such as JUUL, are increasingly popular among adolescents and young adults even though emerging data raise concerns about their health effects. To better understand lung exposure and toxicity, we developed a ventilated artificial lung exposure model in which temperature, humidity, puff volume, puff frequency, and breathing pattern can be independently controlled. The effects of breathing, temperature, and humidity on the fate of inhaled e-cig aerosols were investigated by measuring the particle number concentration (PNC), particulate matter (PM) mass concentration, and size distribution during a 4-puff vaping cycle (33 ml puff every 60s). Samples were collected in real time from the 6L lung chamber. In the absence of breathing, the peak PNC and PM reached 6.9×10^6 #/cm^3 and 111 mg/m^3, respectively. In comparison, the peak PNC and PM were reduced by 23% and 44%, respectively, at 10 breaths/min [38% relative humidity (RH); 25°C]. Five min after the last puff, the PNC and PM were washed out by > 97% in the presence of ventilation, while those only decreased by 60% in the static model. Compared to the 38% RH, 25°C condition, a dry environment (1% RH, 25°C) accelerated the decay process by facilitating evaporation. In a simulated lung environment (85% RH, 37°C), the particle size grew due to the hygroscopic effect, where fewer submicron particles with smaller size were identified while particle levels at 3 µm increased over time. Vaping topography, breath pattern, and airway distribution are also being studied. This work provides novel insight as to the physiochemical transformation that occurs when e-cig aerosols are inhaled and an estimation of organ-specific exposure (and exposure pattern) that is not evident from conventional chamber analysis.

5HA.3

Toxicity Associated with Surface Chemistry of Combustion Produced PM2.5 by in Vitro Assays.

MADHU SINGH, Randy Vander Wal, Patricia Silveyra, *Penn State University*

The International Agency for Research on Cancer (IARC) has labeled diesel exhaust as carcinogenic within class 1. While the mechanism(s) by which soot causes the adverse health effects are not known, a great deal of these harmful effects relate to its ability to cause oxidative stress. Thus, oxidative potential, expressed through reactive oxidative species concentration, can be used as a good estimate for its reactivity and toxicity. Accordingly, physical structure and surface chemistry become surrogate measures of its oxidative potential as together they determine the redox properties and polar/acidic character. Based on this premise, we are testing the role and impact of soot structure and surface chemistry upon interaction with bronchial and alveolar epithelial cells. The proposed project's goal is the identification of toxicity, oxidative, and pro-inflammatory factors in combustion produced soot arising from using alternative fuels, by studying the particles directly instead of studying compounds adsorbed on (and removed from) the soot particles. Model soots with tailored surface chemistry, and specific particle physical structures are being tested for toxicity, oxidative stress markers, effects of lung inflammation and and signaling pathways using cell culture bioassays, as well as protein carbonylation and DNA damage marker assessment.

Treatment of carbon particles with nitric acid and ozone resulted in differential oxygen and carboxylic acid content in the PM2.5 surface. Of the three PM2.5 preparations, BEAS-2B cells exposed to nitric acid-treated carbon resulted in the largest decrease (89% and 96%) of cell viability after 6 hr. and 24 hr., respectively, indicating that both carboxylic acid and oxygen content of the particle surface strongly contribute to PM2.5 toxicity. Additional results showed an increase in gene expression of the inflammatory cytokines IL-1ß, and IL-6, and the oxidative stress markers TLR4 and NRF2 at higher concentrations of PM2.5 exposure.

5HA.4

Comparison of Oxidative Potential of Fine Particles between Urban and Rural Sites.

SEUNGHYE LEE, Ma. Cristine Faye Denna, Minhan Park, Jiho Jang, Joonwoo Kim, Kihong Park, *Gwangju Institute of Science and Technology*

The ambient fine particulate matter ($PM_{2.5}$) was reported to cause various adverse health effects. Oxidative potential (OP), the ability of particles to induce oxidative stress by introducing redox-active components, catalytically producing reactive oxygen species (ROS), and reducing antioxidants in the body can be considered as a measure of $PM_{2.5}$ potential toxicity. The ambient $PM_{2.5}$ samples were collected at three different sites (urban Beijing (China) and Gwangju (Korea) in the winter of 2018, 2019, 2020 and summer of 2019 and rural Gimje (Korea) in the summer of 2020 and winter of 2021). The $PM_{2.5}$ OP was determined by using the dithiothreitol (DTT) assay. Both volume (OP-DTTv) and mass (OP-DTTm) normalized OP were higher at urban sites than the rural site (p-value < 0.05). At all sites, the higher OP-DTTv was observed in the winter compared to the summer. Chemical composition data for $PM_{2.5}$ will be used to investigate major factors affecting the OP at sites.

5HA.5

Size Fractionation of PM2.5 Water-soluble Elements (Iron and Copper) and Oxidative Potential.

YUHAN YANG, Dong Gao, Rodney J. Weber, *Georgia Institute of Technology*

Epidemiological studies have established a link between particulate matter (PM) mass and adverse health-related issues. Particle oxidative potential (OP), referring to the redox ability of PM, is a possible unifying concept that connects a host of adverse health effects. Iron (Fe) and copper (Cu) are often the most abundant transition metals in ambient $PM_{2.5}$ and are important contributors to aerosol OP. A number of studies have shown water-soluble metals are especially toxic, compared to insoluble metal species. In this study, we developed robust liquid spectrophotometric methods for measuring total and soluble Fe and Cu with a single relatively inexpensive analytical system. These methods were applied to 24-hour filter samples collected throughout the year 2017 in urban Atlanta. The water-soluble components, operationally defined as those species in the aqueous filter extract that pass through a 0.45 µm filter, were further characterized by ultrafiltration, which showed that roughly 85% of both the Fe and Cu in the water-soluble fraction was composed of species smaller than nominally 4 nm. For Fe, roughly 23% was in the nominal size range of 2 to 4 nm, whereas for Cu almost all were smaller than 2 nm. OP of the water-soluble fractions is characterized by measured redox potential in simulated epithelial lining fluid. Our results indicate that water-soluble Fe and Cu are composed of dissolved species or very small colloidal particles that are highly reactive and could be important contributors to aerosol OP.

5HA.6

Spatiotemporal Variability in the Oxidative Potential of Ambient Fine Particulate Matter in Midwestern United States.

HAORAN YU, Joseph V Puthussery, Yixiang Wang, Vishal Verma, *University of Illinois Urbana-Champaign*

Oxidative potential (OP) of fine particulate matter ($PM_{2.5}$) has been proposed as an important mechanism for many $PM_{2.5}$-related health outcomes. The spatiotemporal profile of $PM_{2.5}$ OP could be extremely helpful in assessing the regional health effects of $PM_{2.5}$, and such profiles have been developed from many geographical regions of the world. However, no prior studies have investigated the spatiotemporal distribution of $PM_{2.5}$ OP in the Midwestern United States (Midwest US). Here, we conducted the first study on assessing the OP of both water-soluble and methanol-soluble fractions of ambient $PM_{2.5}$ in the Midwest US. $PM_{2.5}$ samples (N = 241) were sampled from five sites located in urban, rural, and roadside environments of Illinois, Indiana, and Missouri within a year. We used five acellular endpoints, including the consumption rate of ascorbic acid and glutathione in a surrogate lung fluid (SLF) (OP^{AA} and OP^{GSH}, respectively), dithiothreitol (DTT) depletion rate (OP^{DTT}), and ·OH generation rate in SLF and DTT ($OP^{OH\text{-}SLF}$ and $OP^{OH\text{-}DTT}$, respectively), for analyzing the OP of all $PM_{2.5}$ samples. Compared to the homogeneously distributed $PM_{2.5}$ mass concentrations, all OP endpoints showed substantial variability both spatially and temporally. In general, both water-soluble and methanol-soluble OP showed elevated levels during summer. The roadside site had the highest activities for most OP endpoints. The distribution trends between mass- and volume-normalized OP were similar for most endpoints indicating only a minor role of mass in controlling the OP. Higher levels were observed in methanol-soluble OP than water-soluble OP, indicating a better efficiency of methanol to extract the redox-active components in $PM_{2.5}$. Correlations between $PM_{2.5}$ mass concentrations and most OP endpoints were generally poor, indicating the inadequacy of mass to represent the health effects of $PM_{2.5}$. Moreover, weak-to-moderate correlations were observed among different OP endpoints, showing significant differences in the intrinsic mechanisms of these endpoints for exerting oxidative stress, and thus supporting the importance for assessing the integrative OP of PM with several OP endpoints.

5HA.7

On the Relative Contribution of Fe and Organic Compounds, and Their Interaction in Cellular Oxidative Potential (OP) of Ambient PM2.5. YIXIANG WANG, Haoran Yu, Joseph V Puthussery, Vishal Verma, *University of Illinois Urbana-Champaign*

Oxidative potential (OP) reflects the capability of ambient PM2.5 to cause ROS imbalance in the biological system and investigating the chemical components linked with OP has been an active area of research. However, most of the studies linking OP to chemical composition have used only the acellular OP assays, while largely ignoring the biological reactions. In this study, PM2.5 samples were collected from several Midwest US sites, and the OP of collected particles was assessed by a cellular ROS assay based on rat alveolar macrophages. Several chemical components of PM2.5 were also measured. Among all the chemical components, only water-soluble Fe and water-soluble organic carbon (WSOC) were significantly correlated with the OP at all sites. Since both of these components (i.e., Fe and WSOC) were also intercorrelated, we developed a novel mechanistic technique using a combination of solid phase extraction columns, to identify the individual contribution of these species in the macrophage ROS response. Results suggested that the hydrophobic fraction, which consists of various aromatic organic compounds was ROS-inactive in the macrophage assay. In contrast, the hydrophilic fraction, which contains most of the water-soluble metals and aliphatic organic compounds, accounted for ~80% of PM2.5 total cellular OP. To further segregate the contribution of aliphatic organic compounds with metals, we passed the hydrophilic fraction through a chelex column, which removed metals but did not affect the organic compounds. The metal-free hydrophilic fraction was ROS-inactive, while the retained fraction on chelex column, which was eluted using HCl contained most of the ROS activity. To further explore the correlation of Fe and macrophage ROS with WSOC, we investigated the water-solubility of Fe by measuring total Fe on the filters. The water-solubility of Fe was found to be tightly correlated with WSOC, indicating the indirect role of WSOC, probably through complexation of Fe, on enhancing its water-solubility and macrophage ROS activity. Our study reveals different roles of two important components of ambient PM2.5 and their interaction through effect modification on altering the cellular OP of ambient PM2.5.

5HA.8

Chemical and Cellular Superoxide Generation upon Respiratory Deposition of Quinones and Secondary Organic Aerosols. TING FANG, Yu-Kai Huang, Jinlai Wei, Jessica Monterrosa, Pascale Lakey, Michael Kleinman, Michelle Digman, Manabu Shiraiwa, *University of California, Irvine*

Deposition of particulate matter (PM) in the respiratory tract causes formation of reactive oxygen species (ROS) which can trigger oxidative stress and inflammation leading to cardiorespiratory disease. PM can form ROS through chemical reactions such as redox cycling and decomposition of organic species, or can stimulate macrophages to release ROS biologically in lung fluid. However, the relative contributions of chemical and cellular ROS are seldom quantified and the mechanisms linking them to adverse health effects remain uncertain. Here we apply a chemiluminescence assay calibrated with an Electron Paramagnetic Resonance spectrometer coupled with a spin trapping technique to quantify superoxide production. We measure cellular ROS release by RAW 264.7 macrophage cells and chemical superoxide generation in vitro by PM components including quinone and biogenic and anthropogenic secondary organic aerosols (SOA). We show that atmospherically-relevant doses of quinone activate macrophages to release massive cellular superoxide and cause lipid oxidation, as revealed by fluorescence lifetime imaging (FLIM) coupled with a phasor approach, while higher doses trigger cellular antioxidant response elements that protect against further oxidative damages. We find that chemical ROS is more important for SOA as macrophages remain mostly inactive after exposures to atmospherically-relevant SOA.

5HA.9

Interactions between Transition Metals in Particulate Matter and Phosphate Buffer Affect Acellular Oxidative Potential Assays.

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

Atmospheric aerosols have a deleterious effect on human health. Amongst the various constituents, transition metals are hypothesized to have enhanced toxicity based on their potential to generate reactive oxygen species (ROS). Acellular methods to measure the oxidative potential (OP) of PM commonly use a phosphate buffer matrix at pH 7.4 and 37 °C to simulate conditions in the human body. In this study, we characterize the precipitation of transition metals in the dithiothreitol (DTT) assay, one of the most widely used measures of aerosol OP. Thermodynamic modeling predicts the precipitation of Fe and Mn at low metal concentrations in the PO4 buffer matrix. Experiments were conducted at low aqueous metal concentrations (0.5- 20 µM) using individual metal salts and using urban particulate matter (NIST SRM-1648a); metal precipitation was measured via chemical analysis of dissolved metals, laser particle light scattering, and SEM analysis with EDS microscopy. The results showed unambiguous evidence for precipitation of Fe and Mn within 5 – 30 min, a timescale relevant for the DTT assay. Although thermodynamic modeling suggests Cu does not precipitate due to its high solubility, Cu removal was observed in the urban PM samples, possibly due to adsorption to Fe precipitates or co-precipitation. Finally, the DTT assay response was evaluated for metals applied in dissolved vs. solid form. The implications of this work for use of OP assays to infer PM toxicity are discussed.

5HA.10

Aerosol Science, Toxicology and Risk Analysis Accomplishments from the Lovelace Organization: 1960-2020.

ROGER MCCLELLAN, *Advisor*

The U.S. Atomic Energy Commission (AEC) In 1957 published an analysis of consequences of a major nuclear reactor accident. The estimated consequences were substantial raising concerns about the use of nuclear reactors to generate electricity. A major uncertainty in the analysis was lack of data on health risks of inhaled fission product radionuclides. To address this void the AEC in 1960 initiated a research program at the Lovelace Foundation in Albuquerque, NM. The first employee in the program was T. Mercer, a highly accomplished aerosol scientist. Mercer quickly developed the aerosol science base that continues to serve as a foundation for the Lovelace research program. In 1966, under my leadership, a strategic plan was developed to conduct a series of lifespan studies in Beagle dogs using beta-admitting radionuclides with varied physical half-lives (90Y, 91Y, 144Ce and 90Sr) in either soluble and the other insoluble. Later, the strategy was expanded to include 239Pu (used in nuclear weapons) and 238Pu (used in Space Nuclear Power Systems) as monodisperse aerosols. The design optimized the opportunity to understand the influences of dose, dose rates, radiation quality and time on dose–response relationships. In the 1970s, the Lovelace program was broadened to include research on emissions from diesel vehicles, combustion of fossil fuels and specific chemicals. A cornerstone of Lovelace research has been the use of a paradigm extending from Source of aerosols to Air concentrations to Personal Exposure to Dose to critical tissues to Disease outcome. Over its first half century of research the Lovelace organization became internationally recognized for its contributions to understanding and control of airborne materials. Many Lovelace scientists have been recognized for their extraordinary achievements. Four have been recognized as AAAR fellows. This presentation will review major accomplishments of the Lovelace program over the first half century of operation.

5HA.11

Respiratory Drug Development and Lovelace Biomedical: 2010-2021. JACOB MCDONALD, Philip Kuehl, *Lovelace Biomedical*

Lovelace Biomedical has a long history of aerosol science research, dating back to 1966. Dr. Roger McClellan has submitted a parallel abstract to define the legacy of aerosol research performed at the organization from 1966-2010. The intent of this presentation is to describe the transition of the focus of the organization over the past decade to the use of aerosols for respiratory drug development, alternative tobacco, cannabis and bioaerosols. This transition was performed to best meet the needs of society and the resources that are available at Lovelace to perform nonclinical and clinical studies under regulatory scrutiny. The laboratory has placed itself as a premier site for the conduct of drug development to target the nose and lung to target myriad diseases. The current emphasis builds on the legacy of work that was performed over the first 50 years, and looks forward to continue to build on a strong foundation in aerosol science and dosimetry. The presentation will review major accomplishments and the transition of the business from 2010-2021

5IA.1

Exposure of Adults and Children to the Released and Resuspended Particles from Nanotechnology-enabled Consumer Products. RUIKANG HE, Jie Zhang, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Nano-enabled consumer products are becoming an important indoor particulate matter source. The release, deposition, and resuspension of particles from such products could be an important contributor to adverse health effects.

This study investigated personal exposures due to the resuspension of two Ag-based and two Zn-based consumer sprays used indoors. The release and resuspension of particles were investigated in a newly constructed $2.8 \times 1.6 \times 2.4 m^3$ chamber. Particles were sprayed at 1.1m height and then resuspended by a walking adult or the motion of a robotic sampler that simulated a child. The measurements of resuspended focused on particles reaching the breathing zone of an adult (1.5 m height) and child (0.3 m height). Button Samplers (SKC Inc.) with 25-mm PTFE filters (SKC Inc.) were used to collect sprayed and resuspended particles. The mass of captured particles was determined by weighing.

During spraying, the released particle concentration ranged from 350 to 30,000 $\mu g/m^3$ at 0.3 m and 14 to 14,000 $\mu g/m^3$ at 1.5 m. The concentrations varied among different products; once the product was sprayed, the concentrations measured at 0.3 m were higher than those measured at 1.5 m at the same time in a vast majority of experiments (94%). When particles were resuspended, resuspension rates ranged from 10^{-4} to 10^{-1} h^{-1}, depending on the product, floor type, and experimenter (e.g., adult and child). When particles were resuspended from the carpet, the resuspension rate for particles resuspended by an adult and reaching their breathing zone was higher than for particles resuspended by a child-simulating robot and reaching the child's breathing zone for 3 of the 4 products. However, when particles were resuspended from vinyl, the resuspension rates measured in the adult's breathing zone were lower than in the child's breathing zone. For both the adult and child, resuspension rates were higher for particles resuspended from carpet compared to vinyl.

The results suggest that children could be exposed to higher resuspended particle concentrations when using consumer products compared to adults. The resulting exposures depend on the product, flooring materials, resuspension force, and breathing zone height.

5IA.2

Assessing Mitigation Strategies to Reduce Potential Exposures to Indoor Particle Release Events. Kathryn Van Valkinburgh, Ali Mohammadi Nafchi, Nigel Kaye, Ehsan Mousavi, Vincent Blouin, ANDREW METCALF, *Clemson University*

As a result of the coronavirus outbreak, many educational institutions 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. Understanding potential air pollution hazards are a particular concern for highly populated indoor environments, such as workplaces and classrooms. This study discusses the results of ventilation testing in several different classrooms on Clemson University's main campus. In each classroom, a particle atomizer was used to release aerosol particles into the air, and multiple particulate measuring devices were placed strategically around each classroom to measure the particle concentration over time. We then assessed how quickly the particles were removed by the ventilation systems with varying ventilation conditions, including the addition of both high- and low-cost portable mitigation devices into the classroom.

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. The results indicate that increasing the air changes per hour in classrooms, whether through centralized air supply, decentralized ventilation units, or portable filtration devices, reduces the particle concentration half-lives. Another goal of this study is to apply the results and findings on particle behavior from the particle release tests to further evaluate the potential personal exposure risk associated with various classroom ventilation setups. The assessment indicates that measures which reduce particle concentration half-lives in the room, such as increasing the air flow through a fan coil unit and/or introducing portable filtration devices, also reduce the estimated total dose of viral particles inhaled during a given time period.

5IA.3

Quantifying Temporal Ventilation Trends in Indoor Air Quality in University Buildings Using Professional Grade Low-Cost Sensors. SABRINA WESTGATE, Daniel Alvarado-Velez, Eben Cross, David Hagan, Nga Lee Ng, *Georgia Institute of Technology*

In recent years, low-cost air quality sensors have become increasingly accessible, expanding opportunities to examine indoor air pollution over extended time periods and with high time resolution. Although we spend the majority of our time indoors, we have much to learn about how various factors, such as occupancy, influence indoor air quality. The rise of aerosol transmissible SARS-COVID19 has further highlighted the need to empirically evaluate - in real time - current ventilation systems and indoor air pollution dynamics in public spaces. This is of especial interest since in-situ carbon dioxide (CO_2) is often used as a proxy for understanding aerosol dynamics and potential SARS-COVID19 transmission. To assess indoor air quality and aerosol dynamics in a university setting, professional grade, low-cost sensors (QuantAQ MODULAIR and MODULAIR-PM) with the capability to detect particulate matter (PM_1, $PM_{2.5}$, PM_{10}), CO_2, and various gas-phase species were installed in rooms across the Georgia Institute of Technology campus beginning in Fall 2020. The rooms examined vary in size, ventilation type (fan coil units vs. heating, ventilation, and air conditioning units (HVAC)), percent outdoor air introduced into the room, and occupancy. In this study, data collected beginning in Fall 2020 was used to understand the variations in indoor air quality as a function of time, occupancy, and pollutant type. Room ventilation rates were estimated from the decays of in-situ CO_2 levels after class times and PM decays after cleaning or human activities. The calculated ventilation rates were compared to each other and to facilities ventilation records. Results show a clear impact of mechanical ventilation schedules on CO_2 and PM decay rates and indicate the applicability of using CO_2 data from room occupancy to estimate room and aerosol ventilation. Moreover, results indicate a relationship between PM size and decay rate, providing insight to indoor aerosol dynamics.

5IA.4

Particulate Matter in Multi-Unit Social Housing: Impacts of Smoking, Season, and Building Retrofits. Alexander Mendell, Alireza Mahdavi, Yuchao Wan, JEFFREY SIEGEL, *University of Toronto*

We investigated $PM_{2.5}$, total suspended particle (TSP), and particle-bound SVOC concentrations in 75 social housing apartments in Toronto before and after energy-reduction retrofits. Smoking (either self-reported on a questionnaire and/or indicated by presence of tobacco odours and apparatus) lead to indoor $PM_{2.5}$ concentrations that were approximately four times greater than in homes without smoking, as well as higher TSP concentrations. Considerable variation in the smoking effect was likely driven by smoking frequency. Seasonality (late fall vs. late spring) was a much smaller impact and was only evident in non-smoking apartments. The building retrofits did not influence particle concentrations, potentially due to the fact that PM sources as well as ventilation were largely unaddressed in the retrofit approach. Particle bound phthalates and PAHs followed similar trends to $PM_{2.5}$ and TSP. When compared to PM2.5 concentrations measured in 20 single-family non-smoking homes in Toronto, the $PM_{2.5}$ concentrations in the non-smoking apartments were approximately a factor of two larger, potentially owing to interunit transport of environmental tobacco smoke and other particle sources. However, the TSP concentrations were higher in the Toronto single family homes, likely due differences in measurement approach, house age, and filtration system operation. Overall, the results suggest that energy retrofits can achieve carbon goals without adversely impacting indoor air quality. Apartment unit compartmentalization and/or other approaches to reduce smoking should be considered in future retrofits of social housing.

5IA.5

Exposure to Indoor and Outdoor Air Toxics and Associated Human Health Risk in Edmonton, Canada. MD. AYNUL BARI, Sanchita Paul, Warren Kinderzierski, *University at Albany, SUNY*

Exposure to hazardous air pollutants (HAPs) or air toxics is of interest due to potential carcinogenic and other adverse health effects. There is a growing awareness and public health interest about the quality of air people breathe in indoor and outdoor environments. While government agencies have emphasized tackling urban ambient air pollution, less attention has been paid in assessing HAPs in indoor and outdoor (e.g., backyard) residential settings – which are key microenvironments for human exposure. The purpose of this study was to evaluate the relationship between indoor/outdoor residential HAPs concentrations and their potential risk to public health. Indoor and outdoor HAPs concentrations, including volatile organic compounds and trace elements in PM1, were measured in 50 non-smoking homes of Edmonton, Alberta in both winter and summer 2010. For assessing risks associated with inhalation exposures, dose response criteria of the USEPA were used to screen HAPs concentrations. For chronic exposure, cancer and non-cancer risks were evaluated using USEPA inhalation unit risk and reference concentrations associated with the concentration for each HAP. Estimated 95th percentile (upper-bound) cancer risks of some indoor HAPs e.g., benzene, 1,3-butadiene, naphthalene, formaldehyde, and cadmium were above recommended USEPA acceptable risk (1x10–6) and Alberta cancer benchmark (1x10–5) targets, but below the USEPA tolerable risk (1x10–4). Estimated indoor non-cancer risks of 1,3-butadiene, trichloroethene, and naphthalene were above a safe level (>1) with the highest being observed for acrolein. Estimated risks for all outdoor HAPs were below the acceptable and safe levels except for acrolein (non-cancer risk). Findings of this study provide key information about current HAPs levels in residential homes and their associated public health risks. This can aid in developing useful information for reducing exposure to HAPs in residential settings through daily activities and household practices.

5IA.6

Indoor PM2.5 as a Function of Outdoor PM2.5, Temperature, Heatwave Period, and Smoking Status.

RUIKANG HE, Ioanna Tsoulou, Sanjeevi Thirumurugesan, Brian Morgan, Stephania Gonzalez, Deborah Plotnik, Jennifer Senick, Clinton J. Andrews, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

$PM_{2.5}$, defined as airborne particulate matter (PM) with a diameter of 2.5 µm or less, is an important indoor pollutant that leads to negative cardiovascular and respiratory effects. Our previous study showed that indoor $PM_{2.5}$ is influenced by outdoor $PM_{2.5}$ levels, human indoor activities such as smoking, and could also be affected by heatwaves (days with t > 90F). However, clear relationships between indoor $PM_{2.5}$ and these factors remain largely unexplored. In our continuing investigation of heatwave effects on indoor PM, we focused on how indoor smoking modifies the influence of outdoor conditions on indoor air quality. Thus, apartments of 8 smokers and 16 non-smokers were monitored from July to September to track the change in indoor $PM_{2.5}$ and relate them with outdoor conditions.

We found that indoor $PM_{2.5}$ levels increased as outdoor temperature increased in 87.5% of non-smokers' apartments and 37.5% of smokers' apartments in both heatwave and non-heatwave days. Slope coefficients of the linear regression between indoor $PM_{2.5}$ and outdoor temperature were statistically significant and positive for 62.5% of non-smokers' apartments and 37.5% of smokers' apartments for both heatwave and non-heatwave days; 25.0% of smokers' apartments showed statistically significant negative slope coefficients for heatwave days. Also, indoor $PM_{2.5}$ levels increased with increasing outdoor $PM_{2.5}$, except for 4 smokers' and 2 non-smokers' apartments. Analysis of the relationship between indoor and outdoor $PM_{2.5}$ showed that in 68.8% of non-smokers' apartments slope coefficients were statistically significant and positive regardless of heatwave; on the other hand, no smokers' apartments showed statistically significant slopes during heatwave days, i.e., the heatwave conditions did not add much $PM_{2.5}$ to already high $PM_{2.5}$ levels in smokers' apartments.

Overall, our data suggest that long-term monitoring in residences could be helpful to the combined research into climate change, indoor air pollution, and resulting human health effects.

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5IA.7

Secondary Organic Aerosol Formation from the Reaction of Decamethylcyclopentasiloxane (D5) with Chlorine Atoms.

ANITA AVERY, Francesca Majluf, Jordan Krechmer, Harald Stark, Lea Hildebrandt Ruiz, William Brune, Manjula Canagaratna, Andrew Lambe, *Aerodyne Research, Inc.*

Indoor emissions of siloxanes from personal care products have been studied extensively, as they often dominate total VOCs in occupied spaces. The oxidative aging of the siloxane decamethylcyclopentasiloxane (D5) by hydroxyl radicals (OH) and corresponding secondary organic aerosol (SOA) formation have recently been characterized. Chlorine atoms (Cl) may compete with OH for the oxidative loss of D5 under certain conditions, particularly following bleach cleaning activities that emit Cl precursors such as molecular chlorine and hypochlorous acid. However, the SOA formation potential of D5 + Cl reactions has not been studied. Here, we characterized the chemical composition and yield of SOA generated from the Cl oxidation of D5 in an oxidation flow reactor at Cl concentrations ranging from approximately $5*10^7$ to $2*10^9$ cm-3 in several minutes' exposure time. D5 + Cl SOA was characterized with several state-of-the-art mass spectrometry techniques, including aerosol mass spectrometry, and a Vocus proton-transfer-reaction mass spectrometer (PTR-MS) with a heated aerosol inlet. Results are compared to SOA generated from D5 + OH using OH concentrations ranging from approximately $5*10^9$ to $5*10^{10}$ cm^{-3} to identify molecular tracers for Cl- versus OH-initiated oxidative aging of D5. These results emphasize the importance of secondary chemistry during and after bleach cleaning activity.

5IA.8

Understanding Outdoor and Indoor Air Quality Implications of 100% Fresh (Ambient) Air Ventilation System. ALVARADO-VELEZ DANIEL, Sabrina Westgate, Eben Cross, David Hagan, Nga Lee Ng, *Georgia Institute of Technology*

Studies have shown that indoor air quality (IAQ) is important to consider at the building design stage due to its impact on human health and work productivity. Some symptoms of poor IAQ include shortness of breath, headaches, and irritation of the respiratory system. Viruses and bacteria can also spread through airborne particulate matter (PM) which is of special concern at the time of this study due to the COVID-19 pandemic. Many buildings utilize ambient air for ventilation, and thus the quality of indoor air is dependent on the quality of the ambient air. Here, we utilize paired QuantAQ MODULAIR and MODULAIR-PM sensors to measure the mass concentration of particulate matter (PM) of different sizes (PM1, PM2.5, PM10) and the mixing ratio of CO2, CO, NO, NO2, and O3 inside and outside a building on Georgia Tech’s campus. The building evaluated uses 100% fresh (ambient) air in ventilation. One pair of sensors was located inside a work office and another pair was located on the roof of the building near the air inlet of the dedicated outdoor air system. Each sensor makes measurements at one-minute intervals. Preliminary results indicate the indoor PM mass concentration in general follows a similar trend to the outdoor concentration. However, the relationships between indoor and outdoor gas species appear to be highly variable. Specific parameters (e.g., time of the day, human activities, etc.) influencing indoor/outdoor gas and particle species are discussed. Results from this study will help elucidate the effects of outdoor air quality on IAQ and could be used to determine steps needed to improve IAQ.

5IA.9

Modeling Indoor Inorganic Aerosol Concentrations during the ATHLETIC Campaign with ISORROPIA. Bryan Berman, Bryan Cummings, Hongyu Guo, Pedro Campuzano-Jost, Jose-Luis Jimenez, Demetrios Pagonis, Peter F. DeCarlo, SHANNON CAPPS, Michael Waring, Douglas Day, Zachary Finewax, Benjamin A. Nault, Anne Handschy, *Drexel University*

Aerosol constituents alter as they are transported through ventilation systems into rooms indoors. For instance, changes in temperature and relative humidity (RH) between indoors and outdoors influence the partitioning of specific aerosol components. Previously, IMAGES (Indoor Model of Aerosols, Gases, Emissions, and Surfaces), a modeling platform that simulates indoor organic aerosol, was extended to incorporate the inorganic aerosol thermodynamic equilibrium model, called ISORROPIA. ISORROPIA estimates partitioning for inorganic aerosols and precursor gases; here, it is applied to outdoor and indoor concentrations of sulfate, nitrate, ammonium, nitric acid, and ammonia. The model was initially evaluated by comparing simulated aerosol to indoor measurements done by Avery et al. (2019) in a classroom during the summer and winter. However, this dataset did not have outdoor or indoor gas-phase concentrations with which to inform and evaluate IMAGES with ISORROPIA. In 2018, the ATHLETIC campaign conducted at the University of Colorado Dal Ward Athletic Center explored how human exercise, chlorine-based cleaners, and other parameters influence indoor air quality (Claflin et al., 2020; Finewax et al., 2020). Using a suite of instruments, they measured inorganic aerosol and gas concentrations in addition to temperature and RH. Herein, modeled inorganic aerosol and gas concentrations were compared to indoor measurements from the ATHLETIC campaign to further evaluate the IMAGES with ISORROPIA model with a complete datasets.

5IA.10

Cookstove Emissions and Performance Evaluation Using a New ISO Protocol and Comparison of Results with Previous Test Protocols. WYATT CHAMPION, Michael Hays, Craig Williams, Larry Virtaranta, Mark Barnes, William Preston, James Jetter, *U.S. Environmental Protection Agency*

In 2018, the International Organization for Standardization (ISO) 19867-1 "Harmonized laboratory test protocols" were released for establishing improved quality and comparability for data on cookstove air pollutant emissions, efficiency, safety, and durability. This is the first study to compare emissions [carbon dioxide, carbon monoxide, total hydrocarbons, methane, nitrogen oxides, fine particulate matter ($PM_{2.5}$), organic carbon, elemental carbon, and ultrafine particles] and efficiency data between the ISO protocol and the formerly employed Water Boiling Test (WBT). The study examines six stove/fuel combinations [liquefied petroleum gas (LPG), pellet, wood fan, wood rocket, three stone fire, and charcoal] tested in the same US EPA laboratory. Evaluation of the ISO protocol shows improvements over previous test protocols and that results are relatively consistent with former WBT data in terms of tier ratings for emissions and efficiency, as defined by the ISO 19867-3 "Voluntary Performance Targets." Most stove types remain similarly ranked using ISO and WBT protocols, except charcoal and LPG are in higher $PM_{2.5}$ tiers with the ISO protocol. Additionally, emissions data including polycyclic aromatic hydrocarbons are utilized to compare between the ISO and Firepower Sweep Test (FST) protocols. Compared to the FST, the ISO protocol results in generally higher $PM_{2.5}$ tier ratings.

5IA.11

Volatilization and Partitioning to Aerosols From Electronic Cigarette Vapor Residue. HENRY COLBY, Erin Katz, Roger Sheu, Peter F. DeCarlo, *Drexel University*

With increasing popularity of electronic cigarettes (E-cigs) and frequent use in the indoor environment it is necessary to study their effect on indoor air quality. While immediate impacts of e-cig use on air quality are visible and have been investigated, little is known about the persistent impact of surface deposited e-cig particles on indoor air quality. Third hand smoke (THS) is the term used for deposited tobacco smoke on surfaces which can evaporate into room air over a longer time scale. These evaporated species, including compounds like nicotine, have been shown to partition to ambient particles where they can accumulate and deposit in the human respiratory system. This same process can occur with E-cig vapor residue. Laboratory experiments using a stainless-steel chamber were performed to demonstrate that semivolatile species deposited from E-cig particles form a residue which can repartition to the gas phase and deposit onto ammonium sulfate seed aerosols. Using a high-resolution aerosol mass spectrometer (HR-AMS), the particle composition of primary vapor was recorded prior to three experiments which analyzed seed aerosols with partitioned species over 5 days. Subsequent experiments with the addition of an Elf-Vocus proton transfer reaction mass spectrometer (PTRMS) allow us to observe the change in concentration of gas phase species as the primary particles are eliminated from the chamber and seed aerosols are introduced. The results of these experiments provide a better understanding of the interaction between gas and particle phases of species like nicotine, vegetable glycerin, propylene glycol, and benzoic acid.

5IA.12

Evaluating the Indoor and Outdoor Air Quality Impacts of Intensive Building Energy Efficiency Improvements.

COLBY BUEHLER, Kenneth Gillingham, Pei Huang, Drew Gentner, Jordan Peccia, *Yale University*

Intensive building energy efficiency improvements can reduce air pollutant and greenhouse gas emissions from electricity generation, improving outdoor air quality and human health, but may also affect indoor air quality through changes in ventilation. This study examines the indoor and outdoor effects of highly ambitious, yet feasible, building energy efficiency upgrades in the United States through 2050. Our energy efficiency scenarios, derived from the literature and modeled using Yale-NEMS (National Energy Modeling System), lead to reductions in outdoor energy-related emissions of 18-25% for $PM_{2.5}$ and 6-11% for CO_2 in 2050. The effects on indoor air quality as a result of the various energy efficiency scenarios were examined using a coupled indoor air quality box model with a Monte Carlo approach across the entire US housing stock based on typical activity patterns and evolving housing characteristics. Due to increasing emphasis on energy savings related to the building envelope, indoor air quality impacts varied across the U.S. housing stock and were dependent on indoor emissions, infiltration air exchange rates, and the presence of $PM_{2.5}$ filtration. While indoor air quality was negatively impacted in some homes, the net effects of changes in indoor and outdoor air quality with intensive energy efficiency scenarios could prevent thousands of premature deaths per year across the United States in 2050, but the results emphasize the need for careful consideration of ventilation policies and investments in improved $PM_{2.5}$ filtration in recirculation systems.

5IM.1

Laminar Flow Sublimation-Deposition Systems for Nanoparticle Growth with MALDI Matrices.

KE' LA KIMBLE, Michelle Heilig, Brock Mitts, Li Li, Kimberly Prather, Christopher J. Hogan, *University of Minnesota*

Aerosol Time-of-Flight Mass Spectrometry (ATOFMS) enables single particle chemical analysis via laser ionization. Traditional laser ionization approaches are well suited towards small molecules, but are challenging to apply to high molecular mass analytes. Conversely, matrix- assisted laser desorption ionization (MALDI) is an established route to ionize peptides, whole proteins, and nucleic acids, i.e., biomolecules. MALDI-MS has been demonstrated for aerosols, but sparingly applied due to the lack of a repeatable, portable method to combine aerosol particles with an appropriate matrix material (material that absorbs laser light and facilitates ionization) without requiring separate particle collection and transfer steps. We have developed a laminar flow sublimation-deposition system to coat individual particles repeatably with MALDI matrix materials in-flight. Based on the operation principle of condenser-saturator systems in laminar flow condensation particle counters, the sublimation-deposition system passes particles over a heated bed (70-90^{o} C) of MALDI powder (ferulic acid and 2,4 dihydroxybenzoic acid in the present effort), leading to a heated, saturated aerosol. Using a water jacket-cooled tube at 0o C, deposition of the matrix material following sublimation proceeds onto particles. We find that particles as small as 15 nm can be grown to near 300 nm using this approach, and that for particles in the 15 nm – 100 nm size range, the resulting size is relatively insensitive to initial particle size, though strongly sensitive to sublimator temperature. As particles in the 300 nm size range can be detected and ionized significantly more efficiently in ATOFMS systems than sub-100 nm particles, matrix sublimation-deposition has the combined effects of (1) enabling MALDI-MS of aerosol particles and (2) improving “hit-rate” for sub-100 nm particles.

5IM.3

Understanding the Physicochemical Evolution of Levitated Particles using Linear Quadrupole Electrodynamic Balance Coupled with Paper Spray Mass Spectrometry.

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

Aerosols are an important component of earth’s atmosphere which influence cloud properties, climate, air quality and health. Due to aerosols’ wide composition range along with reactive environmental conditions, their chemical composition and hence properties are continuously evolving as a result of various physicochemical processes (like heterogeneous reactions, photochemical transformations, and evaporation) happening in/on the particles. Understanding the physicochemical evolution of these particles is crucial to predict their role and impacts in the atmosphere.

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 chemically evolving multi-component levitated aerosol particles. In terms of experimental setup, an array of micrometer sized droplets is levitated in LQ-EDB. The light scattering technique is employed to determine physical properties (like size and RI) using Mie resonance spectroscopy which is then followed by compositional measurements of individual particles using high resolution MS.

Measurements of the evaporation kinetics of two volatile n-ethylene glycols, triethylene glycol and tetraethylene glycol in their binary and ternary mixtures, were made in real-time under dry conditions to understand and relate the evolving size with chemical composition. These measurements were then extended to explore the influence of various humidity conditions on the evaporation kinetics. It is demonstrated that both size and composition evolution follow the expected trend with each other and also when compared against evaporation model predictions. Finally, our results demonstrate that the LQ-EDB-MS platform can accurately and precisely measure the time-dependent physical properties and compositional changes, yielding broad capabilities for studying chemical aging in suspended particles.

5IM.5

Molecular Structure Characterization of Nanoparticles Formed from the Ozonolysis of Alpha-Pinene.

ADAM THOMAS, Véronique Perraud, Michelia Dam, James Smith, *University of California, Irvine*

It is known that a major source of atmospheric aerosol originates from the oxidation of volatile organic compounds, of which monoterpenes represent an important class. In particular, the α-pinene + O_3 system has been widely studied, in large part due to its role in new particle formation. However, there remains much to be learned about the distribution and structural identities of the products of this reaction, particularly as they are observed in the early stages of particle growth. It has been shown in recent years that ultra-high resolution mass spectrometry (HRMS) using an orbitrap mass analyzer features several key advantages over other more widely used approaches applied in the analysis of organic aerosol, including a superior mass resolving power (up to 140,000) and tandem mass spectrometry (MS2) capabilities. Here, nanoparticles were generated from reactions of ozone (1-1.5 ppm) with α-pinene (300-400 ppb) in an 8.5 L flow reactor and collected using a sequential spot sampler before being analyzed offline with an UHPLC-HRMS system consisting of a Vanquish Horizon UHPLC and a Q Exactive Plus orbitrap mass analyzer (ThermoScientific). Collectively, over 100 products with unique retention times were resolved in sub-100 nm diameter nanoparticles sampled during these experiments, with structural insight gathered from the detailed analysis of the MS2 fragmentation patterns collected from some of the most abundant species. We used data collected from these experiments to create and populate an MS2 spectral database which can be used to assist in future laboratory and field studies. Overall, our findings demonstrate the ability of orbitrap MS to highly resolve and structurally characterize compounds found in secondary organic nanoparticles.

5IM.6

Enriching Inlet for Improving Sensitivity and Level of Detection of Reactive Organic Gases by an Order of Magnitude in SCCM-Level Flows. NAMRATA SHANMUKH PANJI, Graham Frazier, Gabriel Isaacman-VanWertz, *Virginia Tech*

A significant portion of the global aerosol load is due to organic aerosols (OA), which are formed in large part when reactive organic gases in the atmosphere, such as terpenes, are oxidized through complex photochemical pathways. Quantitative measurement of these compounds, especially using low-cost methods, is challenging because they are present in sub-ppb to sub-ppt levels. Furthermore, losses to instrument lines and surfaces can compound these challenges. As a result, instruments measuring volatile reactive organics often suffer from high levels of detection and low sensitivities. We have developed a novel enriching inlet to concentrate these gases (by up to an order of magnitude) for low sampling flows. VOCs are sampled through Teflon™ AF-2400 tubing subjected to a pressure differential. Under these conditions, inert gases are driven out of the sampling stream due to selective permeation, leaving behind a stream of concentrated VOCs for analysis downstream. We present here a validated model that links pressure differential, inlet length, sampling flow rate, and analyte permeability, to predict enrichment of a given gas at a given sample flow, with propane (C_3H_8) used as a sample gas. We demonstrate this inlet with enrichment of up to a factor of 10 for a wide range of atmospherically important analytes, including major OA precursors like isoprene (C_5H_8) and α-pinene ($C_{10}H_{16}$). Enrichment is shown to be predictable, and achievable under a wide range of pressurized and sub-ambient flow conditions.

5IM.7

10 nm Exhaust Particle Counting System for Automotive Certification Measurements. HELMUT KRASA, Martin Kupper, Markus Bainschab, Martin Cresnoverh, Mario Arar, Alexander Bergmann, *Graz University of Technology*

Reducing the lower particle size cut point of a particle number emission measurement system: A holistic system optimization.

The current Euro 6 standard limits the emission of non-volatile particle number (PN) for particles larger than 23 nm in diameter. Future European emission legislation for vehicle homologation will reduce the particle size limit to 10 nm in a first step for light-duty vehicles and subsequently for heavy duty vehicle types. In the European H2020 project “DownToTen” (DTT), critical loss mechanisms in the sub 23 nm regime were examined. Based on the findings, a loss-optimized dilution- and sampling system was demonstrated as a suitable exhaust particle probing unit for this size regime.

We present the first steps beyond the project DownToTen incorporating the gained scientific findings into a commercially available state-of-the-art particle number measurement instrument. We substantially improved the AVL Particle Counter (APC) for the measurement of solid particles >10nm with respect to minimal losses and reduced artefact formation. This cannot be achieved by solely reducing the cut point of the employed counting unit. The primary dilution stage supplied by a Rotating Disk Diluter (RDD) was identified as a source of diffusional particle losses. The RDD’s particle loss performance was significantly improved by optimizations of the geometry and the mode of operation, theoretical calculations showed a potential loss reduction up to 45%. Flow path and flow rate optimizations reduced the diffusional particle losses in the system. First experiments showed a further 30% reduction. The performance of the optimized system was characterized experimentally and compared with simulation results.

5IM.8

Optimizing the Activation Efficiency of Sub-3 nm Particles in a Laminar Flow Condensation Particle Counter by Model Simulation.

WEIXING HAO, Mark R. Stolzenburg, Michel Attoui, Jiaoshi Zhang, Yang Wang, *Missouri University of Science and Technology*

The measurement of airborne particles with sizes below 3 nm is critical, as it helps the understanding of atmospheric nucleation and elucidates important particle synthesis mechanisms in the gas phase. Condensation particle counters (CPC) have been widely used to measure the concentration of aerosols. However, it is challenging for the CPC to measure particles below 3 nm due to the insufficient activation of these particles via vapor condensation. Methods have been proposed to increase the saturation ratio of the condensing vapor to promote the detection efficiency of sub-3 nm particles in the CPC. Different working fluids also make a considerable impact on particle detection. Given the various types of parameters and the wide range of values these parameters can take, modeling studies are needed in searching for the optimal operating conditions of a CPC.

In this work, we simulated the sub-3 nm particle activation and growth in a laminar flow CPC using COMSOL Multiphysics, which has advantages of simulating complex flow conditions and interfacing with post-processing software such as MATLAB. Our simulation incorporates the influence of temperature-dependent fluid properties on particle activation and the impact of latent heat and non-continuum effects on droplet growth. The results were compared against the analytical Graetz model [1], and demonstrated excellent agreement (within 0.7%) between these two simulation methods. Our COMSOL simulations show that glycerine, diethylene glycol, ethylene glycol, 2-aminoethanol, and dimethyl phthalate are the best five working fluids achieving the smallest particle size activated among 45 commonly used solvents. We also discussed the effect of CPC operating conditions, such as the condenser geometry and flow conditions, on particle activation for optimizing the performance of the CPC in detecting sub-3 nm particles.

[1] Stolzenburg, M. R., & McMurry, P. H. (1991). Aerosol Sci. Technol., 14(1), 48-65.

5IM.9

Simplified Calibration of CPC Detection Efficiency Using Mono-Disperse Aerosols.

DEREK OBERREIT, Siqin He, *Kanomax FMT, Inc.*

Measurements of Condensation Particle Counter (CPC) detection efficiencies ($N_{sampled}/N_{detected}$) traditionally use a High Resolution Ion Mobility Classifier (HRIMC) to provide an aerosol with a known range of electrical mobilities and a faraday cup electrometer (FCE) to measure the charge concentration of the classified aerosol; however there are several sources of measurement error using this method. While corrections can be made to the measurements, these corrections depend on the raw particle size distribution and an assumption that the charge distribution matches empirically measured values. Existing methods also do not allow for calibration of the activation efficiency independent of transport efficiency, latter of which is size dependent and can skew the result. The transport efficiency of the FCE also leads to errors that are difficult to correct for. Mitigation of these concerns facilitates repeatable, high accuracy calibrations of detection efficiencies.

In this work, we describe a method for calibrating CPC detection efficiencies to fixed diameters using near monodisperse aerosolized proteins with a moderate resolution IMC. We show that these materials can be aerosolized with negligible interference by multiply charged particles or errors due to skewness of the challenge aerosol. We also show concentration as a function of condenser temperature profiles for several different materials and how variations in the stability of the challenge aerosol concentration can be corrected using a reference detector. We also show that by measuring the asymptote of these profiles, the activation efficiency as a function of condenser temperature can be determined. With this method, the transport efficiency and activation efficiency can be decoupled effectively eliminating this source of error from the reference detector.

5IM.10

Optimization of Multiplexed Orthogonal Injection of Ions from Electrospray Sources into a Low Pressure Ion Funnel as a Means to Improve Sensitivity. XI CHEN, Pei Su, Julia Laskin, Carlos Larriba-Andaluz, *IUPUI*

The electrodynamic ion funnel has been widely used to efficiently focus and transmit ions in the expanding gas jet from electrospray ionization (ESI) sources at sub-ambient pressures (0.1–30 Torr). Multiplexing of the ESI emitters is one of the notable techniques used in RF funnels to increase ion current and sensitivity of the detector, in this case a Mass Spectrometer (MS). An experimental system consisting of four injection inlets orthogonal to the funnel axis was studied showing that the total ion current transmitted through to the mass spectrometer was almost proportional to the number of capillaries under some configurations and analyte sets. To optimize the design of the funnel, ion trajectory simulations were studied using SIMION software analyzing the ions movement at different pressures and ion inlets distribution (staggered or aligned, symmetric or otherwise). To aid with the simulation and to mimic the real environment harshness of pushing ions from atmospheric pressure into low pressure with as much realism as possible, the velocity profile inside capillaries and funnel chamber was simulated through the computational fluid dynamic (CFD) software SOLIDWORKS. The flow field was then added to the SIMION field simulations to track ion trajectories and optimize the geometry and orientation of the orthogonal inlets, and the pressure inside the system. Among the different cases studied, the one that performed the best was to split the four capillaries into two pairs on opposite sides of the funnel and aligned so that the flows from the capillaries countered each other. For this configuration, the optimized transmission pressure was found to be 7 Torr. The optimization steps laid out in this work provide a way to optimize the sensitivity of other ion sources in a controlled manner, making the study very useful in many disciplines.

5IM.11

Correcting Bias in Log-linear Instrument Calibrations in the Context of Chemical Ionization Mass Spectrometry. CHENYANG BI, Jordan Krechmer, Manjula Canagaratna, Gabriel Isaacman-VanWertz, *Virginia Tech*

Quantitative calibration of analytes using chemical ionization mass spectrometers (CIMSs) has been hindered by the lack of commercially available standards of atmospheric oxidation products. To accurately calibrate analytes without standards, techniques have been recently developed to log-linearly correlate analyte sensitivity with instrument operating conditions. However, there is an inherent bias when applying log-linear calibration relationships that is typically ignored. In this study, we examine the bias in a log-linear-based calibration curve based on prior mathematical work. We quantify the potential bias within the context of a CIMS-relevant relationship between analyte sensitivity and instrument voltage differentials. Uncertainty in three parameters has the potential to contribute to the bias, specifically the inherent extent to which the nominal relationship can capture true sensitivity, the slope of the relationship, and the voltage differential below which maximum sensitivity is achieved. Using a prior published case study, we estimate an average bias of 30 %, with 1 order of magnitude for less sensitive compounds in some circumstances. A parameter-explicit solution is proposed in this work for completely removing the inherent bias generated in the log-linear calibration relationships. A simplified correction method is also suggested for cases where a comprehensive bias correction is not possible due to unknown uncertainties of calibration parameters, which is shown to eliminate the bias on average but not for each individual compound.

5IM.12

The Dual Polarity Spider: A Fast, Compact, Particle Mobility Spectrometer.

STAVROS AMANATIDIS, Gregory Lewis, Steven Spielman, Ryan Ward, Yuanlong Huang, Benjamin Schulze, Susanne Hering, Richard Flagan, *Aerosol Dynamics Inc.*

Mobility-based particle spectrometers have become the *de facto* reference method for measurement of submicrometer and ultrafine aerosol size distributions. Yet the conventional instruments are large and heavy, and thus not appropriate for field deployments. The “Spider DMA” is a small, radial-flow differential mobility analyzer recently developed for applications requiring high portability and fast time resolution, such as moving platform deployments. The instrument is designed to operate at 0.3 L/min aerosol flow and 0.6 – 1.2 L/min sheath flow, and provides sizing in the 10 – 500 nm range with a moderate resolution of R = 2 – 4.

Here, we present key features of the “*Dual Polarity Spider DMA*”, a next generation design that provides size classification of particles with either positive or negative charge. This is realized by employing a recently developed high-voltage supply that can generate accurate upscan and downscan voltage ramps of both positive and negative polarity. We discuss the key changes incorporated in the new DMA design, that enable robust and efficient classification across its operating voltage range from -5000 V to +5000 V. Transfer functions in scanning-voltage mode are evaluated through finite element modeling, and through tandem DMA experiments with both positive and negative particles. Moreover, we report a comparison of its performance in measuring ambient size distributions against a conventional mobility particle sizer, over a testing period of several days of continuous operation. The data show agreement in the shape, number concentration, and geometric mean diameter for ambient aerosols, corroborating the compact Spider DMA efficacy for fast, accurate ambient size distribution measurements.

5SI.1

Risk Assessment and Mitigation of Aerosol Driven Transmission during Wind Instrument Plays.

RUICHEN HE, Aliza Abraham, Linyue Gao, Jiarong Hong, *University of Minnesota*

Aerosol driven disease transmission has raised significant concerns regarding the safety of wind instrument plays. In collaboration with 16 musicians from Minnesota Orchestra, we provide a systematic examination of aerosol generation from 10 types of wind instruments and the transport of aerosols under the orchestral hall settings. We find the aerosol concentration exhibits more than two orders of magnitude variability across different instruments and depends on the dynamic level, articulation pattern, the breathing techniques used for different instrument plays, etc. Through a comparison with aerosol generation from normal breathing and speaking, we categorize the instruments into low (tuba), intermediate (e.g., bassoon, flute, French horn, etc.) and high risk (e.g., trumpet, trombone, etc.) levels. Brass instrument flow increases with music amplitude and their aerosol production exhibits an inverse response to note duration, while woodwinds emit more aerosols when note pitch increases. The regions where the flow speed and aerosol concentration are above the measurable background level vary among instruments but extend no farther than 30 cm from the instrument outlet for all instruments. Farther away, the upward-moving thermal plume induced by the temperature difference between the human body and ambient air is the dominant source of flow and aerosol transport. Covering the trumpet bell with one layer of acoustic fabric reduces the emitted aerosols by ~60% with little impact on the sound quality. Computational fluid dynamics simulations show that placing an air cleaner above the instrument outlet can reduce the aerosols by 90% owing to the thermal plume driving aerosols upwards. Filtration efficiency further increases considerably (~10%) when lowering the ambient temperature from 25 °C to 20 °C to enhance the thermal plume effect. Overall, our findings provide useful insights into the risk assessment and the corresponding mitigation strategies for various musical activities.

5SI.2

SARS-CoV-2 in Aerosol Particles Exhaled from COVID-19 Infected Patients during Breathing, Talking and Singing.

MALIN ALSVED, David Nygren, Patrik Medstrand, Sara Thuresson, Carl-Johan Fraenkel, Jakob Löndahl, *Ergonomics and Aerosol Technology, Lund University, Sweden*

In the beginning of the COVID-19 pandemic, several super spreader events occurred during singing in choirs, which lead to an increased attention to airborne transmission of SARS-CoV-2, the virus causing COVID-19. Since then, aerosol generation from singing has been studied in more detail, however, only from healthy subjects. In this study, we collected aerosol particles in the exhaled breath of 40 COVID-19 infected patients during breathing, talking and singing, respectively, and analysed the samples for detection of SARS-CoV-2.

Method

Patients that were contacted by the COVID-19 testing service due to a positive test result were asked to volunteer for the study. A team of researchers drove a small truck hosting a mobile laboratory to the home address of the patient to perform exhaled breath aerosol collection using a condensational particle collector (BioSpot, Aerosol Devices) and a two-stage cyclone sampler (NIOSH bc-251, Tisch Environmental). Samples were collected for 10 min each when the patient was breathing, talking and singing, respectively.

All samples were stored at -80°C until RNA extraction and analysis by reverse transcription quantitative polymerase chain reaction (RT-qPCR) targeting the N-gene.

Results

A first screening of air samples collected with the BioSpot showed that SARS-CoV-2 could be detected in the exhaled aerosols from three of nine patients during singing or talking. Two of these samples contained 10^3 and 10^4 viral RNA copies, corresponding to a viral emission rate of approximately 4 and 25 viruses per second, respectively. Samples from the remaining 31 patients are to be analysed during the spring. We hope to contribute to quantifying and understanding the Covid-19 transmission via the airborne route.

This study was approved by the Swedish Ethics Review Authority (2020-07103). This work was supported by AFA Insurances and the Swedish Research Council FORMAS.

5SI.3

Measurements and Simulations of Aerosol Released while Singing and Playing Wind Instruments.

TEHYA STOCKMAN, Shengwei Zhu, Abhishek Kumar, Lingzhe Wang, Sameer Patel, James Weaver, Mark Spede, Donald K. Milton, Jean Hertzberg, Darin Toohey, Marina Vance, Jelena Srebric, Shelly Miller, *University of Colorado Boulder*

Outbreaks from choir performances, such as the Skagit Valley Choir, showed that singing brings potential risk of COVID-19 infection. There is less known about the risks of airborne infection from other musical performance, such as playing wind instruments or performing theatre. In addition, it is important to understand methods that can be used to reduce infection risk. In this study, we used a variety of methods, including flow visualization, aerosol and CO2 measurements, and computational fluid dynamics (CFD) modeling to understand the different components that can lead to transmission risk from musical performance and risk mitigation. This study was possible because of a partnership across academic departments and institutions and collaboration with the National Federation of State High School Associations and the College Band Directors National Association. The interdisciplinary team enabled us to understand the various aspects of aerosol transmission risk from musical performance, and quickly implement strategies in music classrooms during the COVID-19 pandemic. We found that plumes from musical performance were highly directional, unsteady, and vary considerably in time and space. Aerosol number concentration measured at the bell of the clarinet were comparable to singing. Face and bell masks attenuated plume velocities and lengths and decreased aerosol concentrations measured in front of the masks. CFD modeling showed differences between indoor and outdoor environments and that lowest risk of airborne COVID-19 infection occurred at less than 30 minutes of exposure indoors and less than 60 minutes outdoors.

5SI.4

The Effect of Plexiglass Shields on Droplet/Aerosol Transmission of Virus in Indoor Environments. BO YANG, Khaled Hashad, Alfredo Rodriguez, K. Max Zhang, *Cornell University*

Several studies showed the potential airborne transmission of the SARS-CoV-2 virus. Social distancing, facial masks, and handwashing have been emphasized to slow down the transmissions. One specific design is the plexiglass shields, which were installed in many indoor environments such as classrooms, restaurants, and banks. The plexiglass shield is a part of the indoor environmental interior structure, affecting the indoor flow field and the virus-contained particle/droplet trajectories. However, there are very little quantitative data showing the effect of the interior structure on particle/droplet transport and fate. The goal of this study is to simulate the SARS-CoV-2 virus contained particles/droplets dynamics in a room. In the simulation, human talking-generated particle/droplet size ranges from 0.6 µm to 750 µm. Both the particle/droplet evaporation and deposition were modeled using computational fluid dynamics (CFD) coupled with the aerosol dynamics. Given this specific indoor layout, the plexiglass shield can significantly increase the deposition ratio, but cannot decrease the airborne ratio. The particle/droplet exhaust ratio would be decreased correspondingly. Our findings indicate the plexiglass shield could be helpful to the large particles/droplets (>100 µm), but not very effective for smaller ones.

5SI.5

Healthcare Acquired Infections (HAIs), Coronavirus, and Filtration Efficiency. NIKKI SASHER, *AAF Flanders*

Air quality has profound health implications in all indoor environments where the U.S. population normally spends most of their time. Specifically, indoor air can expose humans to hazardous biological and chemical agents. The quality of indoor air is therefore a prominent public health concern that requires a clear understanding of the transmission processes for the development and implementation of targeted infection prevention and control measures. World-wide outbreaks of coronavirus-caused COVID-19 and severe acute respiratory syndrome (SARS), H5N1 bird flu, and H1N1 novel influenza have caused a substantial health impact to the population and have increased public concerns for the spread of viral disease. The global pandemic caused by the novel coronavirus SARS-CoV-2, which causes the disease known as COVID-19, has changed the world in ways no one could have imagined. There is much more to learn about this emerging global threat, however, there are some aspects of the virus that are known. The main route of transmission of the virus is thought to be through respiratory droplets expelled when sneezing, coughing, or even talking. Therefore, there is a strong desire to mitigate risk to the general population. With the goal in mind of evaluating coronavirus filtration efficiency if the transmission mode becomes aerosolized and into an HVAC system, AAF's Biological Research Department launched a study utilizing a safe surrogate for the SARS-CoV-2 virus in order to evaluate the virus removal efficiency of several filters ranging in efficiency ratings of MERV 14-16. Air samples containing surrogate virus were collected upstream and downstream from the filters using aerosol test equipment such as Anderson Cascade Impactors and optical particle counters to be able to separate particles by size (approximately 0.3 to 10 microns). Then the samples were tested by quantitative reverse transcription polymerase chain reaction (RT-PCR) and a fluorometer to estimate mass. For each particle size, the particle size removal efficiency was calculated. The results showed that under the conditions of the study, filter efficiency for SARS-CoV-2 surrogate virus was comparable to filter efficiency using KCl particles (ASHRAE 52.2 standards). In addition, the efficiency of particle removal was similar across the methods used (optical particle counter, fluorometer or PCR).

5SI.6

Assessment of Personal Exposure to Airborne SARS-CoV-2 Using Wearable PDMS Passive Air Samplers.

DONG GAO, Darryl Angel, Kayley DeLay, Elizabeth Lin, Jordan Peccia, Krystal Godri Pollitt, *Yale University*

Exhaled respiratory droplets and aerosols can carry infectious viruses and have been recognized as an important mode of transmission for COVID-19. Virus-containing aerosols can remain suspended in the air over long distances and time. Airborne SARS-CoV-2 particles have previously been detected with active air samplers which typically draw air through a filter using a pump. Wearable passive samplers may be a more effective alternative to conventional active samplers in exposure and health effects studies, given their simplicity, low cost, and portability. In this study, we used a wearable low-cost sampling device for detecting personal SARS-CoV-2 exposure to inform individuals of their potential risk of COVID-19 infection. This device passively concentrated airborne constituents onto a polymeric membrane made of polydimethylsiloxane (PDMS) while being worn by an individual. The collection efficiency of virus-laden aerosol on PDMS was tested within a custom rotating drum using the Phi6 bacteriophage as a surrogate for SARS-CoV-2. To further demonstrate application of the PDMS sampler as a quantitative exposure assessment tool, the samplers were distributed in occupational groups that are potentially at high risk for infection, including healthcare workers and restaurant employees. The constituents were extracted from the PDMS after a 5-day continuous collection and analyzed for the presence of SARS-CoV-2 RNA by Droplet Digital polymerase chain reaction (ddPCR). The results indicated uptake of SARS-CoV-2 by PDMS personal samplers in hospital and restaurant settings, suggesting that the PDMS-based passive sampler may serve as a useful exposure assessment tool for airborne SARS-CoV-2 in a real-world high-risk setting.

5SI.7

Influence of Flow Rates on Pressure Drop and Penetration for Various Masks.

PETER CHEA, Buddhi Pushpawela, Ryan Ward, Richard Flagan, *California Institute of Technology*

Mask-wearing emerged as the primary safety measure to prevent spreading COVID-19. To assess the viability of different materials in filtering aerosols when inhaling, we tested multiple copies of different mask categories: including NIOSH-certified N95 respirators, KN95 masks, procedure masks, and cloth masks. The intact masks were exposed to polydisperse NaCl aerosol of 30-800 nm, and tightly sealed within a chamber to get the upstream and downstream particle counts and pressure measurements. The pressure drop was measured for seven flow rates between 5 and 85 LPM. For all masks, it increased linearly with flow rate with $r^2 > 0.98$. The KN95 and cloth masks had higher pressure drops than the other masks, causing reduced breathability. The penetration was calculated with counts from a differential mobility analyzer and condensation particle counter system for three flow rates: 5, 30, and 85 LPM. For all of the masks, the penetration increased with flow rate, while the most penetrating particle size (MPPS) generally decreased. However, N95 and KN95 electret masks did not exhibit a significant shift in MPPS when the flow rate increased from 5 to 85 LPM. Compared to electret masks, the shift in MPPS for procedure and cloth masks was significant. This behavior shows that, for increased flow rates, the effectiveness of diffusion and electrostatic attraction (mainly affecting small particles) decreases, while that of impaction (mainly affecting large particles) increases. The use of face masks at high flow rates increases the risk to the wearer, and reduces breathability. The reduction of breathability may cause the public to be hesitant to wear masks.

5SI.9

Variability of the Performance of Facemasks. BUDDHI PUSHPAWELA, Stavros Amanatidis, Yuanlong Huang, Richard Flagan, *California Institute of Technology*

COVID-19 is transmitted, at least in part, by airborne particles emitted by infected individuals. Wearing masks is one of the key actions that are required to prevent spreading COVID-19. To understand the variability in the performance, we evaluated the penetration of particles through the masks (a measure of risk), comfort (pressure drop), and the quality factor of 145 masks with multiple copies of 29 different types. The tests were performed at a flow rate of 30 L/min; mean values of the performance parameters were calculated for two different sizes; 120 nm and 300 nm. Of the masks tested, for 120 nm particles, the NIOSH-certified N95s respirators consistently had the lowest penetration 1.7±0.5%, while KN95 masks allowed 3.7±2.6% penetration. In contrast, penetration through pleated procedure masks was 14.7±16.9% due to one outlier - with that outlier removed, penetration decreased to 7.1±4.3%; cloth masks allowed 26.4±9.3% penetration. The corresponding pressure drops at 120 nm for N95s, KN95s, procedure, and cloth masks were 22±4 Pa, 37±14 Pa, 14±5 Pa, and 32±10 Pa. The quality factors for different masks ranged from 15±3 kPa^{-1} to 274±28 kPa^{-1}. Even within the different classes of masks, substantial variability was apparent, with coefficients of variation in penetration of 120 nm particles of 0.08-0.25 for N95s, 0.07-0.99 for KN95s, 0.11-0.42 for procedure masks, and 0.11-0.26 for cloth masks. The respective coefficient of variation of pressure drop was 0.03-0.12, 0.02-0.20, 0.05-0.15, and 0.01-0.20. Tests on multiple copies of different masks demonstrated consistent performance of N95s, but considerably greater variability within the other classes of masks tested, leading to uncertainty in the degree of protection that they would provide. Therefore, quantitative testing is needed along with verifiable labeling to ensure that masks meet specific standards and, thereby, to control the large influx of inferior and counterfeit masks into the market.

5SI.10

Racial Disparities in Fine Particulate Matter Exposure and COVID-19 Spread in the United States. PAYTON BEELER, Rajan K. Chakrabarty, *Washington University in St. Louis*

Minority populations across the United States (US) have been disproportionately affected by 2020 COVID-19 pandemic. However, the underlying reasons for the rapidity of disease spread in minority communities are not clear. Here, we investigate the relative impact of disparities in 28 confounding factors on the basic reproduction ratio (R0) of COVID-19 in twelve major metropolitan statistical areas (MSAs) in the US at the county-level. We infer county-level R0 using an established metapopulation epidemiological model corresponding to the period March 1–April 30, 2020 marked by a rapid surge in COVID-19 cases across the US states and implementation of strict lockdown measures. On average, we find that a 10% increase in long-term, ambient PM2.5 exposure (particulate matter with aerodynamic diameter 2.5 µm or less) is associated with a 7.6% increase in R0, an outsized effect in comparison to other factors. In addition, we find that the largest disparities in PM2.5 exposure and subsequently in R0 are concentrated among Hispanic-American communities, followed by Asian-American and African-American communities, respectively. These findings highlight the effects of longstanding geographic segregation of minority communities. Geographic segregation of minority communities has led to extremely large fluctuations in county-level racial and ethnic minority fractions, in turn leading to large disparities in PM2.5 exposure and COVID-19 spread. We conclude by providing each MSA with a roadmap for identifying which communities should be targeted for PM2.5 mitigation policy implementation.

5SI.11

Inactivation of Escherichia coli in Droplets at Different Ambient Relative Humidity: Effects of Phase Transition, Solute and Cell Concentrations. ZHANCONG LIANG, Wing Lam Chan, Xiaomeng Tian, Patrick Kwan Ho Lee, Chak K. Chan, *City University of Hong Kong, China*

Previous studies have indicated that ambient relative humidity (RH) plays an important role in the inactivation of bacteria and viruses in droplets. However, characteristics of the RH-dependent inactivation between bacteria and viruses have been reported to differ. Furthermore, how the droplet medium and cell concentration influence inactivation remains unclear. In this study, inactivation of the model bacterium Escherichia coli in droplets of Luria-Bertani (LB) broth and artificial saliva (AS) as a function of RH and initial cell concentration was investigated in a flow cell under a well-controlled environment. Phase transition of aqueous droplets of the two media was observed to occur at ~50% RH and their hygroscopicity at different RH were similar. At an initial cell concentration of 10^{10} CFU/mL, relative viability (RV) in AS droplets showed a V-shape dependence on RH with a minimum at 60%, while RV in LB droplets showed a gradual decrease with decreasing RH. As the initial cell concentration decreased from 10^{10} to 10^8 CFU/mL in LB droplets, RV prominently decreased, especially at moderate RH (~60%), and a V-shape RV trend with RH was observed. A drop in RV was also found in AS droplets at a lower initial cell concentration, to below the detection limit in some cases. By considering the bacteria-to-water volume ratio, a high cell concentration in droplets was found to reduce inactivation due to osmotic effect. We conclude that for freshly emitted saliva droplets containing a low concentration of bacteria, an ambient RH of ~60% renders the most effective inactivation.

6AC.1

Formation and Aging of Carboxylic Acids and Dimer Esters in α-Pinene and β-Pinene Secondary Organic Aerosol.

CHRISTOPHER KENSETH, Yuanlong Huang, Nicholas Hafeman, Nathan Dalleska, Brian Stoltz, John Seinfeld, *California Institute of Technology*

Multifunctional carboxylic acids and dimer esters have been identified using advanced mass spectrometric techniques as significant components of secondary organic aerosol (SOA) formed from oxidation of α-pinene and β-pinene. Due to a lack of authentic standards, however, structures of these SOA molecular products are inferred from accurate mass/fragmentation data and, therefore, mechanistic understanding of their formation and aging remains unconstrained. Here, informed by detailed structural analyses (MS and MS/MS, ^{13}C isotopic labeling, and H/D exchange), we synthesize the first authentic pinene-derived dimer ester and elucidate its formation mechanism from a series of targeted SOA formation experiments using chemical ionization mass spectrometry (CIMS) and liquid chromatography/electrospray ionization mass spectrometry (LC/ESI-MS) for analysis of gas- and particle-phase composition. Additionally, we investigate the aqueous-phase (photo)chemistry (kinetics, products, and mechanisms) of six recently synthesized, pinene-derived carboxylic acid and dimer ester homologues at cloudwater-relevant concentrations as a function of pH using LC/ESI-MS. These studies provide a missing link tying the atmospheric degradation of α-pinene and β-pinene to the observed formation of low-volatility compounds capable of driving particle formation and growth, as well as key insight into the dependence of aqueous-phase photochemical processing on molecular size/functionality and applicability of aqueous-phase structure-activity relationships (SARs).

6AC.2

Comparison of Common Vapor Pressure Estimation Methods through Modeling of Alkene OH/NOx Systems.

EMMALINE LONGNECKER, Julia Bakker-Arkema, Paul Ziemann, *CU Boulder*

Modeling of atmospheric reactions is an important tool in understanding the current and future impacts of human activity on the environment. Vapor pressure is a key parameter in modeling these reactions, as it largely determines the ability of a species to transition from the gas to particle phase. However, the vapor pressures of many atmospherically relevant molecules are still poorly constrained. In order to aid modeling efforts, several group contribution methods have been developed for estimating compound vapor pressures. The current study evaluates how four of these methods: SIMPOL, EVAPORATION, SPARC, and Nannoolal, impact the modeled predictions of secondary organic aerosol (SOA) yields for the reactions of C8-C14 1-alkenes and C9-C15 2-methyl-1-alkenes with OH radicals in the presence of NO_x. The models were created in the program KinSim and included detailed reaction mechanisms and branching ratios determined in several previous chamber studies by our research group, as well as gas-particle and gas-wall partitioning. SOA yields predicted using each of the four estimation methods were then compared to the measured values. The results of the models were variable, with the maximum discrepancies ranging from an underestimate of ~40% to an overestimate of ~30% compared to the experimentally determined mass yields. This variability exemplifies the impact of vapor pressure in modeling atmospheric reactions and indicates the need for further research in development of estimation methods.

6AC.3

Differences in Mass Yields and Composition of Secondary Organic Aerosols from Nitrate Radical Oxidation of Isoprene under Various Reaction Conditions.

TIANCHANG XU, Masayuki Takeuchi, Yuchen Wang, Nga Lee Ng, *Georgia Institute of Technology*

Isoprene is the most abundant biogenic volatile organic compounds in the atmosphere. The reaction of isoprene and nitrate radicals (NO_3) at nighttime is important because of the high reactivity of NO_3 with isoprene and the high yields of secondary organic aerosols (SOA). While SOA formation from isoprene and NO_3 reaction has been investigated in previous studies, different SOA yields and product distributions were reported and the underlying reasons have not been fully examined and understood. Here, we conduct laboratory chamber experiments with isoprene and NO_3 formed from N_2O_5 under various reaction conditions to examine their influences on SOA yields and composition. Experiments are conducted under different N_2O_5 to precursor ratios. Further, two different generation methods of N_2O_5 are employed: (1) pre-mixes NO_2 and O_3 in a flow tube before introduction into the chamber and (2) injects NO_2 and O_3 separately into the chamber. The chemical composition of gas- and particle-phase products is measured continuously using a High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS) and a Filter Inlet for Gases and AEROsols coupled to a High-Resolution Time-of-Flight Iodide Chemical Ionization Mass Spectrometer (FIGAERO-CIMS). We observe that SOA yields increase with increasing N_2O_5 to isoprene ratio. This is attributed to the formation of higher-generation products with lower volatility, since the reaction can proceed to a larger extent with higher oxidant exposure. The major higher-generation compounds detected in the particle phase include 2N-monomer $C_5H_{10}N_2O_8$, 3N-monomer $C_5H_9N_3O_{10}$, and 3N-dimers $C_{10}H_{17}N_3O_{12-13}$. We observe that the relative abundance of monomers and dimers changes with precursor to N_2O_5 ratios. Results from this study can offer a better understanding of isoprene nitrate and SOA formation in the atmosphere where the relative abundance of isoprene and oxidants vary.

6AC.4

Volatility Comparison of β-caryophyllene Autoxidation Products with C15 Dimers Using FIGAERO I-CIMS Thermal Desorption.

JENNA DEVIVO, Mingyi Wang, Lubna Dada, Neil Donahue, The CLOUD collaboration, *Carnegie Mellon University*

Trees emit a variety of volatile organic molecules that are important precursors to particle and secondary organic aerosol formation in the troposphere, especially in pristine conditions. Peroxy radicals (RO_2) formed from these emissions undergo autoxidation, increasing the number of oxygen atoms and decreasing volatility. RO_2 molecules can react with each other (dimerize) to decrease volatility. This pathway is important for biogenic molecules with fewer than the twenty carbon atoms typically needed for nucleation. The volatility basis set (VBS) categorizes different molecules into volatility bins based on the extent of oxidation (O:C ratio) and volatility (logC*). However, the VBS often relies on composition-volatility relations to infer volatility of a molecule based on its molecular formula. At the CLOUD chamber at CERN, we used an iodide chemical ionization mass spectrometer and a Filter Inlet for Gases and AEROsols (FIGAERO) for thermal desorption to directly measure the volatility of different biogenic precursors. We found that C15 monomers and dimers had similar volatilities for a given carbon number and O:C, falling in the Low and Extremely Low Volatility Organic Compound classes regardless of whether they were monomers or dimers. The dimers were measured in controlled experiments where RO_2 radicals of isoprene (C5) and α-pinene (C10) autoxidized and reacted together to form C15 species. The monomers were measured in conditions where only β-caryophyllene (C15) was present. These experimental volatilities agree with the work of Stolzenberg et al., 2018. This comparison suggests that a single composition-volatility relation applies to terpene and isoprene oxidation products, regardless of the carbon number of the precursor. This finding supports volatility analysis for mass spectrometry results where molecular structure is unknown. Additionally, the formation of low volatility products from biogenic molecules with less than ten carbons emphasizes the importance of relatively small gas phase molecules for nucleation.

6AC.5

Ambient Chlorine Chemistry in an Oil and Gas Production Region: Evidence from a FIGAERO-CIMS. CATHERINE MASOUD, Nirvan Bhattacharyya, Kristi McPherson, Leif Jahn, Pearl Abue, Kanan Patel, Daniel C. Blomdahl, Pawel K. Misztal, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Unconventional oil and gas development (UOGD) has increased dramatically in the United States. As chlorinated compounds are added to hydraulic fracturing water, UOGD may be a source of chlorine, contributing to atmospheric chemistry and the formation of secondary organic aerosol in these regions. In the spring of 2021, we deployed a suite of instrumentation to Karnes City, Texas, a rural area in the middle of the Eagle Ford Shale, to investigate the impact of UOGD on air quality. We measured airborne pollutants including halogenated and oxygenated species (Cl_2, $ClNO_2$, N_2O_5 and OVOCs) using a High-Resolution Time-of-Flight Chemical Ionization Mass Spectrometer operated in iodide mode (I- HR-ToF-CIMS) and equipped with a Filter Inlet for Gases and Aerosols (FIGAERO). Measurements show several episodes of substantially elevated Cl_2 and $ClNO_2$ levels, consistent with the presence of a local chlorine source. We also find evidence of organic chlorides in the gas and particle phases indicating the contribution of chlorine chemistry in formation of secondary pollutants in the area. We deployed an oxidative flow reactor which conducted Cl-initiated oxidative aging of ambient air and provides markers for Cl-initiated reactions in the ambient air.

The measurement campaign included other instrumentation such as a Vocus-PTR-ToF-MS (with a VIA inlet), aerosol chemical speciation monitor, scanning electrical mobility spectrometer, a photometric ozone monitor, a chemiluminescence NO_x monitor, and a CAPS NO_2 monitor. We utilize data from these instruments to supplement the FIGAERO-I-CIMS data and investigate chlorine chemistry and its role in secondary organic aerosol formation in this inland oil and gas production region.

6AC.6

Chemistry in Heated Cooking Oils and Effects on Gaseous and Particulate Emissions. Manpreet Takhar, Jenna Ditto, Eleanor Vaz, Jonathan Abbatt, ARTHUR W. H. CHAN, *University of Toronto*

Food cooking contributes a significant fraction of volatile organic compounds (VOCs) and particulate matter (PM) in urban atmospheres. Most of these emissions originate from heated oils and food ingredients. In this work, we study the decomposition mechanisms of triglycerides as a source of gas-phase aldehydes and particles emitted from food cooking. Experiments were conducted by heating cooking oils in a temperature-controlled aluminum block. Cooking oils with different triglyceride composition were studied, along with a commercially available homotriglyceride (triolein). VOCs emitted during the heating process were measured using online (PTR-MS) and offline (GC/MS) mass spectrometry. Particle number and volume concentrations were measured using SMPS, and particles were also collected on filters for offline GC/MS analysis with derivatization. Aldehydes are formed from radical-initiated autoxidation. Antioxidants, added by oil manufacturers to increase oil shelf life, were found to suppress aldehyde emissions from oils with larger degree of unsaturation (canola oil) and promote emissions from others (triolein, olive oil, sunflower oil). This effect can be explained using a kinetic model by the relative importance of radical propagation and termination by antioxidant compounds. On the other hand, PM consisted mostly of free fatty acids. The fraction of free fatty acids in cooking oil increased with each heating cycle, consistent with increasing PM emissions. The effect of water in promoting hydrolysis of triglycerides is also investigated. Our results highlight the importance of studying cooking oil chemistry as a basis for understanding food cooking emissions and developing effective strategies for mitigating exposure.

6AC.7

Brown Carbon Formation and Evolution from Aqueous-Phase Nitrate-Mediated Photooxidation of Phenolic Compounds. THEODORA NAH, Junwei Yang, Wing Chi Au, Haymann Law, Chun Hei Leung, Chun Ho Lam, *City University of Hong Kong*

Substantial concentrations of phenolic compounds are emitted during biomass burning. Some of these phenolic compounds are highly water soluble, and can dissolve into atmospheric aqueous phases where they can undergo reactions to form brown carbon (BrC). Inorganic nitrate is a ubiquitous component of atmospheric aerosols, clouds, and fog. Reactive oxygen species (ROS) and reactive nitrogen species (RNS) are produced during the photolysis of inorganic nitrate in atmospheric aqueous phases. We report results from our laboratory investigations of the aqueous-phase photooxidation of a series of phenolic compounds (guaiacol, catechol, 5-nitrocatechol, and 4-nitrocatechol) initiated by inorganic nitrate photolysis under different pH conditions. When illuminated with UV light in the presence of inorganic nitrate, these phenolic compounds reacted rapidly to form BrC. Reaction rates of non-nitrated phenolic compounds were substantially faster than those of nitrated phenolic compounds. The -NO_2 functional group on the aromatic ring of nitrated phenolic compounds likely had a deactivating effect on the ring's reactivity, which contributed to their lower reactivity. Dominant products produced during the initial stages of photooxidation were formed by the addition of -NO and/or -NO_2 groups to the phenolic compounds. These products likely strongly absorbed near-UV and/or visible light, which led to an observed increase in light absorption (i.e., photo-enhancement) in the near-UV and visible range. Greater photo-enhancement was observed during the nitrate-mediated photooxidation of non-nitrated phenolic compounds. For some of the studied phenolic compounds, the pH of the aqueous phase impacted the reactivity of the phenolic compound and the amount of BrC formed. These results highlight how aqueous-phase inorganic nitrate photolysis can drive BrC formation by facilitating the photooxidation of phenolic compounds.

6AC.8

Aqueous-phase Brown Carbon Formation from Limonene SOA: Effects of Drying Conditions and Gas-phase Precursors. NETHMI KASTHURIARACHCHI, Laura-Helena Rivellini, Alex Lee, *National University of Singapore*

Aqueous-phase processing of secondary organic aerosols (SOA) can produce light absorbing organic species, commonly referred to as brown carbon (BrC), via reactions with reduced nitrogen species. While many previous studies have investigated BrC forming reactions of SOA from limonene ozonolysis (limonene SOA) with reduced nitrogen species in bulk solutions, little is known about their formation behaviour in aerosol droplets. This work shows that BrC formation is substantially accelerated upon drying of limonene SOA and ammonium sulfate/glycine mixed droplets. Although water evaporation has been shown to continuously enhance the absorptivity in aqueous bulk solutions, the results show that the mass absorption efficiency (MAE, m^2/gC) of prominent absorbance peaks were highest at ~75% relative humidity (RH) and then decreased at lower RH conditions. Furthermore, absorbance at longer wavelengths (500-520nm), which are the strongest peaks in evaporated bulk solutions, were diminished in evaporated droplets. We hypothesise that rapid re-partitioning of semi-volatile BrC precursors in limonene SOA may occur upon drying, limiting the multi-step oligomerisation mechanism for producing BrC with longer wavelength absorption. Further investigation shows that generating limonene SOA in the presence of other anthropogenic or biogenic volatile organic compounds (VOC) can enhance BrC formation during subsequent drying of bulk SOA extracts mixed with ammonium suflate/glycine. These observations highlight the potential effects of anthropogenic-biogenic interactions on SOA compositions that can subsequently affect secondary BrC formation via aqueous-phase processing.

6AC.9

Effects of Ammonium Sulfate on the Photodegradation of Toluene-Derived Brown Carbon Secondary Organic Aerosol. ALEXANDRA KLODT, Rachel O'Brien, Sergey Nizkorodov, *University of California, Irvine*

Secondary organic aerosol (SOA) derived from aromatic precursors contributes to the pool of atmospheric brown carbon by absorbing solar radiation in the near-UV and visible region of the solar spectrum. Previous studies have observed changes in the absorption spectrum of brown carbon and some other atmospherically relevant compounds with the addition of ionic species. However, there is a lack of consensus on the effect of ionic strength on chromophoric compounds and aerosols. Some studies have shown increased photodegradation rates with increasing ionic strength, while others observed increased absorbance but reduced rates of photobleaching. In this work, toluene SOA produced by photooxidation in the presence of NOx was used to study the effect of ionic strength on photodegradation rates of brown carbon SOA. The SOA was dissolved in aqueous solution at pH 4 and pH 1 and aged with photolysis in the presence or absence of 1 M ammonium sulfate, and UV-Vis spectroscopy was used to monitor the changes in absorption over time in both conditions. In a parallel set of experiments, SOA was photolyzed directly on a filter, and the distribution of functional groups was tracked using FTIR spectroscopy. Electrospray ionization high-resolution mass spectrometry with liquid chromatography separation (LC-ESI-PDA-HRMS) was finally used to observe changes in SOA composition from photolysis in both sets of experiments, allowing analysis of changes in chromophore abundance between the conditions. Preliminary results in the aqueous phase show increased initial absorbance but decreased photobleaching with ammonium sulfate, while the filter experiments suggest that photolysis causes the loss of nitroaromatic compounds as SOA degrades. Results from this study will provide a more complete understanding of the processes influencing the aging of brown carbon aerosol in the atmosphere.

6AC.10

Effects of Different Environmental Conditions on Secondary Brown Carbon Formation from Nighttime Oxidation of Furan. KUNPENG CHEN, Nilofar Raeofy, Raphael Mayorga, Roya Bahreini, Haofei Zhang, Ying-Hsuan Lin, *University of California, Riverside*

Brown carbon (BrC) contributes to a large uncertainty of direct radiation effects of aerosols in the troposphere. Particularly, nighttime oxidation of heterocyclic volatile organic compounds (VOCs) (e.g., furan) may be a potentially important source of secondary BrC aerosols, but the chemical compositions and optical properties are not fully constrained. Here we performed chamber experiments to simulate nighttime oxidation of furan by nitrate radicals (NO3), which was generated from the reaction between nitrogen dioxide (NO2) and ozone (O3). In our study, we explored the effects of different environmental conditions, including low/high concentration ratio of NO2 and O3 (i.e. [NO2]/[O3] = 0.1 or 0.3), the presence of seed particles (ammonium sulfate) and low/high relative humidity (RH < 10% and 50-70%) on BrC formation. Our results showed that under low RH, both high [NO2]/[O3] and the presence of seeds could increase the SOA yield, but different value of [NO2]/[O3] did not affect the size distribution of particles. To explore the light absorption of BrC constituents, we performed ultraviolet-visible (UV-Vis) measurements at 290-700 nm for the aerosol samples extracted by acetonitrile. The calculated mass-normalized absorption coefficient (MAC) indicated that both high [NO2]/[O3] and the presence of seeds could increase the average MAC under low RH. However, analysis of functional groups by attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) suggested that BrC constituents corresponding to high and low [NO2]/[O3] are similar in the presence of seeds, but different in the absence of seeds. The results of high RH experiments, and a comprehensive analysis of molecular compositions and candidates of chromophores by online and offline characterizations (i.e., iodide-adduct FIGAERO-HR-TOFCIMS and UPLC-DAD-ESI-QTOFMS) will be discussed as well. This study demonstrated that environmental conditions may significantly alter the optical properties and chemical compositions of secondary BrC aerosols.

6AC.11

OH Formation during the Photolysis of Polycyclic Aromatic Hydrocarbons.

HEATHER RUNBERG, Brian Majestic, *University of Denver*

Polycyclic aromatic hydrocarbons (PAH) are a ubiquitous atmospheric pollutant, comprising up to 50% of combustion particles. They undergo rapid photo-oxidation to form oxidized PAH products (oxPAH), and eventually, humic-like substances (HULIS). The primary goal of this study was to elucidate the role of hydroxyl radical (OH) formation along the HULIS formation pathway in atmospherically relevant conditions. To do this, anthracene (ANT) and a selection of oxPAH (1-naphthol, 2-naphthol, 1,4-naphthaquinone, 1,4-anthraquinone, and 9,10-anthraquinone) were exposed to simulated sunlight for 16 hours and OH concentration was measured at various time points. OH formation from ANT after a 16-hour reaction was 8.5 ± 0.1 µM OH per mM of starting material. Of the selected oxPAH, 1,4-naphthaquinone (NAPQ) generated the most OH, at 10.0 ± 0.2 µM OH per mM of starting material, significantly more than was seen with ANT.

Additionally, OH formation was measured every five minutes for the first 30 minutes of a 16-hour reaction; incremental formation rates were calculated at each timepoint. NAPQ had an incremental rate at five minutes of 1.10 ± 0.01 µM min^{-1}. The rate steadily declined over the next 25 minutes, with an incremental rate at 30 minutes of 0.28 ± 0.1 µM min^{-1}. Conversely, the OH formation rate during the first 30 minutes of the ANT reaction showed an initial OH burst with a relatively high incremental rate at five minutes of 0.09 ± 0.01 µM min^{-1}, followed immediately by a significantly lower incremental rate of 0.03 ± 0.01 µM min^{-1} at 10 minutes. The incremental rate then steadily increased over the next 25 minutes, with a rate at 30 minutes of 0.12 ± 0.01 µM min^{-1}, suggesting that NAPQ is driving OH formation during the photo-oxidation of ANT.

6AC.12

Examining the Competition Between Oxidation and Deposition in the Fate of Reactive Organic Carbon.

GABRIEL ISAACMAN-VANWERTZ, Chenyang Bi, *Virginia Tech*

Most of the reactive organic carbon in the atmosphere is emitted in the form of a small number of molecules and compound classes, which undergo photochemical oxidation processes in the atmosphere to form the dynamic and complex mixture of tens of thousands of compounds. To tackle this analytical challenge, a wide range of measurement techniques and modeling frameworks have been developed that classify compounds by their physicochemical properties and/or their molecular formulas. By estimating physicochemical properties of modeled and measured atmospheric oxidation products, we examine the predicted timescales for critical atmospheric transformations, particularly deposition and oxidation. To understand the potential impact of deposition on broader atmospheric chemistry, we place real-world smog chamber data into a framework of competition between loss processes and implement a simple description of deposition into a 0-d box model of photochemical oxidation. We further quantify the extent to which the molecular structure of each compounds impacts the transformations and fates of organic compounds in the atmosphere. A substantial fraction of atmospheric organic compounds is found to have competitive timescales for oxidation and deposition, particularly in the case of semi-volatile oxygenated gases that are likely to form aerosol upon further oxidation. Reactive organic carbon in these transition regimes account for a major fraction of both atmospheric reactivity and potential for secondary aerosol formation, suggesting the need for improved constraints on removal processes to reduce uncertainty in modeled aerosol formation.

6HA.1

Aid Pulmonary Disease Diagnosis and Treatment with CFD Modeling and Deep Learning: a New Perspective and Pilot Study. Changjie Cai, YU FENG, *The University of Oklahoma Health Sciences Center*

According to the National Vital Statistic Report, chronic obstructive pulmonary disease (COPD) is the 4th leading cause of death in America, which causes severe breathing difficulty due to airway stiffening, loss of airway deformation capability, and airway blockage induced by inflammation. As the standard COPD treatment, inhalation of therapeutic nano-/micro- particles has illustrated a long-standing drug delivery barrier to achieving desired therapeutic outcomes, i.e., only approximately 25% of the drug particles can be delivered to the deeper lung with most of the particles depositing in the upper airway. To overcome such a barrier and increase the drug delivery efficiency from today's 25% to 90% to the deeper lung for the better therapeutic outcome and reduced side effects, it is imperative to detect the obstruction locations. To achieve better treatment outcomes, it is also beneficial to detect the obstruction sites at earlier stages with noninvasive method. To pave the way to a noninvasive and automatic diagnostic method based on clinically measured intrathoracic medical images, we proposed and test the feasibility of a new noninvasive diagnostic methodology using both computational fluid dynamics (CFD) and binary Convolutional Neural Networks (CNN), i.e., "the expiratory airflow pattern analysis," to identify the obstruction location in left or right lung deeper than generation 6 (G6) by automatic detection of the clinically measurable intrathoracic airflow velocity contour shifts using Hyperpolarized Magnetic Resonance Imaging (MRI). The virtual tracheobronchial (TB) tree employed in this study contains 44 small airway openings in total. To build the training data and test database, 1 of the 44 openings was blocked for each simulation, in order to mimic the least changes in obstruction conditions in human lung compared with the obstructions of multiple openings in left or right lung. We trained the YOLOv4, a state-of-the-art CNN mode to develop the prototype of the diagnosis algorithm, using 34 randomly selected images as the training inputs. The Mean Average Precision of the trained model for the other 10 images was 100% at a threshold (or probability of detection) of 0.5 with the Intersection over Union of 96.65%. However, in this study, only one subject-specific TB tree was employed in the CFD simulation, which neglects the inter-subject variability. Obstructions were assumed to only appears in either the left lung or the right lung in the training and test images, which did not contain the cases with obstructions in both lungs. To enhance the generalized predictability of the deep learning model in the near future, more subject-specific airway configurations will be reconstructed and employed in the CFD simulations to prepare the training and testing images with the effect of inter-subject variabilities.

6HA.2

Droplet Deposition Measurements in a Simplified Mouth-Throat Airway. HUIZHEN YANG, Xiaole Chen, Ting Ding, Jinan Zhang, *Nanjing Normal University*

Portable vibrating mesh nebulizer now becomes an alternative approach generating drug aerosols for the treatment of pulmonary diseases. Its compliance of children and infants is relatively better than injection and oral administration. Experiments carried out using a simplified mouth-throat (MT) airway model under different inhalation flow rate conditions explored the deposition fraction (DF) of droplets. The normal saline droplets were generated from a portable vibrating mesh nebulizer (Youwell HL100A). The experiment system consisted of the VMN, MT airway, a filtration unit, and a vacuum pump. After each droplet deposition test, the MT airway and the filter were washed with distilled water using ultrasonic cleaning. The washed-out solutions were prepared in volumetric flasks, and then the sodium chloride (NaCl) concentrations were measured. Therefore, the droplet DF could be determined. The droplet DFs were measured under different inhalation flow rates, i.e., 15, 22.5, 30, 45, and 60 L/min. The environment of the experiments was controlled at T=26.5°C, RH=50% and PM2.5 = 0 μg/m3. The results indicate that the DF of the droplet does not increase with the increase of the inhalation flow rate, which is different from the dry particle experiments in literature. The DF of the droplets decreases from 25.7% at 15 L/min to 7.3% at 22.5 L/min, and further declines to 6.8% at 30 L/min. Then the DF of the droplets gradually increases from 13.8% at 45 L/min to 14.5% at 60L/min. The high DFs of the droplets at the low inhalation flow rates, i.e., 15 L/min and 22.5 L/min, may relate to the droplet evaporation process in the airway.

6HA.3

Estimation of Ultrafine Particle Respiratory Deposition Using Mobile Aerosol Lung Deposition Apparatus (MALDA).

WEI-CHUNG SU, Jinho Lee, *University of Texas Health Science Center at Houston*

Exposure to ultrafine particles has been and continues to be an essential occupational and environmental health issue. However, due to the limitation of traditional experimental methods, it is very difficult to acquire ultrafine particle respiratory deposition data in human airways. This study employed a newly developed and upgraded experimental approach, Mobile Aerosol Lung Deposition Apparatus (MALDA), to estimate the respiratory deposition of ultrafine particles in main human airway regions. The unique MALDA consists of a set of realistic human airway replicas including a complete head airway (nasal and oral airways), tracheobronchial airways down to the 11th lung generation, and a representative alveolar section. The upgraded MALDA was first evaluated in the laboratory for performance and then deployed in an indoor real-life setting to estimate the ultrafine particle respiratory deposition associated with passive vaping. Experimental data acquired showed that the MALDA approach could provide efficient and systematic ultrafine particle respiratory deposition data in the human respiratory tract. The experimental data aligned closely with conventional respiratory deposition curves. Results obtained from this study demonstrated a great promise on the future application of MALDA in occupational and environmental health related exposure assessments for acquiring on-site ultrafine particle respiratory deposition data.

6HA.4

Effects of Device Type, Liquid Composition, and Emission Level on Characteristics of Aerosol Generated from Tank-Style E-cigarettes and JUUL Pods.

YUENING GUO, Liqiao Li, Yi Luo, Yifang Zhu, *University of California, Los Angeles*

E-cigarettes are increasingly popular among adolescents in recent years. Tank devices and JUUL pods are the newest and most widely-used e-cigarette devices. However, there are substantial differences between their device structures and e-liquid compositions. The characteristics of aerosols generated from these two devices warrant better understanding and cross-comparisons for future human exposure studies and policy making. This work compared the relative effect of device type (Vapor-fi Volt II tank device vs. JUUL pods), type of nicotine used in e-liquids (freebase nicotine vs. nicotine benzoate salt), and emission level (i.e., one and three 4-second puffs) on the characteristics of mainstream e-cigarette aerosols. The e-cigarette aerosol was introduced into a 460-L mixing chamber and then measured for particle number concentration (PNC), $PM_{2.5}$ mass concentration, size distribution, and evaporative properties (i.e., particle lifetime and volatility). The results suggested similar PNC level between tank and JUUL devices. Nevertheless, JUUL generated more than twice of ultrafine particles ($d_a < 0.1$ µm) than tank devices. $PM_{2.5}$ in tank aerosols were more than two times higher than JUUL aerosols. Bimodal size distribution was observed in all samples, with the first mode at 0.06-0.09 µm, and second mode at 0.27-0.31 µm. The change of nicotine type shifted the first mode of size distribution. Device type was a significant indicator for $PM_{2.5}$ ($p < 0.05$) but not for PNC. Nicotine type was only a significant indicator for PNC in 1-puff samples, and it had almost no effect on $PM_{2.5}$. Aerosols generated from tank devices were significantly less volatile than JUUL ($p < 0.05$), while volatility for the two nicotine types has no significant difference. Switching device brought more dramatic effects to aerosol characteristics than switching nicotine source in e-liquids. Future studies on e-cigarette exposures are suggested to treat tank devices and JUUL pods as two distinct emission sources.

6HA.5

Filter Sample Analysis of Metal Contents Generated from Electronic Cigarettes and Potential Secondhand Smoke Emission. KAPIAMBA KASHALA FABRICE, Weixing Hao, Stephen Adom, Wenyan Liu, Huang Yue-Wern, Yang Wang, *Missouri University of Science and Technology*

Electronic cigarettes (ECs) vaping has been on the rise since their introduction two decades ago. EC vapor (nicotine containing aerosols) is generated by vaporizing a liquid that contain, depending on the brand, propylene glycerol, nicotine and flavoring agents. Initially designed to transition tobacco cigarettes' quitters, vaping was believed to have the benefit of eliminating secondhand aerosols and was safer for smokers. However, chemical characterization of aerosols generated by EC devices have revealed higher concentrations of metal nanoparticles that may lead to health complications. Moreover, though EC do not release smoke like tobacco cigarettes, people can still be exposed to secondhand aerosols, exhaled by smokers, that may contain metal species. To date, health effects of being exposed to secondhand e-cigarette aerosol is not well elucidated.

In this study, we characterized the metal content and size distribution of primary and secondhand aerosols generated by two brands of ECs (VOOPOO and blu). We collected the primary aerosols using a standardized puff profile and analyzed the metal contents on the filter samples using the inductively coupled plasma mass spectrometry (ICP-MS). Results show that the mass of Cr, Ni, and Zn are 10.0, 19.5, and 26.1 ng per puff for VOOPOO EC, and 4.4, 1.3, and 1.0 ng per puff for blu EC, respectively. Secondhand aerosols were obtained by passing primary aerosols through a simulated respiratory system, which is composed of a series of filters that mimic lung deposition efficiency. In addition, we assessed metal contents as a function of cycles and found that metal emissions increase with EC ageing. Our findings provide more detailed understanding on the emission characteristics for assessing health effects of EC usage.

6HA.6

The Spatial Distribution of Particles from Little Cigar Smoke Deposited in Rat Lungs. KAISEN LIN, Christopher Wallis, Emily Wong, Patricia Edwards, Laura Van Winkle, Bahman Asgharian, Anthony S. Wexler, *University of California, Davis*

Quantifying the dose of tobacco smoke and the location of this dose in the lung system is important in understanding its toxicity, addiction, and health effects. Several studies have reported contradictory results, i.e. heterogeneous vs. homogenous lobar deposition of inhaled particles, in animal models. However, not many studies have investigated the pulmonary spatial distribution of inhaled particles from tobacco smoke. Even fewer explored the particle size distribution of smoke from little cigars, the total amount of dose, and the lobar deposition of particles. Given the increasing popularity of little cigars, especially in young populations, there is an urgent need to conduct research and collect data on this topic. In our study, we explored the local deposition of particles from combusted Swisher Sweets regular and menthol-flavored little cigar in rat lungs. We exposed 12-week male and female Sprague-Dawley to particles at a mass concentration of 100 mg/m3 for 1 hour. Rats were sacrificed immediately after the exposure and lungs were separated to collect lobe samples. The levels of trace metals, which serve as markers for particle deposition, were quantified with ICP-MS in a lobe-to-lobe resolution. The lobar distribution of deposited particles was determined by comparing the wet mass normalized trace metal concentrations across lobes. To determine the hotspots of deposited particles within each lobe, we will utilize CytoViva hyperspectral microscopy to collect high-resolution data and map particle deposition. The results from this study will also be used to validate and improve the MPPD model, and predict the smoke dose in human lungs.

6HA.7

The Fate of an Inhaled Puff Generated by an Electronic Nicotine Delivery System in The Human Oral and Lung Airways.

AKINA MORI, Owen Price, Shigeaki Ito, Takuya Suzuki, Hitoshi Fujimoto, Hiroaki Suzuki, Bahman Asgharian, *Japan Tobacco Inc.*

The fate of an inhaled puff generated by an electronic nicotine delivery system (ENDS) in the respiratory tract is crucial information in the assessment of its health impact. The puff of ENDS is a mixture of volatile multi-constituent aerosol and vapor constituents. The aerosols undergo continuous phase change. The phase change is expedited by temperature change, vapor uptake, aerosol deposition, and coagulation. Existing ENDS and combustible cigarette models have made strides in filling the gaps between measurements and predictions. To further enhance the dosimetry model for a puff of ENDS, we developed a new generation of dosimetry model that in addition to all previous mechanisms, accounted for the mixing of the puff with the dilution air after the mouth-hold and convective mixing of the puff with the reserved air in the deep lung. In addition, air-tissue interactions were included for medium vapor pressure constituents of the puff such as nicotine and propylene glycol. Model predictions revealed that mixing did not seem to affect uptake but resulted in increased airborne concentration of vapor and aerosols in the lung airways at the end of the puff exhalation. Thus, it increases the opportunity for the mixture to be taken up during the next puffing cycle. In addition, tissue concentrations of nicotine were similar among different generations of the lungs, and the predicted uptake of nicotine throughout the lung, particularly in the deep lung, is significantly higher than the prediction by existing models. We consider that the model enhancement improved matching of predictions with actual, but its confirmation is remained for the future studies. The model developed in this study provides a scientific tool for risk assessment of an inhaled ENDS puff.

6HA.8

A Comparative In Vitro and In Vivo Toxicity Assessment of E-cigarette Aerosols Generated from Sub-ohm Tank and Juul.

TIANCONG MA, Liqiao Li, Tian Xia, Yifang Zhu, *University of California, Los Angeles*

Electronic cigarette (e-cig) is a battery-powered nicotine delivery device that has been widely marketed as an alternative to traditional tobacco cigarettes. However, considering the outbreak of the e-cig, or vaping product use-associated lung injury (EVALI), various attractive flavors, and the constantly evolving e-cig devices, it is necessary to find out the links between e-cig devices, e-liquid components and their potential toxicity. In this study, we prepared e-cig aerosol samples by changing the number of puffs, e-liquid composition, and type of e-cig devices (sub-ohm tank and Juul), and collected samples through an impinger system for biological assays. We tested their effects on THP-1 macrophages, BEAS-2B bronchial epithelial cells, and NF-κB-luc transgenic mice. We found that e-cig samples are cytotoxic to THP-1 cells and BEAS-2B *in vitro*, leading to the production of inflammatory cytokines and cell death. Importantly, the aerosol produced by Juul (3.7 V) is more toxic *in vitro* than sub-ohm tank (7.5 V). For both sub-ohm tank or Juul, higher voltage increased aerosol toxicity. After exposing the e-cig aerosol samples to NF-κB-luc mice by oropharyngeal aspiration, the expression of NF-κB was observed by *ex vivo* imaging, suggesting activation of pro-inflammatory pathways. In addition, e-cig samples induced neutrophil infiltration and IL-1β production in the lung. These results indicate that differences between devices affect pro-inflammatory NF-κB pathway activation and cell death, which are related to e-cig-induced acute lung inflammation. More studies are needed to reveal the potential mechanism of toxicity induced by different devices.

6HA.9

Component Specific Evaporation of Filter Collected E-Cigarette Particulate Matter under Wet and Dry Conditions.

KAITLYN SUSKI, Brad Ingebrethsen, Nagaraja Rao, Huan Wang, *JUUL Labs*

Once e-cigarette aerosol exits the generation device, the aerosol undergoes dynamic changes. The particles, which are typically composed of vegetable glycerin (VG), propylene glycol (PG), nicotine, flavor components, and water, can take up or lose water and volatile components in response to changes in the aerosol dilution state, temperature, and relative humidity. Many online aerosol measurement techniques require dilution or the use of aerodynamic lenses under vacuum, which result in evaporation of volatile and semi-volatile components. The chemical composition and size of the particles can be affected by these measurement artifacts, making the study of e-cigarette aerosol challenging. To minimize instrumentation artifacts, e-cigarette aerosol was collected on filters and analyzed using offline gas and liquid chromatography techniques. To simulate component evaporation during aging, the collected material was flushed with air for different lengths of time (up to 1 hour). Flushing was done at 40 °C with wet (RH ≈ 99%) and dry (RH < 5%) air to simulate particle water equilibration and investigate the effect of water on the evaporation kinetics.

This work shows that under dry conditions, PG is almost completely evaporated from the deposited material over the course of the experiment, while VG is mostly retained. Under wet conditions the deposited material takes up water rapidly, which results in an initial spike in evaporation of PG and nicotine (higher than the dry case). Once water uptake slows, PG and nicotine evaporation are reduced compared to the dry case due to dilution of the deposited mass with water. This experimental approach meaningfully simulates the many changes that can occur to e-cigarette aerosol particles during aging and dilution for 2 limiting cases (RH≈ 99% and RH < 5%).

6HA.10

Temperature Dependence of Emission Product Distribution from Vaping of Vitamin E Acetate.

ALEXA CANCHOLA, Kunpeng Chen, Megan Woods, C.M. Sabbir Ahmed, Jin Y. Chen, Ying-Hsuan Lin, *University of California, Riverside*

The recent wave of e-cigarette or vaping-associated lung injuries (EVALI) demonstrated the potential dangers of inhalation of toxic substances from vaping. Vitamin E acetate (VEA) oil, an illicit diluent of tetrahydrocannabinol (THC) in vape cartridges, is believed to be the main culprit in the myriad of EVALI cases seen. Recent studies have found that thermal degradation of VEA during vaping can result in the formation of toxic products such as ketene and duroquinone (DQ). In addition, the wide range of vaping behaviors – including the e-cigarette model used, puff duration, puff interval, etc. – have been demonstrated to affect the size and volume distribution of aerosols emitted from VEA vaping. However, the impact of applied power and resulting heating coil temperature on the chemical composition of emitted aerosols has not been fully assessed. We hypothesize that elevated temperature of the coil during vaping could enhance thermal degradation of VEA, causing a shift in emission product distribution and toxicity in vapers. To assess the temperature-dependence of VEA emission products, we generated vaping aerosols at voltages ranging between 3.3 to 4.8 V (140 to 280 °C), measured the coil temperatures, and analyzed the size-segregated emission product distribution using a microorifice uniform deposit impactor (MOUDI) and gas chromatography/mass spectrometry (GC/MS). We found that increases in coil temperature are positively correlated with increases in VEA transformation. As temperature increases, production of intermediate products like DQ decreases (-0.067 ± 0.012 (µg-DQ-produced mg-VEA-consumed^{-1}) V^{-1}), while production of lower molecular weight alkenes and oxygen-containing compounds (carbonyls and alcohols) increases. The results from this study highlight the dynamic nature of vaping emissions and will help to inform the public regarding the risk of exposure to toxic vaping emission products and potential vaping-related health concerns.

6HA.11

Iron-facilitated Organic Radical Formation from Secondary Organic Aerosols in Surrogate Lung Fluid.

JINLAI WEI, Ting Fang, Pascale Lakey, Manabu Shiraiwa, *University of California, Irvine*

Respiratory deposition of secondary organic aerosols (SOA) and iron may lead to the generation of reactive oxygen species and free radicals in lung fluid to cause oxidative stress, but their underlying mechanism and formation kinetics are not well understood. Here we demonstrate substantial formation of organic radicals in surrogate lung fluid (SLF) by mixtures of Fe^{2+} and SOA generated from photooxidation of isoprene, α-terpineol and toluene. The molar yields of organic radicals by SOA are measured to be 0.03 – 0.5% in SLF, which are 5 – 10 times higher than in water. We observe that Fe^{2+} enhances organic radical yields dramatically by a factor of 20 – 80, which can be attributed to Fe^{2+}-facilitated decomposition of organic peroxides, in consistency with a positive correlation between peroxide contents and organic radical yields. Ascorbate mediates redox cycling of iron ions to sustain organic peroxide decomposition, as supported by kinetic modeling reproducing time- and concentration-dependence of organic radical formation as well as additional experiments observing the formation of Fe^{2+} and ascorbate radicals in mixtures of ascorbate and Fe^{3+}. ·OH and superoxide are found to be scavenged by antioxidants efficiently. These findings have implications on the role of organic radicals in oxidative damage and lipid peroxidation.

6IM.1

Evaluation of a New Low-Cost Particle Sensor as an IoT Device for Indoor and Outdoor Particulate Matter Monitoring.

ABI ROBERTS, Kathryn Van Valkinburgh, Christopher Post, John Pearce, Elena Mikhailova, Andrew Metcalf, *Clemson University*

Low-cost particle sensors provide an opportunity to increase the spatial and temporal density of outdoor air quality measurements when integrated with an internet of things (IoT) system that is able to report sensor data in near real-time. Many low-cost particle sensors are currently available, but there are serious concerns about data accuracy and precision, sensor reliability, and suitability for outdoor deployment. We evaluate a newly available, low-cost particle sensor from Sensirion AG, which reports having high accuracy with other desirable capabilities, including low power consumption, for the ability for long-term sensor deployment, and measurement of particulate matter (PM) size speciation with number concentration, for less than $50/sensor.

This talk will discuss the testing of this new PM sensor in both a laboratory and ambient setting, efforts to develop an IoT system for both indoor and outdoor deployments, and the evaluation of this sensor to collect measurements of indoor and outdoor PM levels. In all tests, the new sensor was compared to measurements from a DustTrak-DRX Model 8533, and in some tests, to a condensation particle counter, scanning electrical mobility particle sizer, and Federal Reference and Equivalence Methods for PM measurements. Laboratory calibration used particles of known size (PM_1, $PM_{2.5}$, etc.) at various number concentrations (spanning 10^2 to $10^4 cm^{-3}$). Outdoor testing demonstrates performance over a range of airborne PM levels in a relatively humid, rural environment. Time-series plots reveal general agreement in short-term PM variability; however, consistent differences in absolute values reveal that offsets may be required. Time-series analysis techniques are compared to identify similarities between tested sensor output, while spatial interpolation of averaged and event-specific data is used to build maps of PM levels.

6IM.2

Understanding the Sources of Urban Air Quality Using Low-Cost Air Quality Sensors.

LAURA YANG, David Hagan, Jean Rivera-Rios, Zahra Shivji, Eben Cross, Chris Peng, Jennifer Kaiser, Nga Lee Ng, *Georgia Institute of Technology*

Advances in low-cost sensor (LCS) technologies for measuring air quality have provided the public with readily accessible information on their exposure to detrimental air pollutants. Previously, LCS were primarily used to measure air pollution levels, but more recent literature suggests that source apportionment analysis of pollutants is possible. The primary objective of this study is to investigate the sources of urban air pollutants using LCS. The second objective is to determine the capabilities of the different sensors in measuring particulate matter (PM) in an urban area. From November to December 2020, we deployed QuantAQ LCS that measure both gases (CO, NO, NO_2, and O_3) and PM along with Purple Air LCS and various research-grade instruments (Aerosol Chemical Speciation Monitor (ACSM), Scanning Mobility Particle Sizer (SMPS), O_3 and NO_x monitors) in Atlanta, GA. The unsupervised algorithm non-negative matrix factorization (NMF) was then employed to resolve factors that describe the Atlanta air quality. We compare the capability of optical particle sensors and nephelometers and the performance of QuantAQ LCS and Purple Air LCS in measuring PM. We identified three factors (CO-dominated, O_3-dominated, and particle factor) with different temporal trends and properties. The CO-dominated factor correlates well with combustion-related organic aerosol (OA) factors (hydrocarbon-like, biomass burning, and cooking OA) resolved from positive matrix factorization (PMF) analysis of ACSM data. Moreover, the particle factor correlates with inorganics measured from the ACSM. Results from this study exhibit that LCS not only can be used to provide basic mass concentration information but also can be used for in-depth source apportionment studies even in an urban setting with complex pollution mixtures and relatively low aerosol loadings.

6IM.3

Long-term Evaluation of Low-Cost Air Sensors to Measure Indoor and Outdoor Particulate Matter in a Polluted Environment: Strengths and Limitations.

JAEBIN JU, Linh Luu, Danielle Rocco, Esther Morales, Daniel B. Curtis, *California State University, Fullerton*

There has been a recent increase in interest in the field of low-cost air sensors, particularly PurpleAir sensors, due to their low cost, ease of use, ability to share the data online in real time, high time and spatial resolution, and ability to be deployed over wide geographical areas. These advantages have led to wide adoption of the sensors, with over 10,000 PurpleAir sensors deployed in the United States, especially in certain areas, such as California. Many studies have been conducted to test the accuracy and reliability of the sensors in controlled environments and there are increasing number of field studies being conducted. Although several studies have shown that the raw accuracy of low-cost sensors is questionable, the high precision of the sensors may allow for intercomparison studies between sensors. However, there have been only few studies studying performance of the sensors indoors and outdoors at the same location.

This study evaluated the long-term reliability of deploying PurpleAir sensors to compare the indoor and outdoor air quality at California State University, Fullerton, located in a suburban area within the Los Angeles metropolitan area in Southern California. Two PurpleAir sensors were collocated, one indoors and one outdoors, for a two-year period ranging from January 1, 2019 to December 31, 2020, including several very high particle concentration events such as fireworks from the July 4 holidays and several wildfire plumes in the area. A correlation between the outdoor and indoor concentrations was observed, but at roughly half the concentration indoors. In addition, short-term pollution events, suspected to be fireworks from a nearby theme park, were observed. It is shown that after time-averaging the measurement to one-hour periods that the short-term events were not observed, indicating that the high time-resolution of the PurpleAir sensors may allow for better understanding of transient pollution events than reference monitors.

6IM.4

Laboratory Calibration of a Low-cost Particulate Matter Sensor Using Standardized Aerosols. CHING-HSUAN HUANG, Jiayang He, Elena Austin, Edmund Seto, Igor Novosselov, *University of Washington*

Particle deposition in human respiratory tract and the resultant adverse health effects depend on particles' size distribution, making direct measurement of time- and size-resolved particulate matter (PM) concentrations essential to health-related research. Some commercially available low-cost PM sensors provide output as total or size-specific particle counts and mass concentrations. These quantities are not measured directly but are estimated by the original equipment manufacturers' (OEM) proprietary algorithms and have inherent limitations because particle scattering depends on the particles' composition, size, shape, and complex index of refraction (CRI). Furthermore, environmental conditions such as relative humidity can also affect particle light scattering measurements. Hence, there is a need to characterize and calibrate their performance under a controlled environment and standardized test aerosols. Here, we developed calibration algorithms for a low-cost PM sensor as a function of particle size and mass concentration. A standardized laboratory experimental protocol was developed to control the PM concentration, environmental conditions, and sensor-to-sensor reproducibility. The calibration was based on tests when sensors were exposed to different polydisperse standardized testing aerosols. The results suggested linear model without adjusting aerosol properties, including CRI, density, and relative humidity was able to correct the raw, uncalibrated low-cost PM sensor number concentration measurements with normalized mean absolute error within 4.0% compared with the reference instrument. The calibration algorithms developed were most accurate for correcting PM < 2.5 µm (error < 2.9%). Linear models additionally adjusting for particle CRI and density demonstrated slightly lower error for calibration and may be used in scenarios such as industrial environments where specific known aerosols occur, but may be less useful for ambient environmental conditions where the aerosol composition is varied.

6IM.5

Performance of a Hybrid Lower-Cost PM Monitor in West Africa. JULIEN BAHINO, Michael R. Giordano, Eben Cross, James Nimo, Allison Hughes, Emmanuel Appoh, Christian Sewor, Kofi Amegah, Daniel Westervelt, Isaiah Tuolienuo, Melanie A Jackson, Stefani Penn, Rob Pinder, Arsene Ochou, Veronique Yoboue, Matthias Beekmann, R. Subramanian, *OSU-EFLUVE, LISA/CNRS, UPEC, ENPC, UP*

Particulate matter (PM) low-cost sensors (LCS) are widely used to monitor air quality in regions where no reference monitors are available. Nephelometric LCS devices like the Plantower (used in PurpleAir devices) are insensitive to size distribution, as shown in multiple published laboratory studies. In areas where either resuspended or desert dust are significant contributors to ambient aerosol, nephelometric LCS devices can misattribute $PM_{2.5-10}$ to $PM_{2.5}$. Lower-cost optical particle sizers like the Alphasense OPC-N3 claim to measure and size particles up to 40 µm in diameter, making them candidates for lower-cost sensing of dust. But they do not report aerosol sizes below 350 nm. At the same time, published laboratory studies have shown that nephelometric LCS devices respond to 100-200 nm particles, even if the manufacturer's stated detection limit is higher. Hence, a new alternative is the combined use of nephelometric LCS and OPCs, as in the Quant-AQ Modulair PM sensor.

In April 2021, we deployed five Modulair PM units in Ghana and Côte d'Ivoire. In Accra, Ghana, two sensors are collocated with the Ghana EPA's Teledyne T640 monitor ($PM_{2.5}$ and PM_{10}) located at the University of Ghana, and one with the US embassy BAM ($PM_{2.5}$). In Côte d'Ivoire, the Modulair units are collocated with a BAM-1022 ($PM_{2.5}$) at the Université Félix Houphouët-Boigny, Abidjan, and with a TEOM (PM_{10}) at Lamto, a remote location. Preliminary results from Accra indicate decent performance for $PM_{2.5}$ using just the as-reported data, while the sensor performance for PM_{10} is weaker and needs to be corrected. We shall present results on the performance of the sensors across West Africa, corrections for the sensors, and the ability of this new lower-cost device to distinguish between $PM_{2.5}$ and PM_{10} in equatorial and dust-influenced climates.

6IM.6

Particle Measurement on Mobile Platforms: Considerations in Using Reference-Grade Monitors, Low-Cost Particle Sensors, and Particle Trajectory Modeling. WILTON MUI, Berj Der Boghossian, Ashley Collier-Oxandale, Steven Boddeker, Jason Low, Vasileios Papapostolou, Andrea Polidori, *South Coast Air Quality Management District*

Mobile air monitoring is gaining popularity as a technique for collecting ambient air pollution data at high spatiotemporal resolution, with potential savings in capital and labor through the reduction of the number of air monitoring instruments, compared to stationary air monitor deployment. Even more substantial cost reductions can be realized if low-cost particulate matter (PM) sensors are employed instead. However, obtaining a representative air sample can prove challenging in a non-stationary deployment scenario; the use of low-cost PM sensors can introduce additional challenges since the data quality can be further degraded in a mobile deployment. The Air Quality Sensor Performance Evaluation Center (AQ-SPEC) at the South Coast Air Quality Management District is advancing the field of knowledge surrounding the use of reference-grade monitors and low-cost PM sensors on mobile platforms. Through successive iterations of monitoring vehicles, AQ-SPEC has practical experience to share regarding various aspects of design, planning, and development of mobile platforms. In addition, AQ-SPEC has published the first-ever mobile testing protocol for low-cost sensors, which tests the performance of sensors in three broad deployment scenarios: 1) within a controlled-flow sampling duct, 2) within a partially-controlled rooftop enclosure, and 3) completely exposed on the vehicle rooftop. Through pilot-testing this protocol with a PM sensor (PurpleAir PA-II), performance issues were revealed that would otherwise not be revealed from stationary testing. Finally, AQ-SPEC is utilizing advanced methods to improve particle sampling on its newest-generation mobile platform, such as computational fluid dynamics and particle trajectory simulations using free and open-source tools to allow for maximum accessibility.

6IM.7

Cloud Condensation Nuclei (CCN) Activity Analysis of Low-Hygroscopicity Aerosols Using the Aerodynamic Aerosol Classifier (AAC). KANISHK GOHIL, Akua Asa-Awuku, *University of Maryland*

In this research, we present a method for Cloud Condensation Nuclei (CCN) activity analysis of aerosols using an Aerodynamic Aerosol Classifier (AAC). The AAC is a novel instrument that size-selects/classifies aerosols based on their mechanical mobility. This is done by measuring the relaxation time of particles within the AAC to determine their aerodynamic diameter. Past studies have developed theoretical models for characterizing AAC-based particle classification. Furthermore, AAC has been used for numerous applications including calibration of Optical Particle Counter (OPC), determination of particle mass, effective density and shape factor, and separation of particles. However, the utility of AAC for CCN activity analysis of aerosols has not yet been explored. Traditionally, a Differential Mobility Analyzer (DMA), which classifies aerosols based on electrical mobility, is used to obtain size-resolved measurements in CCN experiments. The classification requires aerosol particles to acquire a unit charge before being subjected to an electrostatic field while they move along the DMA column. Despite the utility of a DMA-based setup, there are issues related to particle multiple charging artifacts that introduce uncertainties in measurements and CCN activity predictions. Substituting the DMA with an AAC can help minimize these uncertainties as classification using an AAC does not require particle charging. This can potentially improve aerosol size-selection and CCN activity predictions, particularly of low-hygroscopicity species. Previously, the AAC transfer function has been used for expressing the AAC resolution and uncertainties associated with particle relaxation times. Here, we extend a similar transfer function analysis to examine the variability in AAC resolution in terms of aerosol aerodynamic diameter to facilitate quantification of size-dependent uncertainties corresponding to aerosol aerodynamic diameter. This is shown to be effective for reducing disparities in size-resolved measurements, therefore increasing the accuracy in predicting CCN activity of low-hygroscopicity aerosols.

6IM.8

Validation of Integrating Cavity Absorption Spectroscopy for Cloud and Aerosol Mass Concentration Measurement. MONIKA GRAFL, Benjamin Lang, Alexander Bergmann, *Graz University of Technology*

Instruments expanding the capabilities to characterize cloud properties, such as cloud mass fractions of liquid water droplets (liquid water content, LWC) and ice crystals (ice water content, IWC), are of continued interest to the research of cloud radiative properties, the prediction of cloud and precipitation formation, as well as the research of aerosol-cloud interactions. Further applications of such instruments include certification aspects in aviation, where the representative experimental simulation of clouds for the certification of aircraft for flight in icing conditions is still a work in progress.

As total condensed cloud water content measurement is routinely performed using evaporative probes, a tempting approach to solve the challenge of separating liquid and ice fractions of water is to directly determine the relative fractions of both condensed states via the different absorption spectra.

By using a flow-through integrating cavity with nearly Lambertian (diffuse) and highly reflective inner walls, as commonly used in integrating nephelometers for aerosol light scattering measurement, a homogeneous, isotropic light field is generated inside the cavity, ideally eliminating the influence of scattering effects on the absorption measurement of optically thin clouds and aerosols.

To ensure absorption proportional to the mass fractions for large water droplets and ice crystals with diameters above 1 mm, near-infrared radiation is preferable for such measurements.

We present a broadband near-infrared integrating cavity absorption spectroscopy setup for mass concentration measurement of ice crystals and liquid water droplets. The working principle is demonstrated by the analysis of the absorption spectrum measured for a stream of water droplets with defined sizes in the 100 µm range and constant mass fractions, generated by a customized, piezoelectric actuated droplet generator.

6IM.9

A Miniaturized, Lower Cost, Cloud Condensation Nuclei Counter. ALEKSANDRA VOLKOVA, J. Alex Huffman, Donald R. Huffman, Ezra Levin, Gavin McMeeking, Matt Freer, Ben Swanson, Anna Hodshire, *University of Denver*

The impacts of aerosols on cloud properties remains a major obstacle to better understanding Earth’s changing energy budget. Cloud condensation nuclei (CCN) have a potentially major impact on cloud droplet number and size, thereby affecting cloud radiative properties, cloud lifetime, and precipitation. Improving observational capabilities for airborne CCN measurements is required to advance understanding and extend current measurements into a wider geographic region, including under-sampled regions, and for longer time periods. There is also a need for smaller, lower-cost, and lightweight instruments capable of measuring CCN for use on rapidly advancing unmanned platforms, including unmanned aerial vehicles as well as tethered and free balloons. To address these needs, we are developing a simple, lower cost, low power consumption and small footprint CCN counter based on a miniaturized version of the DH Associates CCN counter. The mini-CCN counter, termed the Handix Scientific “CloudPuck”, is based on the well-established static diffusion chamber design but has been significantly improved to take advantage of developments in extremely low-cost digital cameras, lasers, mechanical hardware, electronics, computers, and image processing software. The CloudPuck prototype is radically reduced in size and weight from the currently commercially available CCN counters (approximately 6-inches cubed and < 500 g) and has performed initial proof-of-concept testing with size-selected aerosol of known composition. We will present results from tests designed to determine the ability of the instrument to operate on moving, airborne platforms, including large-scale motion and vibration tests. We also discuss results from a pilot study performed in and around the Storm Peak Laboratory in Steamboat Springs, CO to investigate its performance and examine patterns in CCN concentrations over an extended measurement period under real-world sampling conditions.

6NM.1

Modeling Nanoparticle Charge Distribution in the Afterglow of Non-thermal Plasmas and Comparison with Measurements. Vikram Suresh, LI LI, Joshua Redmond Go Filipe, Ranganathan Gopalakrishnan, *The University of Memphis*

A modeling approach to investigate the charge distribution of aerosol particles exiting flow-through non-thermal plasmas and the afterglow region is presented. Understanding the effect of plasma concentration, discharge parameters, plasma temperature, diffusivity of the charged species, and reaction rate constants on the resulting particle charge distribution, is critical in relevant applications, notably in materials synthesis and processing. In this work, collision kernel (β_{pi}) models developed in prior work by analyzing particle-ion trajectories calculated using Langevin Dynamics based simulations, are incorporated into species transport equations for ions, electrons, and charged particles in the afterglow. The developed collision rate constant models are validated by comparing predictions of particle charge against measured values in stationary, non-thermal DC plasma from past PK-4 campaigns (published in Phys. Rev. Lett. 93(8):085001 and Phys. Rev. E 72(1): 016406). The comparisons reveal excellent agreement within ±35% for particle of radius 0.6,1,1.3µm in the gas pressure range of ~20 – 150 Pa. The atmospheric-pressure flow-through plasma experiments by Sharma et al. (J. Physics D: Appl. Phys. 53(24): 245204) to probe particle charge distributions are modeled using the experimentally validated particle-ion collision rate constant models and the calculated charge fractions are compared with measurements. The comparisons reveal that the ion/electron concentration and gas temperature in the afterglow critically influence particle charge and the predictions are generally in qualitative agreement with the measurements. Modeling assumptions and challenges will be highlighted. Situations where particle charge states at the entry of the afterglow region are in the order of ~1000e- require a different computational treatment and this research is afoot. Published in the J. Physics D: Applied Physics (doi: https://iopscience.iop.org/article/10.1088/1361-6463/abf70c). Funding for this work was provided by US National Science Foundation (NSF) PHY Grant Award Number 1903432 and US Department of Energy Office of Science Grant Award Number DE-SC0021206.

6NM.2

Molecular Dynamics based Investigation of Aerosol Deposition versus Thermal Spray Deposition. GUANYU SONG, Huan Yang, Christopher J. Hogan, *University of Minnesota*

Aerosol deposition (AD) is a coating technique leading to thick ceramic coatings by accelerating particles to supersonic speeds and impacting them with a substrate at reduced pressure and room temperature. AD can be contrasted with thermal spray deposition, wherein particles velocities are lower but thermal energies (temperatures) are higher. To better understand the differences between AD and thermal spray generated coatings, we perform large-scale (>10^5 atoms) molecular dynamics simulations of both the AD and thermal spray processes, as well as conditions intermediate to the two processes. Specifically, using yttria-stabilized zirconia (YSZ) nanoparticles (3-6 nm) as model materials on YSZ substrates, we examine the effects of deposition on the nanoparticle internal energy distribution, residual stress, and strain during deposition. These parameters are also examined for the substrate. Uniquely, AD and thermal spray deposition are simulated at equal translational plus thermal energies (i.e. the sum of half the impact velocity squared and 1.5 Boltzmann's constant x temperature are equal in all simulations). The local internal energy distributions for nanoparticles during impaction show that in AD the bottom region of the nanoparticle is heated much more than the upper region when the nanoparticle reaches its maximum penetration into the substrate. Conversely, in thermal spray, particle internal energy distributions are much more uniform, as the degree of translational-to-thermal energy conversion is lessened. AD results in higher degrees of plastic deformation and residual stress than thermal spray at comparable total energy. Substrate temperatures increase to higher values in thermal spray deposition as compared to AD. Simulation results suggest that both processes can lead to strongly adhered, consolidated coatings from particle deposition, but that coating microstructure is affected by translational-to-thermal energy conversion during deposition processes.

6NM.3

Vapor-Phase Synthesis and Assembly of Reactive Metal Nanoparticles for Energetic Applications. PANKAJ GHILDIYAL, Prithwish Biswas, Steven Herrera, Reza Abbaschian, Michael Zachariah, *University of Maryland, College Park*

Nanoscale reactive metals such as Mg, Al, Fe, and Ni are emerging candidates for designing materials for plasmonics, hydrogen storage, and energetic composites. Assembly of their nanoparticles (NPs) into well-defined structures is also highly desirable due to their collective properties that are sensitive to size, structure, and organization of particles in such assemblies. Aerosol synthesis provides a scalable route to continuous production of high-purity nanoparticles and their assemblies by circumventing the need for stabilizing agents typically employed in colloidal approaches. Here, we present a vapor-phase synthesis approach – electromagnetic levitation and heating – based on controlled-evaporation of bulk reactive metals to not only generate NPs of reactive metals but also assemble them into different aggregate assemblies. Using this approach, we have generated highly reactive Mg NPs with tunable sizes from ~20-500 nm.

We have evaluated the size-dependent reactivity and energetic performance of the synthesized Mg NPs as a fuel for different nanoscale oxidizers. Through in-situ time-of-flight mass spectrometry coupled with ignition and constant-volume combustion-cell measurements, we demonstrate that the Mg-release, ignition temperatures, reactivity, and energy release rates of the energetic composites can be controlled by tuning Mg particle size. We also show that the magnetic field employed in this technique allows for on-the-fly, vapor-phase assembly of metal nanoparticles into aggregates with different fractal dimensions that exhibit distinct morphologies and porosities. This method, therefore, enables scalable synthesis *and* assembly of nanoscale metals, opening possibilities for large-scale manufacturing of materials with tunable reactive behavior as well as morphological and structural features.

6NM.4

Langevin Dynamics Simulation of Porous Particulate Film Deposition with Polydisperse and Agglomerated Particles. JIHYEON LEE, Christopher J. Hogan, *University of Minnesota*

Aerosol synthesis methods are often coupled with deposition in an effort to manufacture particulate coatings. The structural properties of such coatings are largely dependent on the size and morphology of depositing particles, along with the physics governing particle transport to the deposition substrate. This study investigated the effects of the polydispersity and morphology of depositing particles on resulting particulate films on a flat substrate via Langevin dynamics simulation. In simulations, individual particle trajectories were monitored as a constant force drove particles to the substrate, accounting both for particle inertia and thermal (Brownian) motion. Particles were assumed to bind upon contract with the substrate or with previously deposited particles. Deposited films were characterized via analysis of their pore size distributions and porosities. To demonstrate how such structural parameters can effect film physical properties, a thermal conductivity model accounting for non-continuum conduction within pores was constructed and used to predict deposit thermal conductivities. In deposition simulations, we considered partial coalescence, polydispersity, and extent of aggregation for depositing particles. Polydisperse particles were sampled from a log-normal distribution with assigned geometric standard deviations, while aggregates were composed of a prescribed number of primary particles. The deposition of polydisperse and aggregated particles broadened the pore size distribution and increased the mode pore size. Thermal conductivity predictions suggest that particulate films can achieve thermal conductivities comparable to that of conventional aerogels.

6NM.5

Flame Aerosol Synthesis of Mesoporous Silica and Porous Ceramic Nanospheres. Shuo Liu, Satyarit Rao, Mihir Shah, MARK SWIHART, *University at Buffalo - SUNY*

Over nearly three decades since Mobil researchers developed the self-assembled template method for synthesis of mesoporous silica, this class of materials has been broadly applied in catalysis, separation and purification, sensors, and biomaterials based upon its high porosity, ordered pore morphology, and tunable surface groups. Later, researchers developed the aerosol-assisted self-assembly method to produce mesoporous silica in a process similar to spray drying. Until now, no such high porosity mesoporous silica has been produced by flame aerosol technology because the high temperature typical of flame synthesis would destroy the organic template and collapse the pores. Moreover, flame synthesis of silica, e.g., production of fumed silica, generally proceeds by a gas-to-particle conversion route that is inherently incompatible with templating. Here, we report the production of nanoparticles of mesoporous silica using a unique flame aerosol reactor configuration that separates the flame chemistry and particle formation process into different regions, which allows a much lower reaction temperature. In this process, a liquid solution of precursor and surfactant is injected into the throat of a converging-diverging nozzle, placed downstream of a hydrogen-oxygen flame. The nozzle accelerates the hot combustion gases, which atomize the precursor solution. Solvent evaporation, surfactant self-assembly and silica formation occur in each droplet, during the ~50 ms residence time in the aerosol reactor downstream of the nozzle. The droplets are much smaller and the residence time is much shorter than in traditional aerosol-assisted self-assembly processes. With this approach, after calcination to remove the surfactant template, we produced mesoporous silica with a BET surface area of more than 1000 m^2/g, entirely in the form of submicron spheres. This approach is also generalizable to other materials, and we are preparing other mesoporous metal oxides by the same process.

6NM.6

In-Situ Laser Diagnostics for the Characterization of Nanoparticles Synthesized with the Reactive Spray Deposition Technology (RSDT). EVANGELOS K. STEFANIDIS, Thomas A Ebaugh, Stoyan Bliznakov, Leonard Bonville, Francesco Carbone, Radenka Maric, *University of Connecticut*

The Reactive Spray Deposition Technology (RSDT) is a single-step flame-based process used to manufacture highly active catalyst nanoparticles in a flow reactor and deposit them on a target substrate. The optimization of the RSDT methods can be performed by adjusting some operative parameters, such as the spray flowrate, to tailor the properties of the synthesized nanoparticles. The characterization of the nanoparticle products can be performed ex-situ at the end of the deposition process. However, the optimization of the process parameters and the ability to time stage the deposition process can benefit significantly from in-situ laser-based diagnostic capabilities. In this study, we use the second harmonic of a pulsed Nd:YAG laser with a wavelength of 532nm to illuminate a millimeter-sized measuring volume and collect the stimulated emission of light at an angle of approximately 45° from the incident beam through a series of optical elements into a spectrograph equipped with a fast gated and intensified CCD camera. Measurements were performed while synthesizing iridium oxide nanoparticles and two classes of platinum nanoparticles of different sizes, which have been already used to manufacture fuel cells. We obtained repeatable results independent of the laser illumination fluence in terms of both calibrated static Rayleigh scattering cross-section and particle Laser-Induced Incandescence (LII) signal. Data analysis allowed us to estimate the nanoparticle sizes and number concentrations at different positions in the reactor for the three considered deposition processes. The results are consistent with those of extra situ microscopy analyses. Additionally, we acquired inelastic Raman spectra to get information about the evolution of the chemical nature of the synthesized iridium oxide nanoparticles in the reactor.

6NM.7

Laser Pyrolysis Synthesis and Applications of Rare-Earth Fluorides for Optical Upconversion. Mohammad Malekzadeh, Khirabdhi Mohanty, Vishvajeet Mane, MARK SWIHART, *University at Buffalo - SUNY*

Nanoparticulate rare-earth fluorides have been traditionally synthesized by solution-phase methods that require multiple steps to obtain the final products, and that employ organometallic precursors, costly ligands, and large volumes of organic solvents. Laser pyrolysis, a flexible aerosol nanosynthesis technique, provides a green single-step route to synthesize a wide variety of metal fluoride nanoparticles by a single method. Because most precursor molecules cannot absorb the 10.6 µm CO_2 laser that drives the laser pyrolysis, a photosensitizer is used to absorb light and transfer energy to the precursors. The most common photosensitizer is sulfur hexafluoride (SF_6) which is inert, non-toxic, and has exceptionally strong absorbance at the laser wavelength. Under focused illumination, the SF_6 can also decompose and serve as a fluorine source. This allows us to use spray delivery of low-cost fluorine-free metal salts as precursors for metal fluorides. Among the materials we have prepared by this approach are rare-earth based optical upconverting nanoparticles that absorb multiple infrared photons and emit at shorter wavelengths. We synthesized $NaYF_4:Yb^{3+}/Er^{3+}$ nanoparticles that upconverted near-infrared light into visible-light range with sharp green (550 nm) and red (650 nm) emission. Varying processing parameters led to emission of green, yellow, and red light under 980 nm diode laser illumination of dispersions of nanoparticles in various solvents ranging from highly polar to highly non-polar. In addition, we synthesized $NaYF_4:Yb^{3+}/Tm^{3+}$ nanoparticles with sharp near-infra-red emission at 800 nm and $NaYF_4:Yb^{3+}/Ho^{3+}$ nanoparticles with sharp green emission at 550 nm. Because we are not using any hydrophobic ligands during the synthesis process, our upconverting nanoparticles are directly dispersible in water. Accordingly, we used them in water-based nano-inks without any further coating process. The variety of upconverted emission wavelengths achievable by these nanoparticles, alone and in combination makes them useful in anti-counterfeiting and related applications, allowing one to embed images visible only under 980 nm illumination within other images. This presentation will discuss the synthesis, emission optimization, and printing of these nanoparticles.

6NM.8

Synthesis of Graphene Nanosheets from Controlled Explosion of Liquid Precursors. SHUSIL SIGDEL, Justin Wright, Jose Covarrubias, Christopher Sorensen, *Kansas State University*

The explosions of benzene, toluene and xylenes were carried out in a 16.7 L chamber in the presence of O2 at different fuel-rich molar ratios such that an aerosol of elemental carbon is produced. The product was a powder at higher oxygen content and an aerosol gel at lower oxygen where the carbon yield was larger. The explosion temperature was measured by a Spectrometer that detected black body, Planck radiation analysis of which indicated temperatures in the range 2000 - 2400 K. The product collected was characterized by Raman, XRD, BET, TEM, and etc. Raman showed two types of products, the amorphous soot at a lower temperature and multilayer graphene at a higher temperature. BET showed the graphene sample is highly porous (half pore width, 18nm) and has a high specific surface area, 388 m^2/g. We conclude that chamber explosion of aromatic hydrocarbons can produce graphene and the high explosion temperature during the reaction is the primary reason graphene is formed rather than soot.

6NM.9

Controllable Synthesis of Charged Lignin Nanoparticles as Nanocarriers by Electrospray. HAO ZHOU, Sujit Modi, Pratim Biswas, *Washington University in St Louis*

In the field of agriculture spraying and drug delivery, nanocarriers is a critical aspect because it can increase the bioavailability and control the release kinetics of effective chemicals. To obtain efficient targeting, better bioavailability, and reduced side effects, several factors remain to be optimized such as particle size, morphology and charge. However, until now, little work has been done for fabricating charged nanocarriers. Considering the great advantages of charged nanocarriers such as improving the deposition rate and tuning the retention time, in this study, the generation of charged carriers with controllable size, and morphology is conducted by using the electrospray system. Lignin is chosen as the carrier materials due to its low price, environmental friendliness, good biocompatibility, and high stability. Firstly, we control the size and charge distribution of as-prepared nanoparticles by tuning the operation parameters and precursor properties. The particle charge is measured by using tandem scanning mobility particle sizer (SMPS). The particle size is measured by SMPS and TEM. The most important parameters are the liquid flow rate, the initial concentration and the electrical conductivities. Then the influences of the evaporation rate and the coulombic fission events on the particle morphology are studied. Different morphologies including spherical solid, elliptical solid and spherical hollow are synthesized by using the electrospray. Finally, the experimentally measured results are correlated to the theoretically models developed in our previous work. This study suggests a novel strategy for fabricating charged lignin nanocarriers for the drug delivery and agriculture spraying.

6NM.10

Size Effect on the NIR Sheilding of Sodium Tungsten Bronze Particles. HAO TU, Wei-Ning Wang, Da-Ren Chen, *Virginia Commonwealth University*

Because nearly half of the energy in solar radiation is in the infrared (IR) range, it is very desired to have transparent media with the NIR (Near-Infrared) shielding function in order to save energy for the air conditioning of buildings and vehicles. Tungsten bronze oxides (MxWO3), which could be applied to transparent media, e.g., glasses, are one of potential candidates for accomplish the above task. We had previously introduced an aerosol-assisted method to produce crystalline tungsten bronze particles in one step and without any aftertreatment. In the effort to search for the NIR shielding performance optimization of MxWO3 particles, we found the previous works were primarily focuses on the effects of elemental species and crystal phases. The size effect on the NIR shielding of MxWO3 particles is very scattered. In this investigation, we obtain particle samples in different sizes and tungsten bronze species through the aerosol processing after tungstenbrone particles are produced by our aerosol-assisted method. The transmission spectrum of prepared samples (in VIS-NIR range) were measured. It is found that the smaller the tungsten bronze particle size the higher the visible light transmittance (VLT). Through the engineering of the size distribution and species, the VLT and NIR shielding of tungsten bronze particles could be optimized. The detail of our preparation method and the findings will be presented in this presentation.

6NM.11

Freeze Spray Drying for the Encapsulation of Active Proteins. ALBERTO BALDELLI, Aylin Cidem, Yigong Guo, Hui Xin Ong, Daniela Traini, Anubhav Pratap-Singh, *The University of British Columbia*

Proteins have inherent low stability due to their high molecular weight and complex structure, making protein delivery challenging. Freeze spray drying allows the encapsulation of several proteins. In this study, the influence of the formulation on the properties of freeze spray-dried encapsulated proteins microparticles and their physic-chemical stability is presented.

Formulations used for the encapsulation of proteins through freeze spray drying involve a polymer for shell formation, carriers for preserving the stability of proteins, and amino acids for promoting the particle formation. The components selected were polyvinylpyrrolidone (PVP) as polymer, α-lactose, D-mannitol, and trehalose as carriers, and leucine, trileucine, arginine, tyrosine, and glutamine as amino acids. Several proteins were investigated: Bovine Serum Albumin (BSA), pea protein, whey protein, hemoglobulin, and Angiotensin-converting enzyme 2 (ACE2). Formulations were first sprayed, at -10°C using a double-flow atomizer in liquid nitrogen and, later, freeze-dried.

All analyzed proteins were encapsulated by using PVP, with a molecular weight of 1300 kDa, mannitol, and leucine with ratios of 6:9:2. By decreasing the molecular weight of PVP to 360 and 55 kDa, the stability of BSA decreased of the 55 and 88 %, by analyzing infrared spectra. Employing lactose or trehalose produces microparticles with broken shell and unsuccessful encapsulation. Other amino acids, with a weight percentage of 15 to 25 %, generates similar results; glutamine is the amino acid decreasing BSA stability of 40 %. After performing ELISA, ACE2 encapsulated using a ratio 6:9:2 of PVP, mannitol, and leucine showed to maintain 87% of activity.

We confirmed the impact of the formulation on the stability of proteins encapsulated using freeze-spray drying. We determined the optimal formulation components that maintain the stability and activity of several proteins, including ACE2, a potential treatment for SARS-CoV-2.

6SI.1

Personal Protective Equipment: Efficacy in Containing and Shielding Particulate Matter with a Diameter between 1 and 5 µm. ALBERTO BALDELLI, Kevin Heieis, Steven Rogak, Andrew Poznikoff, Robert Purdy, *The University of British Columbia*

Airborne viruses, such as SARS-CoV-2, can spread by droplets and aerosols. Besides social distancing, using personal protective equipment (PPE) is assumed to reduce the probability of both transmitting and contracting airborne viruses.

To test the shielding efficiency of different types of PPE, a 0.9% saline solution was nebulized into the upper respiratory tract of a manikin. Five face masks and three shields were tested. An optical particle sizer was used to measure particulate matter (PM) with a diameter between 1 and 5 µm at the mouth of the receiving manikin with simulated breathing. The eight types of PPE were: medical mask, medical mask with eye shield, N95, KN95, cloth mask, cloth mask with valve, disposable face shield, 3D printed pivot face shield, and a shop shield. Samples were collected over 5 minutes at three separate distances (2, 4, 6 ft) and were repeated at three angles (0, 45, 90 degrees). A room baseline and baseline with aerosols being freely generated was measured.

We validated that the distance between the aerosol source and receiving manikin was important. When compared to the aerosol baseline, a cloth mask was found to reduce average PM by 20% over the three distances. The worst shielding efficacy is seen with the disposable face shield, which increased the PM concentration by 33% and 7%, at 2 and 4 feet respectively. In contrast, the best performing PPE with our model was a medical mask, which reduced average PM by 63%. When a disposable medical mask was placed on both the receiving and aerosol manikins, the concentration of PM was reduced to the room baseline at all distances, with the lowest value of 7 µg/m3 at 6 feet. The effectiveness of any given PPE was highly influenced by their fit on the face of our model in these results.

6SI.2

Respiratory Aerosols and Droplets in the Transmission of Infectious Diseases. MIRA L. PöHLKER, Ovid O. Krüger, Jan-David Förster, Thomas Berkemeier, Janine Fröhlich-Nowoisky, Wolfgang Elbert, Ulrich Pöschl, Gholamhossein Bagheri, Eberhard Bodenschatz, Simone Scheithauer, J. Alex Huffman, Eugene Mikhailov, Christopher Pöhlker, *Max Planck Institute for Chemistry, Mainz, Germany*

Knowing the physicochemical properties of exhaled droplets and aerosol particles is a prerequisite for a detailed mechanistic understanding and effective prevention of the airborne transmission of infectious human diseases. Public health recommendations can benefit from an improved understanding of the respiration particle properties such as number and volume size distributions, the sedimentation time for different diameters, and the chemical composition, which influences the viral load but also the drying time after exhalation.
We provide a critical review and synthesis of scientific knowledge on the number concentrations, size distributions, composition, mixing state, and related properties of respiratory particles emitted upon breathing, speaking, singing, coughing, and sneezing. We derive a parameterization of respiratory particle size distributions based on lognormal modes related to different origins in the respiratory tract, which can be used to trace and localize the sources of infectious particles. This approach may support the medical treatment as well as the risk assessment for aerosol and droplet transmission of infectious diseases. It was applied to analyze which respiratory activities may drive the spread of specific pathogens, such as *Mycobacterium tuberculosis*, influenza viruses, and SARS-CoV-2 viruses. The results confirm the high relevance of vocalization for the transmission of SARS-CoV-2 as well as the usefulness of physical distancing, face masks, room ventilation, and air filtration as preventive measures against COVID-19 and other airborne infectious diseases (Pöhlker et al. 2021, arXiv:2103.01188).

6SI.3

Dynamics of Size Distribution Evolution of Human Expelled COVID-19 Droplets for Coughing and Speaking: A Simulation Study. JOSHIN KUMAR, Yang Wang, Benjamin Sumlin, Esther Monroe, Nishit Shetty, Rajan K. Chakrabarty, *Washington University in St. Louis*

The dynamics of the size distribution of virus-containing human expelled droplets is significant because it determines the deposition pattern in the human respiratory system, the lifetime of droplets in the indoor and outdoor spaces, and consequently, the transmission of respiratory diseases such as COVID-19.

Recent experimental studies have produced data on the initial size distribution for various expiratory activities. This initial size is often used directly for lifetime calculations which underestimates the lifetime of droplets. Hence, we must account for the size dynamics of droplets containing the COVID-19 virus to produce more realistic results.

Here, we present the results of a simulation study on the size distribution evolution of expelled droplets as reported by Prof. Lidia Morawska’s group in previous publications. In our model formulation, we have accounted for the environmental parameters such as evaporation, relative humidity, and room temperature while establishing and solving non-linear coupled differential equations for heat and mass transfer across the droplet and environment.

We show that considering the heat and mass transfer, the virus-containing human expelled droplets tend to shrink to smaller sizes, allowing them to stay unsettled in undisturbed indoor spaces for as long as a week. Also, modeling the dynamics enables us to see the transition states of size distribution as the droplets undergo evaporation and shrink to steady-state sizes within the order of ~0.1 seconds.

6SI.4

Effect of Filtration Area on Aerosol Penetration through Personal Protective Equipment. CHETHANI ATHUKORALA, Hunter Hardy, Suresh Dhaniyala, *Clarkson University*

Personal protective equipment (PPEs) such as masks are critical to filter microbes and pollutants from the air we breathe. With the on-going pandemic, there has been increased interest in evaluating different PPE material with a range of test aerosol. Methodologies to characterize particle penetration through filter media have largely been standardized, but the recent pandemic has shown the need to understand if test methodologies are sensitive to small changes in the setup such as test aerosol material, area of test filter, etc. Here, we use a well characterized filter test setup and evaluate a range of filter material using different aerosol types, charge states, and filter holder sizes to determine the robustness of penetration results as a function of face velocity. We will present our experimental setup and results of our study at the conference.

6SI.5

Studying the Novel SARS-CoV-2 for Aerosol Transmissions. WAJIH UR REHMAN, *COMSATS University Islamabad*

Aerosol transmission from SARS-CoV-2 have always been a conundrum for modern scientific study. In this article, we would discuss about various transmissions from novel SARS-CoV-2 and how they are different in different settings, such as in hospitals where SARS-CoV-2 patients are being treated, in buildings, schools and in outdoor environments. Further, the effect of ventilation in indoor environments will also be studied. The focus of this work is to find the transmission routes and patterns of novel SARS-CoV-2 in various environments (indoors and outdoors) so that the effect of virus spreading can be studied and transmission of virus can be curtailed.

7AC.1

Production of Formate via Oxidation of Glyoxal Promoted by Particulate Nitrate Photolysis.

RUIFENG ZHANG, Masao Gen, Tzung-May Fu, Chak K. Chan, *City University of Hong Kong*

Particulate nitrate photolysis can produce oxidants (i.e., OH, NO_2, and NO_2^-/HNO_2) in aqueous droplets and may play a potential role in increased atmospheric oxidative capacity. Our earlier works have reported on the SO_2 oxidation promoted by nitrate photolysis to produce sulfate. Here, we used glyoxal as a model precursor to examine the role of particulate nitrate photolysis in the formation of secondary organic aerosol (SOA) from particle phase oxidation of glyoxal by OH radical. Particles containing sodium nitrate and glyoxal were irradiated at 300-nm. Interestingly, typical oxidation products of oxalic acid, glyoxylic acid, and higher molecular weight products reported in the literature were not found in the photooxidation process of glyoxal during nitrate photolysis in the particle phase. Instead, formic acid/formate production was found as the main oxidation product. At glyoxal concentration higher than 3 M, we found that formic acid/formate production rate increases significantly with increasing glyoxal concentration. Such results suggest that oxidation of glyoxal at high concentrations by OH radicals produced from nitrate photolysis in aqueous particles may not contribute significantly to SOA formation since formic acid is a volatile species. Furthermore, recent predictions of formic acid/formate concentration from the most advanced chemical models are lower than ambient observations at both ground-level and high altitude. The present study reveals a new insight into the production of formic acid/formate as well as a sink of glyoxal in the atmosphere, which may partially narrow the gap between model predictions and field measurements in both species.

7AC.2

SOA and Organic Nitrate Formation from the Reaction of α-Pinene with NO3 under Simulated Nighttime Conditions.

Kelvin Bates, James Cope, Guy Burke, TRAN NGUYEN, *University of California, Davis*

α-Pinene+NO_3 is a major oxidation pathway at night, and thought to be responsible for the large number of terpene-derived organonitrates observed in mixed biogenic/anthropogenic areas, including in the aerosol phase. However, previous laboratory studies on SOA formation from this pathway have shown a big discrepancy on yields, which are likely due to the broad spectrum of chemical and physical conditions used in previous chamber studies, many of which were performed under conditions with excessively large [NO_3] concentrations. Here, we perform a series of atmospheric chamber experiments to characterize the reaction of α-pinene + NO_3 under a range of atmospherically relevant conditions. Specifically, we vary the reaction partners of the first-generation peroxy radicals (NO_3, NO, HO_2, RO_2) and measure the SOA yields from each individual pathway. We show that the RO_2 + RO_2 pathway produces large quantities of SOA (up to 90% mass yield), while the other pathways have much lower SOA yields. To further characterize the chemical pathways by which these oxidation reactions occur, we use chemical ionization mass spectrometry to quantify yields of some gas-phase products, and collect filters for offline sampling of particle composition using high-resolution Orbitrap mass spectrometry with electrospray ionization. We show that dimer formation is the primary mechanism of SOA production for the RO_2 + RO_2 pathway, and remains highly competitive with other RO_2 fates under simulated nighttime conditions. We present SOA and organic nitrate yields from each RO_2 fate branch, and propose mechanisms consistent with the products observed. These results provide important constraints for atmospheric models of aerosol and nitrate formation, and shed light on the factors controlling nighttime SOA production in mixed biogenic/anthropogenic areas.

7AC.3

Observations of Nitrate Radical Initiated Oxidation of Various Monoterpenes in a Laboratory Chamber Using NO3-CIMS. MICHELIA DAM, Danielle C. Draper, Andrey Marsavin, Juliane Fry, James Smith, *University of California, Irvine*

Chemical ionization mass spectrometry with nitrate reagent ion (NO3-CIMS) was used to probe the composition of nitrate radical initiated monoterpene oxidation products in laboratory chamber experiments for four different monoterpene systems (a-pinene, b-pinene, d-carene, a-thujene). The major species in each system were distinctly different, showing the effect of monoterpene structure on the oxidation mechanism. By comparing groupings of products based on ratios of elements in the general formula CwHxNyOz, the dominance of specific mechanistic pathways (fragmentation, termination, radical rearrangement) were observed for each system. Additionally, the time series of the highly oxidized reaction products gives insight into the ratio of relative production and loss rates of these high molecular weight products. Measured effective O:C ratio of reaction products were anti-correlated to observed particle formation for each system. Monomer:dimer ratio of species did correlate, however. Gas phase yield of oxidation products measured by NO3-CIMS and total gas phase alkyl nitrate yield measured with a thermal dissociation cavity ring-down spectrometer (TDCRDS) corresponded to particle number measured with a scanning mobility particle sizer (SMPS) for each monoterpene system, with the exception of the a-thujene system, which produced a considerable concentration of low volatility products, but no particles. Speciated wall loss interactions were measured with NO3-CIMS and found to be highly variable among oxidized reaction products in our stainless steel chamber. The information gained from this detailed comparison of gas phase composition with currently established mechanisms provides additional insight into the NO3 radical initiated monoterpene oxidation process and further elucidates the effect of these species on particle formation and growth.

7AC.4

The Effect of Viscosity on Rate of Fresh SOA Seed Particles Grown by α-Pinene Ozonolysis. DEVON HAUGH, Michael S. Taylor, Murray Johnston, *University of Delaware*

Atmospheric nanoparticle formation and growth is a significant source of cloud condensation nuclei. To accurately predict future climate, it is important to understand particle growth mechanisms under varying ambient conditions. Nanoparticle growth is dominated by the condensation of condensable organic vapor (COV), as produced in biogenic secondary organic aerosol (SOA). However, it has been recently established by our group that particle phase reactions play a key role in the growth of aqueous ammonium sulfate droplets in the 40-100 nm size range. These reactions cause droplets to grow from α-pinene ozonolysis products at a rate about 50% faster than inert, solid particles under identical conditions. The work presented here investigates this enhanced growth rate by incorporating freshly generated α-pinene SOA as the seed substrate. Fresh SOA can be glassy- or liquid-like, depending on the relative humidity, which allows for a more inclusive range of viscosity to be studied than inorganic salts. Additionally, fresh SOA seeds are peroxide-rich, and therefore, highly reactive. The work to be presented features a dual flow tube reactor setup and investigates the role of seed viscosity on particle growth rate. Results from these experiments compare effloresced fresh SOA seeds under varying relative humidity conditions as well as deliquesced seeds. Growth rates and mechanisms will be discussed in the context of diameter growth rates of the seed particles.

7AC.5

Molecular Composition Changes in α-Pinene SOA Due to the presence of PAHs.

SIMEON SCHUM, Lynn Mazzoleni, Kaitlyn Suski, Alla Zelenyuk, *Michigan Technological University*

Terpene emissions, such as α-pinene, contribute to the formation of a large proportion of biogenic secondary organic aerosol (SOA) in the atmosphere. When emitted near anthropogenic emission sources (cars, power plants, industrial processes, etc.) these compounds will interact, which may lead to compositional changes in the organic aerosol and changes in how the aerosol interacts with the environment (light absorptivity, volatility, viscosity, etc.). Recently, α-pinene ozonolysis SOA was formed in the in the presence of various gas-phase PAHs. The data indicate that the presence of PAHs results in significant changes in the aerosol evaporation rates, viscosity, and yields of formation. Low resolution mass spectrometry results also indicated significant changes in the composition of the resulting aerosol, though the extent of the changes in aerosol molecular-composition was difficult to determine. Here we report the analysis of these samples using multiple ionization types (ESI and APPI) and modes (negative/positive) with ultrahigh resolution mass spectrometry (Orbitrap Elite) for a more detailed look at the molecular composition of these samples. We found that the most obvious change in composition occurred for the mixture of α-pinene and pyrene, showing a cluster of oligomers containing a single oxidized pyrene and one or more α-pinene molecules. Additionally, the use of APPI allowed the observation of low-oxygen oligomers of α-pinene that have not been reported previously in experiments with non-acidic seed aerosol. These low-oxygen oligomers seemed enhanced by the presence of benzo[a]anthracene, but were also present in "normal" α-pinene SOA. The presence of these compounds raises questions about the potential for an additional pathway for SOA formation outside the typical oxygen-increasing reaction described in most SOA studies. Here we will present the results of the mass spectrometric analysis of these samples and discuss their potential implications for the understanding of SOA formation and the interaction between biogenic and anthropogenic aerosol sources.

7AC.6

Formation and Properties of Secondary Organic Aerosol Particles Generated by Oxidation of Cyclic and Acyclic Terpenes.

ALLA ZELENYUK, Robert VanGundy, David Bell, *Pacific Northwest National Laboratory*

Monoterpenes and sesquiterpenes are some of the most common biogenic volatile organic compounds (VOCs) that contribute to formation of significant fraction of atmospheric secondary organic aerosol (SOA). Model treatment of these classes of biogenic VOC emissions and chemistry that leads to SOA formation are typically based on laboratory experiments conducted on a very limited number of SOA precursors (e.g. α-pinene, limonene, β-caryophyllene). Recent studies indicate that plants emit a large variety of both, cyclic and acyclic terpenes, which have different potentials to form SOA. It was shown that SOA formation yields decrease as the fraction of acyclic terpenes in complex VOC mixtures increases, often as a result of environmental stresses from drought, insects, or air pollution. These findings clearly highlight the importance of better understanding oxidation chemistry of acyclic terpenes and the properties of the resulting SOA particles.

We will present the results of a recent study focused on the comparison of formation (yields, size distributions, mass loadings), and properties (composition, density, shape, volatility, viscosity) of SOA particles formed by ozonolysis of cyclic (α-pinene and β-caryophyllene) and acyclic terpenes, including β-ocimene, β-myrcene, and α-farnesene. We find that, consistent with previous studies, SOA yields from ozonolysis of α -farnesene are lower compared to those for β-caryophyllene with the same concentration. Moreover, preliminary data indicate that concentration of VOC strongly effects the viscosity and volatility of SOA particles from both cyclic and acyclic sesquiterpenes. SOA particles formed at lower VOC concentrations are more viscous and less volatile. We show that larger size-selected SOA particles are often aspherical, nearly fractal agglomerates of nanoparticles. However, with time these particles coalesce to form spherical particles, making it possible to estimate particle viscosity as a function of relative humidity.

7AC.7

Reaction Products and Pathways of Alkoxy Radicals in the Condensed Phase. VICTORIA BARBER, Yaowei Li, Alexander Zaytsev, Francesca Majluf, Jordan Krechmer, Frank Keutsch, Jesse Kroll, *MIT*

Condensed phase processes, such as aerosol oxidation aging and aqueous-phase oxidation, are critical in understanding the composition and properties of atmospheric aerosol. Organic radicals including alkoxy (RO) and peroxy (RO2) radicals are key intermediates in these processes. Because most mechanistic studies of organic radical reactions take place in the gas phase, the underlying radical chemistry that governs these condensed phase processes is comparatively poorly understood. The condensed phase represents a much more complex environment, because locally high concentrations may facilitate additional reactions between organic species, and solvent effects may alter relevant potential energy surfaces. Here, we investigate the condensed-phase chemistry of a photolytically-generated RO radical, which allows for the selection of a specific RO radical isomer, greatly simplifying the subsequent chemistry as compared to oxidation via traditional routes. We generate the 1-pentanoxy radical via photolysis of a 1-pentyl nitrite precursor in hexafluorobenzene. The photolyzed reaction mixture is fed at a constant, low flow rate into an atomizer and nebulized directly into a suite of mass spectrometric instruments, providing real-time chemical kinetics information as well as molecular-formula level identification of the reaction products. Consistent with previous work, the results suggest that the nascent RO radical undergoes only unimolecular reaction, independent of the concentration of the RO radical precursor, and even in the presence of a high concentration of a reaction partner with abstractable H-atoms. This unimolecular reaction produces an alcohol-substituted peroxy radical, with a variety of available product channels, including one that involves successive intramolecular H-atom transfer of RO2 radicals, leading to highly oxidized products. The kinetics and branching ratios associated with these product channels are investigated, and compared to recent gas-phase results for similar systems, providing insight into the effects of the solution-phase environment on organic radical chemistry.

7AC.8

Impacts of Salted Aqueous Phase on Monoterpene SOA Produced under Different Atmospheric Oxidants. SANGHEE HAN, Myoseon Jang, *University of Florida*

Typically, the terpene SOA formation during daytime is attributed to the oxidation with both OH and O_3 while at night, this can be dominated by the reaction with O_3 and NO_3 radicals. Thus, daytime terpene products differ from those in nighttime due to the different oxidation pathways of monoterpenes under varying NO_x levels. To date, the impact of inorganic salted aqueous phase on the terpene SOA formation produced in different oxidation pathways was not well understood. In this study, the SOA formation in both daytime and nighttime is simulated by using the UNIfied Partitioning Aerosol phase Reaction (UNIPAR) model that predicts the SOA mass via multiphase reactions of hydrocarbons. The oxidation products of terpenes are predicted by using the explicit gas mechanism (MCM v3.3.1) and autoxidation which forms low volatility products. The resulting products are lumped based on volatility and reactivity and distributed in gas, organic and inorganic aqueous phases to form SOA via multiphase partitioning and heterogeneous reactions in both organic and inorganic phase. The simulated SOA mass is compared to experimental data that are performed under varying conditions in the UF-APHOR chamber. Three different monoterpenes (α-pinene, β-pinene, and d-limonene) react with ozone at nighttime with NO or NO_2 in the presence and the absence of inorganic salt aerosol. The nighttime terpene SOA mass is compared to the SOA that is produced via the photochemical reaction of terpene. The sensitivity of the SOA mass production to NO_x levels and inorganic seed types is characterized by using the UNIPAR model for different SOA formed via different oxidation pathways. Overall, daytime SOA is more influenced by aqueous reactions than nighttime SOA.

7AC.9

Multiphase Ozonolysis of Unsaturated Lipids – Exploring its Mechanism and Product Reactivity. ZILIN ZHOU, Pascale Lakey, Manabu Shiraiwa, Holly Barrett, Hui Peng, Jonathan Abbatt, *University of Toronto, Canada*

Unsaturated lipids are commonly found in atmospheric aerosol and on indoor surfaces. It is well known that these lipids decay rapidly under ozone, following the Criegee mechanism. Here, we studied the heterogeneous ozonolysis reactions of oleic acid and their derivatives (esters and triglycerides) on surfaces. The quantitative analyses of the products suggest that, under dry conditions, up to 80% of the products in the condensed phase are secondary ozonides, whose formation is significantly suppressed by elevated relative humidity (RH). This is due to the reaction between Criegee intermediates (CI) and water, forming gas-phase hydrogen peroxide (H_2O_2) via hydroxyhydroperoxides (α?HHP) intermediates. Such behavior in product composition is well predicted by a kinetic model of triolein (a triglyceride derived form oleic acid). The secondary ozonides derived from triglycerides and phospholipids exhibit high stability in the ambient air and in the aqueous phase. However, mass spectral analyses demonstrate their slow decomposition in ferrous solutions, similar to the Fenton mechanism. Furthermore, an addition of cysteine accelerates the iron redox cycle. The implications of this chemistry will be discussed from the perspectives of oxidative aging of lipids in the environment and potential health effects caused by the oxidation of pulmonary surfactants.

7AC.10

Vapors are Lost to Walls, Not to Particles on the Wall: Development of Artifact-Corrected Parameters and Implications for Global Secondary Organic Aerosol. KELSEY BILSBACK, Charles He, Jeffrey R. Pierce, Nga Lee Ng, John Seinfeld, Shantanu Jathar, *Colorado State University*

Secondary organic aerosol (SOA) is formed through the oxidation of volatile organic compounds and makes up a large fraction of fine particulate matter. Chemical transport models typically rely on SOA parameters derived from environmental chambers that are subject to experimental artifacts. These artifacts include losses of particles to the walls and the losses of vapors to the particles on the wall and the wall directly. Accurately accounting for these artifacts is critical to representing organic aerosol (OA) evolution in models. To investigate these artifacts, first, we used the Statistical Oxidation Model (SOM) with Two-Moment Aerosol Sectional (TOMAS) model and data from chamber experiments to develop artifact-corrected parameters for important SOA precursors (e.g., isoprene, monoterpenes, aromatics, and IVOCs). We found that the parameters produced larger SOA mass yields as we accounted for losses of particles and vapors to the walls but the parameters and SOA mass yields were unaffected by the losses of vapors to the particles on the wall because this process is much slower. Additionally, we found that our schemes substantially impacted the SOA mass yield, depending on the SOA precursor, NO_x condition, and OA mass concentration. Next, we ran pseudo atmospheric simulations using the artifact-corrected parameters, the output of which was used to develop d volatility basis set (VBS) parameters at atmospherically relevant OA concentrations. The updated VBS parameterizations were implemented in GEOS-Chem to evaluate how the artifact-correction schemes impacted global SOA concentrations. Preliminary GEOS-Chem results also suggested that updating the yield parameters for α-pinene alone can change estimated OA by up to 22% in some regions. Overall, we developed a novel systematic method for developing artifact-corrected SOA parameters for chamber studies and demonstrated the effects of these schemes in a global chemical transport model. We expect our results will lead to improved measurement-model agreement for OA.

7AC.12

Photochemical Candy: Use of Isomalt as a Proxy Matrix for Secondary Organic Aerosol. AVERY DALTON, Sergey Nizkorodov, *University of California, Irvine*

Secondary organic aerosol (SOA) is a complex form of particulate matter that has been found to exist as a liquid, a semi-solid, and an amorphous solid. The roles that chemical environment and viscosity play in the photochemical fate of molecules in SOA are poorly understood. In this work, we characterize the photolysis of 4-nitrocatechol (4NC) in a variety of matrices, including liquid water, liquid isopropyl alcohol, and semi-solid isomalt. The rate of photochemical loss of 4NC was obtained by monitoring the absorbance decay using a custom UV-Vis spectroscopy setup. The photochemical rate constants were found to be greater in an organic environment than in an aqueous solution. The quantum yield of photolysis was found to be smaller in an isomalt glass than in liquid isopropyl alcohol, suggesting photochemical reactivity is affected by matrix viscosity. Ultra-performance liquid chromatography was used in tandem with a photodiode array UV/vis spectrophotometer and high-resolution mass spectrometer to propose photolysis products of 4NC. The primary products formed appeared different between matrices. In solution, most products appeared to result from oxidation of 4NC, in contrast to photoreduction and dimerization products which were more prevalent in solid isomalt. We conclude that the photochemical fate of 4NC, and presumably of other nitrophenols, depends on whether they are in a liquid or semi-solid organic particle.

7CT.1

Reevaluating the Filter Pressure Drop Model for Modern Respirators. PATRICK O'SHAUGHNESSY, Zoe Harris, Matthew Purdy, *The University of Iowa*

Among several mathematical models developed to estimate respirator pressure drop, a semi-empirical model by Davies developed in 1952 is still commonly used in the scientific literature. In addition to predicting pressure drop, that model is also used to determine an “effective” fiber diameter – a single fiber diameter that best represents the influence of all fiber diameters on pressure drop. Furthermore, the effective diameter is often applied to equations developed to estimate the particle collection efficiency of a filter because it influences the forces of diffusion, interception, impaction and static charge. Having an accurate pressure drop model is therefore important for predicting both pressure drop and effective diameter.

A study was developed to determine the physical characteristics of filter media associated with modern filtering facepiece respirators (FFRs) and to determine whether adjustments to the Davies model are needed to enhance its accuracy when used to predict pressure drop, and, conversely, the effective diameter of modern FFRs. This study focused on the primary filter layer of 10 FFR models. The pressure drop of 3 filter samples of each filter was measured at 4.7 cm/s and 10.5 cm/s; face velocities associated with low and high breathing rates. Filter thickness and solidity were measured for each FFR model. The median of fiber diameters were measured from 100 fibers counted using photos from a scanning electron microscope.

The measured results did not align with the expected curve from the Davies model. An adjustment was made to that model by minimizing the RMSE (root mean square error) between measured and modeled data. The adjusted equation provided a more accurate prediction of fiber diameter relative to measured diameter. Furthermore, the adjusted model reduces the estimate of filter pressure drop 16-fold, if median diameter is known, relative to the Davies model.

7CT.2

An Improved Filtration Model for Gasoline Particulate Filters (GPFs). PENG WANG, Da-Ren Chen, *Virginia Commonwealth University*

Gasoline particulate filters (GPFs) have been widely used as the aftertreatment devices to control the PM emission from gasoline-powered vehicles in recent years. Compared to those emitted from diesel engines, the PM emitted from gasoline engines are typically smaller in the sizes and higher in the number concentration, resulting in the rare chance for the formulation of soot cake. The collection efficiency of GPFs is highly related to the microstructure of their wall substrates. The “Unit Cell” model assuming the wall substrate of GPFs is made up of different spherical collectors has been commonly employed to estimate the collection efficiency of clean GPFs. However, the collector size distribution of GPFs’ wall substrates was typically derived from the measured pore size distribution in the previous studies, which introduced great uncertainty in the derived collector size distribution. In this study, the Nano-computed tomography (Nano-CT) was employed to reproduce the 3D microstructure of the GPFs’ wall substrate. The size distribution of unit collectors was evaluated directly from the 3D images. The filtration model based on the direct-measured collector size distribution was developed by comparing the predicted collection efficiency with the experimental data. This study demonstrates that the filtration model for GPFs can be improved by characterizing the microstructure of the wall substrate using Nano-CT.

7CT.3

Effective Relative Humidity on Textile Mask Filtration Efficiency and Breathability. JOELLE SEGOVIA, Ching-Hsuan Huang, Nanhsun Yuan, Mei-Yu Liao, Jiayang He, Igor Novosselov, *University of Washington*

During the COVID-19 pandemic, a worldwide mask shortage resulted in many having to create reusable masks out of various materials and fabrics. The reusable masks reduce the waste stream associated with disposable masks and can potentially increase the mask use by the population. However, it is unknown how well these masks can protect the wearer or the people in the vicinity over a range of breathing rates and relative humidity. This study evaluates the effectiveness and ease of breathing through a number of readily accessible materials used for masks. Mask effectiveness is described as the measured filtration efficiency with breathability quantified as the pressure drop is recorded across the material. Natural and synthetic materials such as cotton, silk, rayon, and polyester were tested in the aerosol chamber; sodium chloride particles were used as challenge aerosol. Filtration of particle sizes in the range of 0.5-2 micron was evaluated. Filtration efficiency was determined by comparing particle concentration in the filtered flow against reference measurement taken by aerodynamic particle sizer. To mimic variability in the environmental and in the exhaled breath condition, the chamber was set to three different humidity levels (RH= 40%, 60%, and 80%) along with four different face velocities (0.18 m/s, 0.24 m/s, 0.28 m/s, and 0.34 m/s) to simulate different breathing rates. The filtration efficiency and pressure drop were recorded and used to determine the quality factor of the materials; these data are presented as a function of relative humidity and particle size. The quality factor is a figure of merit relating the filtration efficiency to the pressure drop recorded for each material and compared against that of surgical grade masks. Multiple layers of several materials are also analyzed to determine if there is an increase in filtration efficiency and difficulty in breathing.

7CT.4

Improving Filtration Performance of Ceramic Wall-flow Filters with Heat Resistant Membrane by a Two-step Coating Method.

QISHENG OU, David Y. H. Pui, *University of Minnesota*

Gasoline direct injection (GDI) technology improves fuel efficiency but produces higher PM emissions. Gasoline particle filters (GPF) could be necessary for reducing exhaust particles to meet the emission standards. GPF has difficulty to grow and sustain “soot cake layer” and relies more on porous structures of its own substrate wall to ensure efficiency while keeping back pressure low, which is suboptimal and can be challenging at low mileage. Silica-based nano-scale membrane material is developed for improving filtration performance of ceramic wall-flow GPFs, which can sustain high exhaust temperature, be cost-effective, and user and environmentally friendly. The direct coating of silica membrane in a single-step process has a suboptimal tradeoff between efficiency and backpressure – achieving significant efficiency improvement at high backpressure penalty, which is attributed to the deep penetration of silica coating into substrate micropores. A two-step coating method is then successfully developed, starting from a 1st-step coating of removable porous material to occupy the micro-pore structure, followed by a 2nd-step coating of membrane material on top of the 1st coating. Subsequent regeneration removes 1st coating, leaving the 2nd-step membrane coating staying on top of the substrate. Membrane coated ceramic wafers by the two-step coating method show better efficiency-backpressure tradeoff and soot loading capability than the single-step method with the same coating materials. This two-step coating method is tested on a wall-flow core sample, showing significant efficiency enhancement with less than 30% of backpressure penalty. The developed two-step coating method can be potentially used on other filtration substrates, for improved filtration performance in high-temperature air and/or liquid filtration applications.

7CT.5

Modeling of Heterogeneous Dustcake Effects by PAC Injection in a Cylindrical Electrostatic Precipitator for Mercury Emissions Control at Coal-Fired Power Plants.

ERIC MONSU LEE, Herek Clack, *Northern Illinois University*

Injection of powdered activated carbon (PAC) upstream of an electrostatic precipitator (ESP) is the mature mercury emissions control technology at coal-fired power plants (CFPPs). Based on National Energy Technology Laboratory (NETL)-funded full-scale testing results with PAC injection, conducted by ADA-ES, increasing the rate of PAC injection can potentially promote penetration of submicrometer PAC particles through an ESP, indicated by darkened PM filters from sampling of stack emissions. PAC injection into utility ESPs leads to formation of a heterogeneous dustcake layer on the collection electrodes because of different particle deposition patterns between coal fly ash and PAC. The present study aims to model the effect of such a heterogeneous dustcake in a cylindrical ESP to characterize the induced vortex flows under conditions associated with high electrohydrodynamic (EHD) numbers and its effect on the formation of particle clusters and ESP collection efficiency. A multiscale ESP model is established in COMSOL Multiphysics based on a Euler-Lagrange numerical scheme by considering the effect of particle drag on the fluid flow (i.e. two-way coupling). The heterogeneous dustcake is modeled by imposing a boundary condition assuming spatially varied powder resistivity along the collection electrode surface. The results serve to optimize the process of PAC injection in terms of reducing the PM emissions from ESPs.

7CT.6

Dual-Geometry Pore-Size-Resolved Wall-Flow Filter Deep-bed Loading Model. WEIQI CHEN, Qisheng Ou, Xin Liu, Matti Maricq, David Kittelson, David Y. H. Pui, *University of Minnesota*

Gasoline particulate filter (GPF) is an effective wall-flow technique for gasoline-engine particulate matter (PM) emission control mainly via deep-bed filtration of ceramic walls within the honeycomb cell channels. An analytical filter model is desired for understanding efficiency and pressure drop condition throughout the usage as it is tied to emission regulation and engine performance. Most existing models either oversimplify the filter geometry or do not extend to the soot loading regime such that filter microstructure is modified by particle deposition, leading to altered filter performance. A new advanced loading model is developed based on the classic cell model in this study, which can model the filter wall structure and particle dendritic deposition as two co-existing geometries based on their natural morphologies. On top of it, the pore size distribution of the filter is taken into account throughout the loading process, so the evolution of pore-size-resolved aerosol flow, filtration efficiency, mass loading, particle packing density, and effective fibrous dendritic size can be simulated. In addition, the pore-clogging condition can be estimated without the use of empirical or adjustable parameters. The model validation using filter loading experimental data shows that the model can provide fairly good predictions on both filter efficiency and pressure drop at the same time during deep-bed loading for different wall-flow filters under different operation conditions. By using the model, the change in morphology of particle dendritic structure in different pores for deep filtration was investigated. The impacts of pore size distribution and pore-clogging condition were studied, which suggest that improving the pore size uniformity can improve filter performance in both clean and loading filtration regime.

7CT.8

Continuing Development and Testing of the Electrostatic Battery for Emissions Control (ESBEC). TAEWON HAN, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

We recently developed a novel diesel emissions control device, Electrostatic Screen Battery for Emissions Control (ESBEC), where diesel exhaust particles are removed using an electrostatic mechanism. As part of the continuing development of this technology, we have made the following changes to ESBEC's design: 1) metal collection screens with high porosity for a more even distribution of captured diesel exhaust, 2) redesigned screen holder for easy assembly, 3) device's body constructed from heat-resistant materials (up to 460 ^oF). The size of the current ESBEC prototype is 3 inches in diameter and 10 inches in length. ESBEC was challenged with diesel particulate matter (DPM) exhausted from a diesel electric power generator (6000-watt diesel generator) operated with no electrical load. Tested mass concentrations were 38-187 mg/m^3 and the air flow rates passing through ESBEC were 220-410 L/min; these long-term tests were conducted over 8 days (about 49 hours of sampling and measurement). The collection efficiency of ESBEC was determined every 30 to 60 minutes by comparing DPM concentration upstream and downstream of ESBEC using a pDR-1200 photometer.

The average ESBEC collection efficiency of close to a 100% was maintained for 26 hours, during which 60 g of DPM was accumulated. After that, its performance gradually decreased as more DPM was accumulated (up to 102 g); after 47 hours of operation, ESBEC's collection efficiency decreased to CARB (California Air Resources Board) Level 3 (85%) and the pressure drop across it increased to 57 Pa. The collection efficiency was restored when the charger section was cleaned using isopropyl alcohol for 10 min. In the next tests, we will investigate the removal of DPM from ESBEC's collection screens as a function of different loading/washing protocols.

7CT.9

In-Use Emission Measurements from Two High-Speed Passenger Ferries Operating in California. CHAS FREDERICKSON, Wei Liu, Mark Villela, Kent Johnson, David Quiros, Heejung Jung, *University of California, Riverside*

In 2007, the California Air Resources Board (CARB) adopted an in-use regulation to reduce emissions from Commercial Harbor Craft (CHC), which includes ferries, tug boats, barges, and other vessel categories. After full implementation of the CHC regulation in 2022, many CHC vessels operating in California will be equipped with engines certified to the U.S. Environmental Protection Agency (EPA) Marine Tier 2 or Tier 3 standards. Although the CHC regulation will have achieved substantial emission reductions by accelerating turnover to cleaner engines, no marine engines are originally equipped with diesel particulate filters (DPF) to control particulate matter (PM). Consequently, CHC are expected to remain one of the top three seaport sources of cancer risk due to exposure to diesel PM.

In this study, we measured in-use particulate matter (PM) and gaseous emissions – including carbon monoxide (CO), carbon dioxide (CO_2), nitric oxide (NO), and nitrogen dioxide (NO_2) from two high-speed passenger ferries in the San Francisco Bay Area: one equipped with Tier 2 engines with 18,096 hours, the other equipped with Tier 3 marine engines with 6,392 hours at the commencement of the study. Whereas marine engines are certified by United States (U.S.) Environmental Protection Agency (EPA) over the ISO 8178 E3 steady-state cycle, we used Portable Emissions Measurement Systems (PEMS) to measure emissions during normal revenue service, which includes some transient and some steady-state operation. Emissions were below relevant certification limits; average in-use NO_x emissions were 4.62 and 3.62 g/bhp-hr for the Tier 2 and Tier 3 engine, respectively, and PM emission were 0.044 g/bhp-hr for the Tier 3 engine. The second vessel, equipped with Tier 3 standards engines, was also equipped with an aftermarket selective catalytic reduction (SCR) and diesel oxidation catalyst (DOC) system. In-use data in this study can be used to further evaluate the need for transient versus steady-state certification test cycles, support emission inventory development, and underscores the complexity of aftermarket control of NO_x using SCR.

7CT.10

Liquid Sheet Breakup and Droplet Evolution in Agricultural Sprays. IAROSLAV MAKHNENKO, Long Nguyen, Elizabeth Alonzi, Steven Fredericks, Christine Colby, Cari Dutcher, *University of Minnesota*

Spraying is a common process in everyday life with applications in agriculture, drug administration, printing, and painting. For agriculture purposes, small droplets are needed to enhance coverage of agricultural sprays, but not so small that they cause drift of the sprayed pesticides. Spray drift can cause the deposition of chemicals to undesired areas with a negative impact on livestock, ecosystems, and human health. In this work, different factors influencing spray breakup and droplet size distributions are discussed. Herein we experimentally measure the droplet size distribution of sprays from agricultural spray nozzles. The sprays were both homogeneous as well as emulsion containing, and the dynamic surface and interfacial tensions were varied to identify their influence on spray volume fraction below 150 µm, which is correlated with the spray drift risk, and on the volume median diameter, which is correlated with the spray deposition. The results of this work will help to understand the factors affecting a droplet size during a spraying process, towards increased efficacy of spraying pesticides.

7CT.11

Measurement of Aerosolized HMWO Nanoparticles and Its Application in Liquid Filter Retention Efficiency Characterization. SIQIN HE, Derek Oberreit, Gary Van Schooneveld, *Kanomax FMT, Inc.*

High molecular weight organics (HMWOs) and their presence as a particle or particle precursor in ultra-clean environments, such as ultrapure water (UPW) systems, have been a rising concern in critical particle contamination control processes, whereas there is limited understanding about how these materials lead to nanoparticles found in processes using UPW. It is therefore of great worth and significance to investigate particle size distributions (PSDs) of specific HMWOs and how these PSDs change due to environmental factors, such as temperature and pH values. Meanwhile, it is also as important to know how efficient the liquid filters will be in removing these particles from ultra-clean environments as well as their performance in loading capacity.

In this work, HMWO solutions were prepared at various concentration and property conditions, and a Liquid Nanoparticle Sizer (LNS) system (Kanomax 9310) was used to aerosolize the solutions and characterize the formed nanoparticles for their particle size distributions (PSDs). PSD results were summarized to exhibit the effects of concentration, temperature, and pH on HMWO nanoparticle formations. The same solutions were also used to challenge a few liquid filter units, with the LNS system installed inline to monitor the upstream and downstream particle size distributions and their respective changing trends. The results were used to demonstrate a continuous and online apparatus to evaluate the performance and health of liquid filters.

7HA.2

Influence of Extreme Air Pollution Episodes on the Oxidative Potential of Ambient Particulate Matter in Delhi, India. JOSEPH V PUTHUSSERY, Ashutosh Shukla, Jay Dave, Sreenivas Gaddamidi, Atinderpal Singh, Dilip Ganguly, Neeraj Rastogi, Sachchida N. Tripathi, Vishal Verma, *University of Illinois Urbana-Champaign*

The oxidative potential (OP) of ambient particulate matter (PM) is a health metric used to estimate PM toxicity. In this study, we measured the real-time OP of ambient fine PM (or $PM_{2.5}$) in Delhi, India. $PM_{2.5}$ mass concentrations in Delhi peak during the months of October - January, because of various extreme air pollution episodes (such as biomass burning, Diwali fireworks, and the winter haze events), occurring during that period. Here, we investigated the effect of these pollution episodes on the $PM_{2.5}$ OP and identified the emission sources contributing to $PM_{2.5}$ OP. We measured the hourly averaged real-time OP of ambient $PM_{2.5}$ based on a dithiothreitol assay using a custom-built automated OP measurement instrument which was designed in our lab. The chemical composition of $PM_{2.5}$ was also measured using various collocated online instruments such as a high-resolution time-of-flight aerosol mass spectrometer, aethalometer, and Xact®625i. We sampled ambient $PM_{2.5}$ at Delhi intermittently from October 11, 2019, to January 8, 2020 (~50 days).

Both $PM_{2.5}$ mass concentration and OP_v peaked during the winter/haze period [327 (±163) μg/m^3, 5.3 (±4) nmol/min/m^3, respectively]. However, the mass normalized OP was highest (43±30 pmol/min/μg) during Diwali. Positive matrix factorization analysis results showed that sulfate-rich aerosols and biomass burning aerosols together contributed to more than 50% of the total OP_v during the fall period, followed by dust (19%). However, fireworks became a significant source during Diwali, driving more than 20% of OP_v. Biomass burning (~40%) and sulfate-rich aerosols (~40%) dominated the OP_v during the winter/haze period. These findings reveal substantial temporal heterogeneity in the redox properties of PM and highlight the importance of determining the PM chemical composition along with its mass concentrations for predicting the overall health impacts associated with aerosol exposure.

7HA.3

Spray Aerosol Emissions from Harmful Cyanobacterial Blooms in the Chowan River, NC. HALEY E. PLAAS, Karsten Baumann, Ryan Paerl, Kimberly Popendorf, Colleen Karl, Jill Paxson, Naomi Chang, Joel Sanchez, Huang Hwa, Malcolm A. Barnard, Daniela Maizel, Hans W. Paerl, *University of North Carolina at Chapel Hill*

In addition to obvious negative effects on water quality, recent findings suggest that harmful cyanobacterial blooms (CHABs) impact air quality via primary spray aerosol emissions carrying cyanobacterial cells and cyanotoxins. The objective of our study was to quantify CHAB toxins and examine CHAB DNA sequence diversity in the airshed of the Chowan River, a eutrophic estuary in coastal North Carolina facing recurrent CHABs. Our field campaign (Summers 2020—2021) was the first to evaluate inhalation as a potential exposure pathway to cyanotoxins in NC. From June—October 2020, several two-week integrated, daytime (diel (24h) cycle) $PM_{2.5}$ samples were collected using medium-volume samplers. Offline analytical methods were applied to examine DNA and toxins in water and aerosol samples. Physicochemical water parameters, ambient $PM_{2.5}$ mass concentration, and meteorological conditions were also recorded down to 1 minute resolution. In 2020, CHAB genera dominated algal biomass, but maximum toxin concentrations and toxin-encoding genes (mcyA) in water samples were low (<<1 µg/L), yielding aerosol concentrations below the limits of quantification. However, two cyanotoxin congeners demonstrated to be enriched in aerosol, MC-LA (microcystin leucine-alanine) and MC-LR (leucine-arginine), were quantified in water samples. Airborne CHAB populations are still being evaluated based on DNA sequencing. Summer 2021, we refined our aerosol collection approaches to better characterize the physicochemical properties of airborne CHAB toxins. Due to the ecological properties of cyanobacteria, and their toxins primarily detected intracellularly, we hypothesized that toxins are aerosolized within intact cells and concentrated in the coarse mode. Using high-volume samplers, we simultaneously collected $PM_{2.5}$ and PM_{10}, and performed the same offline toxin analyses. We also used a Biospot 300-P Bioaerosol Sampler to evaluate the viability of CHAB cells in aerosol. Biospot aliquots were cultured as mixed assemblages for later DNA-based identification.

7HA.4

Assessment of PM Exposures during Commute in Megacity of Karachi, Pakistan. HAIDER KHWAJA, Kamran Khan, Sumayya Saied, Azhar Siddique, Saiyada Masood, *University at Albany*

Karachi is the largest city of Pakistan, with a population of more than 20 million. The rapid and continuing increase in the population, urbanization, automobiles, and industries combined with climate change and geogenic conditions have resulted in severe ambient air pollution problems in Karachi with serious health impacts. No systematic measurements of air pollution in urban cities of Pakistan have been done until now. To assess the extent of personal exposure and quantification of the particulate matter (PM) concentration, we conducted the first mobile PM monitoring campaign in Karachi. A portable laser-operated aerosol mass analyzer AEROCET 531 was used to record geo-located size-segregated PM mass (TSP, PM10, PM7, PM2.5, and PM1) concentrations. Seven in-vehicle tracks in different commercial regions of Karachi were studied. All routes are characterized by heavy traffic volumes with a variety of vehicles running with different type of fuels. Maps of routes were generated by using ArcGIS 10.1® software and IDW tool was used to generate the spatial interpolations of the PM. Mean concentrations across the seven tracks were: TSP (685.3 µg/m3), PM10 (527.1 µg/m3), PM7 (385.5 µg/m3), PM2.5 (51.9 µg/m3) and PM1 (8.7 µg/m3). PM concentrations showed strong spatial variability along each track. High volume of traffic, industries, construction work, and re-suspension of particles all collectively gives rise to high PM concentrations and posing the threatening effect to micro- environment and human health.

7HA.6

Real-Time Measurement and Source Apportionment of Five Different Endpoints of the Oxidative Potential of Ambient Particulate Matter at an Urban Site.

JOSEPH V PUTHUSSERY, Haoran Yu, Yixiang Wang, Ian Cornejo, Vishal Verma, *University of Illinois Urbana-Champaign*

The oxidative potential (OP) of ambient particulate matter (PM) has recently gained wide acceptance as an alternate metric for estimating the toxicity of ambient PM. Various studies have reported the OP based on different cellular and acellular assays. However, these studies have been limited to the OP measured on the integrated filter samples collected offline, which usually have poor time resolution. Moreover, different assays capture different combinations of the redox-active PM components, and there is currently no consensus on a standardized OP measurement protocol, which can provide a comprehensive picture of the total PM OP.

In this study, we developed a real-time multi-endpoint online system for measuring the OP of ambient PM based on five different acellular endpoints: oxidation of dithiothreitol (DTT) and ·OH generation in DTT assay; glutathione (GSH) consumption, ascorbic acid (AA) consumption, and ·OH generation in surrogate lung fluid (SLF, mixture of GSH, AA, uric acid and citric acid). We coupled an analytical automated instrument with a mist chamber particle collector and deployed it at a roadside site in Champaign, Illinois for ~2 months. We determined the diurnal trends in the ambient PM OP with a 3-hour time resolution and investigated their association with various chemical species in PM. We found a strong correlation (r >0.8) between ·OH generation rate and the concentration of water-soluble Fe. Additionally, the water-soluble organic carbon was strongly correlated with the DTT consumption rate. We are currently combining the OP data with the PM chemical composition to perform source apportionment analysis. The highly time-resolved OP data obtained from this study would provide a better mechanistic understanding of the redox activity of PM and provide new insights into the best combination of OP endpoints that most comprehensively represent the different aspects of the oxidative properties of ambient PM

7HA.7

Aerosol transmission of Respiratory Viral Diseases.

DISHA TRIVEDI, *MVS Pharma*

Viral infections of the upper and lower respiratory tracts are among the most common illnesses in humans. Humans have witnessed severe viral pandemic like Spanish influenza, H1N1, SARS-CoV, MERS-CoV and most recent and most severe SARS-CoV-2. Understanding of the modes of respiratory viral diseases transmission is of extreme importance for policy making for prevention and treatment of diseases. Airborne transmission via aerosols allows some of these viruses to spread efficiently among humans, causing outbreaks that are hard to control. Published evidence shows that aerosol transmission of viruses like influenza and corona virus can be an important mode of transmission, which has obvious implications for pandemic planning. We here summarise an overview of the available data from experimental and observational studies on the aerosol transmission of respiratory viruses between humans. This type of studies provides information about aerosol transmission based on which new treatment opportunities can be developed.

7HA.8

Sampling Masks for Source-Receptor Determination. DAVID ALBURTY, Ryan Pletka, Shula Jaron, Brian Patch, *InnovaPrep LLC*

This study describes the development and testing of surface and aerosol sampling methods for SARS-CoV-2 and Influenza using a duplex qPCR assay. Surface swabs were used tandem with a novel wearable sampling mask design that features separable added electret sampling filters on both the inside and outside of the mask. A total of 20 surface swabs were collected aboard commercial aircraft, and 38 sampling masks were collected from wearers in homes and commercial aircraft in October, November, and December 2020. Mask filter analysis indicated positive SARS-CoV results for some subjects whose clinical testing results were positive that wore masks for as little as ten minutes. In some cases, testing at a second time point appeared to correlate to the time progression of the illness. In some cases, those who tested clinically positive did not indicate positive results from the mask. Surface swabs taken aboard aircraft were negative or inconclusive. Influenza analysis results were all negative. The mask method shows promise for the identification of those who could potentially be aerosol “super-spreaders” if not wearing masks.

7HA.9

Assessing Residential Bioaerosol and Black Carbon-Related Air Contaminants in the Context of the COVID-19 Shutdown. YAO ADDOR, Reshmi Indugula, Darrel Baumgardner, Tiina Reponen, *University of Cincinnati*

Overview: Bioaerosols (BA) and black carbon (BC) are associated with adverse respiratory and cardiovascular health effects. The built environment is of focus as people spend about 90% of their time indoors. The COVID-19 pandemic restrictions could impact indoor air quality due to an increase in human activities within this environment. In contrast, reduced traffic and industrial activities outdoors could lead to reduced outdoor air pollution.

Objective: We assessed indoor and outdoor BA and BC at a residential site during the COVID-19 shutdown period from July through September, 2020, to compare their characteristics and trends.

Methods: Two cutting-edge, direct-reading instruments, the fluorescence-based Wideband Integrated Bioaerosol Sensor (WIBS-5/NEO) and the light scattering and absorption-based Photoacoustic Extinctiometer (PAX), were used to monitor BA and BC levels, respectively. Air monitoring was conducted indoors and outdoors at a residential site. We analyzed hourly and daily trends to compare the indoor and outdoor BA and BC levels. Also, historical air pollutant data were acquired from air quality network databases for six nearby monitoring stations, to compare 2020 to prior years data.

Results: Preliminary data analysis suggests: 1) Average levels of outdoor NO_2, $PM_{2.5}$, SO_2, pollen and mold in 2020 were lower than the prior 3-year averages in most monitoring stations; 2) BA levels were higher indoors than outdoors while BC levels were higher outdoors; 3) Type A fluorescent particles (mostly bacteria) were dominant indoors, whereas type B (mostly fungi and pollen) dominated outdoors; and 4) Most fluorescent particles sized on average 2 µm indoors and 3 µm outdoors.

Significance: This study is significant in understanding the air quality during the COVID-19 shutdown. Our findings will serve as a reference for further aerosol and air quality studies.

7HA.10

When Aerosol Science Meets the Respiratory Tract: An Update for Inhaled Particle Modeling. ROBERT PHALEN, Mark Hoover, Roger McClellan, *University of California Irvine*

Inhaled aerosol particle deposition models are important for designing inhaled medications, estimating risks from air pollutants, and understanding respiratory tract biology and diseases. Following the seminal publication of W. Findeisen that applied four deposition mechanisms to smooth solid spherical particles passing through a simplified airway structure, a large number of improved inhaled aerosol deposition models have emerged. Improvements, driven by practical needs, involved introducing more-complex aerosols, new deposition mechanisms, more-complete and detailed airway models, and new exposure scenarios. Although the new models have improved medical treatments, risk assessments, and our basic understanding of the respiratory tract, additional improvements are needed.

Advances in aerosol physics have allowed for adding many particle types to models, including fibers, agglomerates, nano-sized, charged, volatile and semi-volatile, liquid, high- and low density, and biological. Also, environmental scenarios, such as altered gravitational and magnetic forces, temperature and humidity extremes, and highly-concentrated aerosol systems are becoming better understood.

Anatomy and physiology data are essential inputs to inhalation models. These change according to age, gender, ethnicity, disease state, species, exertion level, aerosol exposure history and environmental conditions, to name a few. These factors are being added to the deposition models as data become available, but what is unknown exceeds what is known. This hampers applying aerosol deposition calculations to individuals and new exposure scenarios.

A recent multi-disciplinary international conference in Irvine, CA produced research-related recommendations for improving inhaled aerosol deposition modeling. These recommendations included improvements in the aerosol science, anatomy, physiology, and other aspects of the models as well as the need for new collaborations, focusing on health-related applications, establishing data repositories, and attracting new talent to the field.

7IM.1

Condensation Particle Counting in Micro-gravity: Measurements Aboard the International Space Station. Gregory Lewis, Nathan Kreisberg, Steven Spielman, SUSANNE HERING, Marit Meyer, *Aerosol Dynamics Inc.*

Long-term monitoring of ultrafine particle concentrations aboard spacecraft is a challenge. The instrument must be capable of measuring low concentrations of the order of 1 - 10 particles per cubic centimeter that characterize background levels in the filtered cabin air, as well as concentrations approaching 100,000 arising from sources. This concentration range is most easily spanned through condensation particle counters (CPCs). However, the liquid reservoirs required for long-term CPC operation are incompatible with the micro-gravity environment of space craft. Nor are the organic vapor emissions from alcohol-based CPCs allowed.

Presented here is a new, wick-sensor equipped, water-based condensation particle counter specifically designed for long-term use aboard the International Space Station. This NASA-MAGIC CPC uses the three-stage, “cold-warm-cold” architecture of the MAGIC® CPC wherein the walls are lined with a single wick. This wick serves as the water reservoir. Within the cold stages the wick captures water from the flow, and within the warm stage water evaporates from the wick to create the supersaturation needed for particle activation and growth. The wick transports water among these stages via capillary action. With correctly controlled operating temperatures, and with sufficient humidity in the sampled air stream, the net water consumption is zero. The NASA-MAGIC CPC incorporates a sensor to detect the wick moisture level, and this signal is used to regulate the operating temperatures to maintain a fully moistened wick while avoiding excess condensation. The instrument also has a priming mode that enables an initially dry wick to moisten itself from the humidity within a sampled air flow, a feature that allows the system to be launched with a dry wick.

NASA-MAGIC was launched in October 2020, and was deployed aboard the International Space Station in late November. Since that date, a period of 5 months at the time of this writing, NASA-MAGIC has returned a continuous stream of 1-s particle number concentration data.

7IM.3

Calibration of an Optical Sensor for Lunar Dust Measurements: Atmospheric and Vacuum Conditions.

ABHAY VIDWANS, Brad Jolliff, Jeffrey Gillis-Davis, Pratim Biswas, *Washington University in St Louis*

Lunar dust is a major obstacle to future lunar missions. Anticipated issues include visual obstruction, settling onto sensitive power and optical components, and inhalation hazards. To properly mitigate these issues on future missions, NASA has identified submicron dust characteristics as a key target for investigation [1]. Dust concentrations and size distributions near the lunar surface area remain poorly understood, despite several, primarily high-atmosphere, missions [2]. In addition, a spatiotemporal variation of dust characteristics is anticipated due to the highly transient plasma environment of the Moon, causing size and charge-dependent particle lofting and levitation [3]. Measurement of near-surface particles requires a precise, low-cost sensor, capable of measurements in both a vacuum and pressurized environment, to characterize dust in the natural lunar environment and in the pressurized environment where the inhalation hazard exists.

In this study, a low-cost optical sensor (Sharp GP2Y1010AU0F) is calibrated to measure aerosolized lunar simulant concentrations and size distributions at both atmospheric and vacuum pressures. In the first aim, the sensor is placed in two atmospheric-pressure chambers of different volumes filled with aerosolized lunar simulant (JSC-1A). A GRIMM particulate monitor is connected to each chamber to provide reference mass concentrations and size distributions. In the second aim, the sensor is calibrated in a cylindrical vacuum chamber, capable of reaching 10-6 Torr. A dust sample is aerosolized using intense pulses of a He-Ne laser. A SEM stub is placed underneath the sensor as the reference for total integrated particles counted and size distribution. Sensor output readings are correlated against the reference readings to assess the ability of the low-cost sensor to retrieve these critical lunar dust characteristics in-situ.

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7IM.4

Single-Particle Optical Trapping as a Standalone Micro-Reactor for the Study of Particle Loss, Formation, and Chemical Reaction.

CHUJI WANG, Yukai Ai, Haifa Alali, Yong-Le Pan, Gorden Videen, *Mississippi State University*

From the early optical-tweezers approach, which uses a single tightly focused laser beam to levitate dielectric or absorbing micron-sized particles, to the recently developed universal optical trap, which can trap particles of arbitrary chemical and physical properties in different media, optical trapping has evolved significantly over the last decades. One of the most recent developments in optical trapping is the combination of optical trapping with advanced laser spectroscopic techniques to achieve on-trap single-particle measurements. As single particles can be trapped stably in the universal optical trap for long periods of time, temporal evolution of the chemical and physical properties of trapped particles can be monitored. We study chemical reactions of a single particle under controlled atmospheric environments. In particular, we use the universal optical trap to trap single airborne particles, such as pollen grains, fungal spores, droplets, etc., in an air-tight cell and measure time-resolved Raman spectra of the single particles exposed to different relative humidity and ozone concentrations. Chemical reactions of the single particles are revealed by time-evolutions of the Raman spectral intensity and Raman band structure. Further, we propose to use cavity ringdown spectroscopy to track concentrations of reactants and or reaction products in situ, in near-real time. Results suggest that single-particle optical trapping can serve as a standalone micro-reactor for the study of loss, formation, and chemical reaction of single particles in their near-native states.

7IM.5

Realtime Digital Inline Holography for High Fidelity, in Situ and Non-intrusive Aerosol Measurements.

JIARONG HONG, Ruichen He, Rafael Placucci, Lei Feng, *University of Minnesota*

The analysis of particle concentration, size, and shape distribution is critical in many engineering applications and fundamental research, including spray coating, pollutant monitoring, cellular identification, and sorting, etc. Unlike conventional techniques, such as laser diffraction and phase Doppler analysis, the emerging digital inline holography (DIH) technique could provide imaging-based quantification of particle size and shape using a simple and inexpensive setup without knowledge of particle characteristics. Nevertheless, DIH is computationally expensive. In this presentation, we introduce a novel mobile DIH device for high-precision in situ non-intrusive characterizations of particles. Compared to conventional DIH, the proposed system leverages machine-learning, multi-threading programming, and embedded graphic processing units (GPUs) to achieve real-time hologram acquisition and processing. Here we present our recent works applying DIH techniques for aerosol measurements. Specifically, we will first demonstrate the application of DIH for measuring the respiratory droplets generated from normal breathing. The measurements reveal two distinct types of particles in the respiratory flow, i.e., round and faceted, with an average size of 1.7 µm and concentration varying significantly across different individuals. Particularly, the fraction of faceted particles changes from 26% to 40% across different participants and correlates with the peak of normalized exhaled flow rate. Moreover, the real-time DIH has also been used to quantify the aerosols generated from an ultrasonic scaling procedure used in dental operations and offers a robust assessment of the effectiveness of different preventive strategies (e.g., saliva ejector, high volume evacuator, and extraoral local extractor) on mitigating the spread of aerosols over a wide range of sizes. Additional applications including real-time indoor air monitoring will be presented. Overall, we show that real-time DIH can be widely employed in various aerosol diagnostics and environment monitoring involving particles over a broad range of size (from submicron to millimeter), morphology, and concentration.

7IM.6

Methods for Optical Trapping and Active Orientation Control of Airborne Microparticles.

JESSICA ARNOLD, Aimable Kalume, Gorden Videen, Chuji Wang, Yong-Le Pan, *U.S. Army Research Laboratory*

Manipulating microparticles through rotation has a wide range of applications including creating micro-motors, controlling the orientation of biological and chemical samples, and nanofabrication. Various methods have been invoked to trap and rotate particles suspended in liquid. However, when developing techniques for the detection and identification of aerosols, it is advantageous to directly study particles trapped in air. A limited number of studies on manipulating airborne particles have focused on periodic circular motion of trapped particles. In these cases, the observed rotational motion was a consequence of combined angular momentum and forces applied on the trapped particle, and the rotational periodicity is dependent on fixed properties including the particle shape, absorptivity, and laser beam configuration/power. Once the particle and trapping laser configuration are determined, the rotation frequency is fixed and cannot be controlled.

We present innovative methods for controlled rotation of optically trapped particles in air. We show examples of inducing circular or rotational motion by shaping the trapping beam with a liquid crystal on silicon spatial light modulator (SLM). Absorbing particles can be manipulated using the SLM to place a hollow ring onto the center of a Gaussian beam. The hollow beam is distorted into an elliptical shape and passed through a focusing lens. Once a particle is trapped at the focal point, the pattern is rotated which induces a circular, rotational motion in the particle. Another method is to create the hollow trapping beam before it reaches the SLM using two axicons. The SLM is then used to dim the intensity at two sets of diametric points (four total) which are then rotated. With both of these techniques the rotation rate of the trapped particle is externally controlled, and a given orientation of the trapped particle can held for data collection over the required length of time.

7IM.7

Optical-Trapping of Particles in Air Using Parabolic Reflectors and a Hollow Laser Beam: From Submicron to Supermicron Aerosol. AIMABLE KALUME, Jessica Arnold, Yong-Le Pan, *U.S. Army Research Laboratory*

We present an advanced optical-trapping method that is capable of trapping arbitrary shapes, any properties (transparent and absorbing) and sized from nanometer to super micron particles in air. Two parabolic reflectors were used to reflect the inner and outer parts of a single hollow laser beam, respectively, to form two counter-propagating conical beams and bring them into a focal point for trapping. This novel design demonstrated high trapping efficiency and strong trapping robustness with a simple optical configuration. Instead of using expensive microscope objectives, the parabolic reflectors not only achieved large numerical aperture (N.A.) focusing, but were also able to focus the beam far away from optical surfaces to minimize optics contamination. This design also offered a large free space for flexible integration with other measuring techniques, such as optical-trapping Raman spectroscopy, for on-line single-particle characterization.

7IM.8

Comparing Multiple Types of Machine Learning for Characterizing TEM Images of Soot. TIMOTHY SIPKENS, Hamed Nikookar, Max Frei, Frank Einar Kruis, Steven Rogak, *University of British Columbia*

TEM imaging is a mainstay in the characterization of aerosols, like soot. One of the largest barriers to population-wide statistics is the often-labor-intensive manual approach to image analysis. This work examines a series of machine learning approaches to distinguishing soot from the background in TEM images, including (1) unsupervised k-means clustering, (2) a convolutional neural network, and (3) trainable Weka segmentation, via the Fiji image analysis package. Classifications are compared to a largely-manual, in-house method where a user-specified threshold is applied in local regions of the image. Methods show a marked improvement over existing classifiers across a range of images, with over 99% classified pixel accuracy and only a small number of falsely identified aggregates. We also present sensitivities of a range of automated primary particle sizing techniques to the chosen classifier, which is a step towards fully automated analysis of soot TEM images. We conclude by examining the relationship between primary particle size and projected-area equivalent diameter of soot.

7IM.9

Effect of Particle Size on Measurement Uncertainty in Quantification of Chemical Components Using Infrared Absorption.

KABIR RISHI, Pramod Kulkarni, Bon Ki Ku, Chen Wang, Orthodoxia Zervaki, Elizabeth Ashley, *Centers for Disease Control and Prevention, NIOSH*

Infrared (IR) absorption measurement is commonly used for quantification of chemical components of aerosols. Quantification of analyte requires calibration using a standard reference material. Since light scattering, and hence absorption, depends on particle size, the calibration curve generated is specific to the reference material used. Standard methods, such as NIOSH method 7603 for crystalline silica quantification, recommend the use of NIST standard reference material, which have a polydisperse size distribution in the respirable size range. Measurement uncertainty can be significant if the unknown aerosol has a different size distribution compared to that of the calibration aerosol. Previous studies have probed the effect of particle size on analyte quantification in infrared absorption measurements (Bhaskar et al., 1994; Udvardi et al., 2017; Yabuta and Ohta, 2003; Chen et al, 2013); however, they lacked adequate size-resolved measurements over an extended particle size range. The objective of this study was to probe the particle-size induced artifacts in infrared absorption measurements and determine resulting uncertainty in analyte quantification. Aerosol particles of crystalline silica, polymers, and metallic powders were size classified using a cascade impactor in the size range 0.045 µm to 9 µm. Each size selected fraction was extracted into an aqueous suspension and was redeposited on a PVC filter for infrared absorption measurement. For particle sizes ranging from 0.4 µm to 9 µm, an 8-stage Andersen impactor operated at a flow rate of 28.3 L/min was used. To extend the collection to the sub-micron size range, where the particulate mass was << 1 µg, a 6-stage quartz crystal microbalance (QCM) impactor with cut sizes ranging from 0.045 µm to 0.96 µm was used. The measured absorption, at characteristic vibrational frequency, was normalized by the total particulate mass probed by the infrared beam to allow comparison across samples with different particle size distribution. Mass normalized absorption for IR as a function of aerodynamic particle size showed an increasing trend below 1 µm and a decreasing trend above 1 µm, with another broad peak at about 5 µm diameter. Calculations were performed to obtain infrared absorption spectrum using single and multiparticle Lorentz-Mie light scattering theory. Comparison of experimental and theoretical absorption spectra and implications for method calibration and overall measurement uncertainty will be presented and discussed.

7IM.10

Design and Characterization of Triple-Tube, Laminar-Flow Condensation Nano Spot-Collector: Application to Microscopy and Spectroscopic Analysis of Aerosols.

ORTHODOXIA ZERVAKI, Braden Stump, Patricia Keady, Pramod Kulkarni, Dionysios D. Dionysiou, *HELD-NIOSH*

We describe performance evaluation of an aerosol nano spot-collector designed for direct electron or optical microscopy, and laser spectroscopic analysis of nanoparticles and aerosols in the size range 5 nm to 5 µm. The instrument uses water-based laminar-flow condensational growth of particles, followed by gentle impaction for dry spot sample collection directly onto an electron microscopy stub or grid. The spot sample collector was designed for a small logistical footprint while maintaining a high flow rate required to achieve good sampling statistics for microscopy analysis. It uses three parallel laminar flow growth tubes, each with a sample flow rate of 0.4 L/min, providing a total sample flow rate of 1.2 L/min. The laminar flows merge into one flow and exit through a converging nozzle to allow impaction collection on a substrate. The aerosol stream passes through a three-temperature stage growth tube to achieve the desired water vapor supersaturation profile and exit dew point. Experiments were conducted to determine the size-dependent collection efficiency, particle wall losses, uniformity of spot deposit, surface density distribution for particles, and aerosol concentration effects of the three-tube nano spot-collector. Particles as small as 5 nm could be activated as seed condensation nuclei and grow up to 3 µm droplets. During dry collection, the droplets impact onto the warm surface of a SEM stub or a TEM grid forming a spot deposit of approximately 1-mm diameter. The resulting spot particle samples were analyzed using electron microscopy, infrared, and Raman chemical imaging to quantify the size distribution of aerosol and the analyte concentration. Spot samples were analyzed to probe the preservation of the particle size distribution of sampled aerosol.

Keywords: Aerosol nano spot-collector; nanoparticles, condensation growth; supersaturation; aerosol microscopic analysis

7IM.11

Open-Hardware Design and Characterization of an Electrostatic Aerosol Precipitator. SABIN KASPAROGLU, Timothy Wright, Markus Petters, *North Carolina State University*

Electrostatic precipitators (EPs) are devices that remove charged particles from an air stream. In EPs, charged particles are passed between two electrodes that create an electrostatic field. Charged particles are deflected toward or away from the electrode. Some fraction of those particles will be removed from the stream. In this study, we present the design and characterization of an EP. The assembly of the device is simple enough that non-engineering graduate students can build the device from scratch. All components can be directly purchased from vendors, and the device can be assembled with standard tools. Generic components are used to allow the repurposing of parts for other uses. The computer-controlled high-voltage power supply box associated with the project can be used for other common high-voltage applications in Aerosol Science and Technology, including serving as data acquisition and control system for scanning mobility particle sizers. Computational fluid dynamics simulations are used to quantify the 3D flow field through the device. The transfer function describing the transmission efficiency as a function of electrical mobility is characterized through modeling and experiments. Observed deviations of the transfer function from the theoretical prediction are attributed to distortions of the flow near the inlet and outlet of the instrument. Singly charged particles up to 624 nm and 253 nm can be completely removed at a flow rate of 0.5 L min^{-1} and 1 L min^{-1}, respectively. We provide several options to further reduce the cost which we believe would significantly increase the accessibility of the technique to a broader audience.

7IM.12

Development of Aerosol into Liquid Sampler for Collecting Nanoparticles by Combining Particle Size Magnifier and Wet Cyclone. SOICHIRO KATO, Yayoi Inomata, Takafumi Seto, *Kanazawa University*

It is well known that exposure of ambient particles causes the adverse health effects. To analyze health impact of aerosol, in vitro studies have been conducted by submerging particle-liquid suspension against cell culture. Conventionally, such suspension has been prepared by extracting the particles collected on the filter surface into solvents by mechanical dispersion and sonication. However, it is difficult to quantify exact amount of particles in the liquid because a part of solid particles remain on the filter surface by van der Waals force. In this study, a high flow rate aerosol wet sampler, that can collect airborne particles directly into liquid, was developed by combining the Particle Size Magnifier (PSM) and wet cyclone. The water-based PSM was developed to enhance particle size by condensational growth of water vapor. The micron-sized droplets that contain aerosol particles can be collected by centrifugal force generated by a swirling flow in the cyclone. We have designed two types (cut-off diameter) of cyclones with flow rate of 80 L min-1. The collection efficiency of ambient particles from <0.1 to 10 µm is evaluated with changing operation parameters of the PSM and cyclone.

7UA.1

Intra-city Factors Obtained from Dispersion-normalized Multi-time Resolution Factor Analyses of PM2.5 in an Urban Environment.

Uwayemi Sofowote, Robert Healy, Yushan Su, Jerzy Debosz, Michael Noble, Anthony Munoz, Cheol H. Jeong, Jonathan Wang, Nathan Hilker, Greg J. Evans, Jeff Brook, Gang Lu, PHILIP K. HOPKE, *University of Rochester*

Ambient fine particulate matter data of continuously monitored species at two air monitoring sites within Toronto were used to gauge the intra-city variations in PM composition over a two-year period. One location was beside a major highway while the other was an urban background location. In this work, we specially pretreated the concentrations of the measured species (dispersion-normalization) to reduce the influence of local meteorology before applying multi-time resolution factor analysis to identify and quantify source contributions. Factors found were pSO4, pNO3, secondary organic aerosols (SOA), and crustal matter (CrM) that were common to both sites, a hydrocarbon-like organic matter (HOM) exclusive to the urban background site, three black carbon related factors (BC, BC-HOM at the highway site, and a brown carbon rich factor (BC-BrC) at the urban background site), biomass burning organic matter (BBOM) and brake dust (BD) at the highway site. This talk will discuss the dispersion-normalization and present the differences in PM2.5 composition for the regional and local factors between these two locations that were only 10 km apart. Site-specific factors are of greater interest for control policy design. Thus, regressions with potential explanatory, site-specific variables were performed for results from the highway site. Three regression model approaches were explored (MLR, GRG regression, and the generalized additive model GAM). GAM gave the largest R2 for the locally-sourced factors. Heavy duty vehicles were most important for explaining the black carbon (BC and BC-HOM) factors. Light-duty vehicles were dominant for BD. Auxiliary modelling for the local factors showed that the traffic-related factors likely originated along the main roadways at their sites while the more regional factors, - pSO4, pNO3, SOA, - had sources that were both regional and local. These results will be useful in understanding ambient particulate matter sources on a city scale.

7UA.2

Dynamics, Composition and Origin of Submicron Atmospheric Aerosol Measured at Suburban and Traffic Site in Prague, Czech Republic.

PETRA POKORNá, Nadežda Zíková, Petr Vodicka, Jakub Ondráček, Jaroslav Schwarz, Philip K. Hopke, *ICPF CAS, Prague, Czech Republic*

To improve the air quality in urban areas, the underlying causalities need to be well understood, particularly when it comes to aspects such as PM concentrations and sources. The aim of this work was to determine submicron aerosol dynamics, chemical compositions, and origins at two urban sites in the Czech Republic capital.

A parallel measurement campaign was conducted in June-December 2020 at a suburban and a traffic site in Prague. Number size distributions in the range 15.1 – 593.5 nm at the suburban and 14.6 – 495.8 nm at the traffic site were measured every 5-min using an SMPS (TSI). 2-h PM_1 elemental and organic carbon concentrations with a field semi-online OCEC analyser (Sunset Laboratory Inc.) as well as 1-h PM_{10} by a Beta gauge (MP101M, Environnement SA) along with gasses and meteorology were recorded. Also, 24-h/12-h PM_1 samples (suburban/traffic) by a Leckel (LVS-3, Sven Leckel Ingenieurbüro) for a subsequent chemical analysis (water-soluble ions and sugars) were collected. The monthly medians of SMPS total number and mass concentrations were tested by Dunn's test [1].

During the six-month campaign, no 24-h PM_{10} EU limit exceedance (50 µg/m3, 35x in the year) occurred. The monthly PM_{10} median at suburban and traffic sites ranged between 11 – 19.5 µg/m3 and 14 – 24 µg/m3 (June/November), respectively. For most months and both number and mass median concentrations based on the SMPS data at both stations differed. Further, more complex data analysis is needed to fully assess the submicron aerosol concentrations, compositions, and origins at the Prague stations.

Project LTAUSA19006 of the Ministry of Education, Youth and Sports of the Czech Republic is acknowledged for financial support.

[1] Dunn, O. J., Multiple comparisons using rank sums. Technometrics, 6, 241–252, 1964.

7UA.3

State of Gaseous Air Pollutants and Resulting Health Effects in a Developing Country of Southeast Asia (Karachi, Pakistan). OMOSEHIN MOYEBI, Fatim Sannoh, Zafar Fatmi, David Carpenter, Azhar Siddique, Kamran Khan, Jahan Zeb, Mirza M. Hussain, Haider Khwaja, *University at Albany, Albany, New York*

Karachi is a megacity with severe air pollution problems. There are high emissions of air pollutants from vehicular traffic, industrial activities, and biomass burning in Karachi. The numerous emission sources and rapid growth in population makes Karachi a priority site for air pollution research. The objectives of this study are to i) investigate the levels of gaseous air pollutants in Karachi ii) determine temporal and seasonal variation in levels of various air pollutants, and iii) perform a health impact assessment. Daily samples of gaseous pollutants were collected for six consecutive weeks in each of the four seasons for a year at the Tibet Center. Samples were analyzed for pollutants by ion chromatography. Maximum daily concentrations of NO_2 (28.1 ppbv), NO (90 ppbv), O_3 (57.8 ppbv), and SO_2 (331 ppbv) were recorded in fall, while the highest concentration of HNO_3 (9129 pptv) was recorded in spring. Seasonal average concentrations were high in winter for NO_2 (4.84 ± 3.35 ppbv), NO (9.47 ± 7.82 ppbv), and O_3 (8.92 ± 7.65 ppbv), while HNO_3 (629 ± 1316 pptv) and SO_2 (20.2 ± 39.4 ppbv) were high in spring and fall, respectively. This reflected the influence of seasonal environmental characteristics such as photochemical activities, meteorological conditions, and source and sink strength. The observed SO_2 seasonal average in fall was 5 times higher than the summertime. Health impact assessment estimated an increase of 1200 and 569 deaths due to short-term exposure to SO_2 in fall and spring, respectively. Chronic daily intake estimated risk per 1000 were 0.99, 0.47, 0.45, and 0.26 for SO_2 in fall, NO and O_3 in winter, and NO_2 in spring. This study confirmed the effect of poor urban air quality on human health and demonstrated the influence of photochemical activity on the formation of secondary pollutants.

7UA.4

Modeling Air Quality in Los Angeles During the COVID-19 Pandemic Using CMAQ: Organic Aerosol Chemistry, Speciation, and Source Apportionment. ELYSE PENNINGTON, Yuan Wang, Karl Seltzer, Jiani Yang, Benjamin Schulze, Meemong Lee, Havala Pye, Benjamin Murphy, Christopher Kenseth, Benjamin Moul, Lelia Hawkins, Harrison Parker, John Crounse, Paul Wennberg, John Seinfeld, *California Institute of Technology*

The COVID-19 pandemic had large impacts on human behavior and air quality in urban areas around the world. Modeling these changes on a regional scale has been difficult due to the complex nature of pandemic-induced variations in emissions, meteorology, and multi-phase atmospheric chemistry. Here we utilize the Community Multiscale Air Quality (CMAQ) model version 5.3.2 with new chemical mechanism updates to understand air quality in the Los Angeles Basin during March-June, 2020. We use a random forest regression model to incorporate real-time traffic data into an existing emissions model, yielding accurate mobile source emissions that are specific to our simulation period. Volatile chemical product (VCP) emissions are provided by the VCPy framework, and sensitivity simulations are performed to understand the effect of local shutdowns on VCP emissions and the resultant air quality. The chemical mechanism of CMAQ was updated to include secondary organic aerosol (SOA) formation from VCPs and mobile source intermediate volatility organic compounds (IVOCs). Model predictions of $PM_{2.5}$, ozone, and speciated SOA are compared to concurrent measurements made in Pasadena, Claremont, and routine monitoring stations throughout the Los Angeles Basin. The impacts of meteorology (e.g. temperature and precipitation) on elevated ozone and reduced particulate matter (PM) concentrations are investigated using sensitivity experiments in the Weather Research and Forecasting (WRF) model. We aim to understand the primary emissions sources and atmospheric oxidation pathways of organic aerosol (OA) by investigating the individual components of SOA and use 1x1 km resolution to explore fine-scale spatial variations. Understanding the impact of COVID-19 on human behavior and the subsequent changes in air quality provides an unparalleled opportunity to predict the impact of future policy changes on air quality and human health.

7UA.5

Factors Influencing Ambient Particulate Matter in Delhi, India: Insights from a Machine Learning Model.

KANAN PATEL, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Concentrations of ambient particulate matter (PM) depend on various factors including primary sources, meteorology, and chemical transformations. The concentrations/composition, sources and dynamics of PM can be estimated by combining ambient field measurements with machine learning and statistical analysis tools. New Delhi, India is the most polluted megacity in the world and routinely experiences extreme pollution episodes. As part of the Delhi Aerosol Supersite Study, we measured online continuous PM_1 (Particulate matter of size less than 1µm) concentrations and composition using an Aerosol Chemical Speciation Monitor (ACSM) for 4+ years, starting January 2017. PM_1 is typically composed of organics as well as inorganics such as chloride, ammonium, sulfate, and nitrate ion species. To understand the factors that influence PM_1 variability, we built a machine learning model using random forest regression that estimates PM_1 species concentrations by using ambient temperature, relative humidity, planetary boundary layer height, wind speed, wind direction, precipitation, agricultural burning fire counts, and solar radiation. We used hour of day, day of week and month of year to account for emissions specific to certain times (e.g., emissions from traffic may be more important during vehicular rush hours). We demonstrate the applicability of this model to 1) capture temporal variability of the PM_1 species, 2) to understand the influence of individual factors/features via sensitivity analyses, which is otherwise difficult to interpret because of multicollinearity between the variables and 3) to predict the PM_1 concentrations during the COVID-19 lockdowns and use the differences between predicted and actual concentrations to quantify the role of activity restrictions during the COVID-19 lockdowns on air quality. Overall, our model provides novel insights into factors influencing ambient PM_1 in new Delhi, India, demonstrating the power of machine learning models in atmospheric science applications.

7UA.7

Hourly Measurements of Organic Aerosol Chemical Species (TAG-GC-MS) at a Receptor Site in Mexico City.

Y. MARGARITA MARTíNEZ-DOMíNGUEZ, Armando Retama-Hernández, Olivia Rivera-Hernández, Tania Müller-García, Omar Amador-Muñoz, *Atmospheric Science Center, UNAM*

The determination of specific compounds of the Organic Aerosol (OA) provides information on emission sources and secondary organic chemical species formation. In this work, the organic chemical composition analysis of the particles ≤2.5 µm (PM2.5) with hourly time resolution was carried out using a Thermal desorption Aerosol coupled to a Gas Chromatograph - Mass Spectrometer (TAG-GC-MS). The sampling campaign was carried out from November 5 to December 15, 2018 at southwest of Mexico City, considered as a receptor site. The analysis included 82 compounds grouped into: polycyclic aromatic hydrocarbons (PAH), oxy-PAH, n-alkanes, phthalates, and aldehydes. Its diurnal/nocturnal variations showed characteristic features that represent the corresponding activities of the emission sources. PAH were emitted from vehicular sources, except retene, a PAH originated from biomass burning observed throughout the season. Oxy-PAHs were emitted by mobile sources (benzanthrone) and formed overnight (anthraquinone). Phthalates were emitted by sources associated with plastic industrial activities, except for dicyclo-hexyl-phthalate, which apparently was originated from mobile sources. Aldehydes showed both primary origin and secondary formation, where n-alkanes <C23 apparently act as precursors of their formation via OH free radicals during the day. The origin of n-alkanes was both, petrogenic and biogenic. n-alkanes <C23 (petrogenic) were abundant during the day, while n-alkanes ≥C23 (mainly biogenic) were abundant during the night.

n-alkanes contributed with 71% on average of the total mass of all determined species, aldehydes contributed with 13%, phthalates with 10%, PAHs with 4% and oxy-PAHs with 2%. The total amount of all found species contributed only ~0.2% of the total PM2.5 mass, highlighting the particle complexity. PM2.5 mass concentration was quite constant between December and November; however, 2-3 times higher PAH and oxy-PAH levels were observed in December respect to November, which marks a differential in the toxicity of the particles. Acknowledgments: Financial support: Environmental Ministry (SEDEMA) of Mexico City Government, PAPIIT IN102519, UC MEXUS-CONACyT CN-1987.

7UA.8

On-Road Vehicle Emissions Now Account for a Minor Fraction of Organic Aerosol in Los Angeles. BENJAMIN SCHULZE, Christopher Kenseth, Elyse Pennington, Paul Van Rooy, Karl Seltzer, Afsara Tasnia, John Crounse, Barbara Barletta, Simone Meinardi, Donald Blake, Kelley Barsanti, Havala Pye, Paul Wennberg, John Seinfeld, *California Institute of Technology*

Regulatory policies aimed at controlling emissions from on-road vehicles have substantially reduced aerosol mass loadings in Los Angeles over the last seventy years. Despite continuing investments in vehicle emissions controls, however, the rate of decline in organic aerosol (OA) mass loadings has slowed in recent years. Although the increasing relevance of non-traditional sources of urban volatile organic compounds (VOCs) such as volatile chemical products (VCPs) has been advanced as a potential explanation for this observation, the relative importance of individual emission sources to the current urban OA budget remains unconstrained. Here, we compare high resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) measurements of aerosol mass loading and composition in Pasadena, CA from meteorologically similar periods in 2010 and 2020 to the results of a detailed 0-D box model of OA formation to gain insight into urban OA sources. Positive matrix factorization (PMF) is applied to the OA mass spectral dataset to distinguish mass loadings of urban and regional background OA. The model incorporates recently published inventories of OA precursor emissions in LA County in 2010 and 2020 as well as state-of-the-science parameterizations of emission volatility (e.g., I/SVOCs) and secondary OA (SOA) formation using a volatility basis set framework. Model results reproduce measured OA mass loadings within measurement uncertainty for both years, and suggest that on-road vehicle emissions in 2020 accounted for less than 20% of urban OA. No individual emission source is predicted to be responsible for a majority of ambient OA. Rather, VCPs, cooking-related sources, non-road combustion engines, and asphalt all contribute significantly to urban OA loadings. Simulations of future emission scenarios suggest that only minor reductions to the urban OA burden will occur over the next decade, and demonstrate that effectively reducing urban OA will require increased focus on emissions from non-road and area sources.

7UA.9

Direct Measurements of Secondary Organic Aerosol (SOA) Response to NOx and VOC Perturbations in the Ambient Atmosphere. SHENGLUN WU, Christopher Cappa, Qi Zhang, Benjamin Schulze, John Seinfeld, Michael Kleeman, *University of California, Davis*

Secondary organic aerosol (SOA) is the dominant component of organic aerosol that significantly impacts climate change and human health. Complex components and formation mechanisms make it difficult to predict SOA response to emissions perturbations. Volatile organic carbon (VOC) compounds are the major precursor for SOA, but complex interactions with oxides of nitrogen (NOx) can impact the SOA formation in different ways. Furthermore, O3 formation that depends on NOx/VOC will also affect SOA formation. Here we directly investigate the SOA formation in the ambient atmosphere under changing NOx/VOC conditions. The sensitivity of SOA to NOx and VOC perturbations was directly measured using a mobile trailer equipped with three identical Teflon smog chambers (each 1 m3) filled with ambient air. One chamber was used as the basecase measurement, one chamber had NOx added, and one chamber had a surrogate VOC added (ethylene, m-xylene, n-hexane). A High-resolution time-of-flight aerosol mass spectrometer and scanning mobility particle sizer was installed to measure the organic aerosol in the chambers. O3, NOx, temperature, and relative humidity were also measured. Two weeks of measurements in Sacramento in April 2020 shows that both NOx and VOC perturbation suppress the SOA formation relative to the basecase conditions. The perturbed SOA formation appears to respond to both oxidant levels and to the SOA formation potential of the parent VOCs. However, the O:C ratio has an inverse response to total SOA perturbation response, suggesting more complex chemical reactions are active. These results indicate that the NOx and VOC have a large impact on SOA formation and they provide insight into how SOA formation in the ambient atmosphere will change with current emission control strategies.

7UA.10

Secondary Organic Aerosol Formation in Regional Scales by Using Multiphase Reaction of Hydrocarbons.

ZECHEN YU, Myoseon Jang, Soontae Kim, Jiwon Choi, Azad Madhu, Sanghee Han, Jinsoo Park, *University of Florida*

Secondary organic aerosol (SOA) is one of the major components in ambient fine particulate matter. This SOA is formed through atmospheric oxidation of volatile organic compounds (VOCs) emitted from both anthropogenic and biogenic sources. To date, the prediction of SOA in regional and global scales is traditionally performed by using gas-particle partitioning models. SOA can also be formed by the heterogeneous reactions of semi-volatile organic compounds in aerosol phase. In particular, SOA formation increases via aqueous reactions in the presence of inorganic salted wet aerosols. However, the current air quality models have no features to process aqueous reactions of a variety of oxidized organic products from different hydrocarbons. Using the Unified Partitioning-Aerosol phase Reaction (UNIPAR) model, our research team recently launched the simulation of SOA formation by multiphase reaction of various hydrocarbons in the presence of inorganic aqueous salts under varying NO_x, SO_2, humidity, and temperature. In this work, the UNIPAR model is incorporated with the Comprehensive Air Quality Model with Extensions (CAMx) to predict the regional concentration of SOA under different urban atmospheres. The model parameters in UNIAPR are unified and optimized for various products originating from the oxidation of different precursors (i.e., aromatics, terpenes, and alkanes) and environmental conditions (i.e., NOx levels and aging). The CAMx-UNIPAR model simulates the air quality appeared during the Korean-United States Air Quality (KORUS-AQ) campaign between May and June in 2016. The predicted SOA is compared with field observations from ground sites and aircraft measurements in different meteorological conditions (dry to wet conditions for inorganic salts) to understand the significance of organic aqueous reactions. The contribution of biogenic emissions and automobile emissions on SOA formation is also evaluated by using CAMx-UNIPAR.

7UA.11

Investigating the Impact of Biomass Burning Aerosols on Urban Air Quality in Los Angeles.

MITCHELL ROGERS, Benjamin Schulze, Christopher Kenseth, John Crounse, Paul Wennberg, John Seinfeld, *California Institute of Technology*

The frequency and severity of wildfire events have escalated dramatically in recent years, particularly in the western United States. Despite the ubiquity and effects of wildfires, however, there is a limited understanding of how biomass burning aerosols impact urban air quality, particularly in regions with pervasive air pollution. Here, we characterize the influence of wildfire emissions on urban aerosol mass loadings and composition measured in Los Angeles, CA using a high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) during the 2020 Bobcat Fire. Positive matrix factorization (PMF) is employed to identify and apportion sources of airborne particulate matter typical of urban atmospheres (e.g. combustion and cooking) as well as those unique to biomass burning. Wildfire plume transport and aging is evaluated using HYbrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) backward air mass trajectories. Compared to typical levels in Los Angeles, non-refractory submicron organic aerosol concentrations increased by over a factor of 10 during periods impacted by smoke from the wildfire. Future work will reconcile results with past models of simulated aerosol formation and chamber measurements.

7UA.12

Improved Prediction of Near-Road Vehicle Emissions for Gasoline and Diesel Vehicles Between Emission Simulators and Measured Data 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 temperatures and dilution ratios that are 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 studies and current emission simulators could be due to MOVES, and other emission simulators, treating OA as non-volatile and not adjusting the PM based on the 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 is a continuation of data that was presented last year and uses published volatility basis set (VBS) data coupled with a newly developed model to improve the prediction of near-road PM2.5 from gasoline and diesel vehicles. Using the VBS approach, the gas-particle partitioning of OA from gasoline and diesel vehicles were modeled using Python to create a correction factor and empirical formula that can work with the outputted MOVES EF to correct for primary PM2.5 from vehicles. This correction factor helps to bridge the gap between regulatory model estimations and what is measured near-road. 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 sampling dilution & temperature (from the PEMS and dynamometers), ambient temperature & background PM, distance from the vehicle, and the vehicles EC/TC ratio, and shows that there is a bias in predicted roadside PM using the current transportation models.

8AC.1

Nitrate Photolysis in Mixed Sucrose-Nitrate-Sulfate Particles at Different Relative Humidities.

ZHANCONG LIANG, Ruifeng Zhang, Masao Gen, Yangxi Chu, Chak K. Chan, *City University of Hong Kong, China*

Atmospheric particles can be viscous. The limitation in diffusion impedes the mass transfer of oxidants from the gas phase to the particle phase and hinders multiphase oxidation processes. On the other hand, nitrate photolysis has been found to be effective in producing oxidants such as OH radicals within the particles. Whether nitrate photolysis can effectively proceed in viscous particles and how it may affect the physicochemical properties of the particle has not been much explored. In this study, we investigated particulate nitrate photolysis in mixed sucrose-nitrate-sulfate particles as surrogates of atmospheric viscous particles containing organic and inorganic components as a function of relative humidity (RH) and the molar fraction of sucrose to the total solute (F_{SU}) with an in-situ Micro-Raman system. Sucrose suppressed nitrate crystallization, and high photolysis rate constants ($\sim 10^{-5}$ s^{-1}) were found, irrespective of the RH. For F_{SU}=0.5 and 0.33 particles under irradiation at 30% RH, we observed morphological changes from droplets to the formation of inclusions and then likely "hollow" semi-solid particles, which did not show Raman signal at central locations but at the edges. Together with the phase states of inorganics indicated by the full width at half maxima (FWHM), images with bulged surfaces, and size increase of the particles in optical microscopic imaging, we inferred that the hindered diffusion of gaseous products (i.e., NOx, NOy) from nitrate photolysis is a likely reason for the morphological changes. Atmospheric implications of these results are also presented.

8AC.2

Photodegradation of Secondary Organic Aerosols, the Formation of a Photo-Recalcitrant Fraction and Its Effects on Mass, Composition, and Viscosity.

VAHE BABOOMIAN, Giuseppe Crescenzo, Yuanzhou Huang, Fabian Mahrt, Allan Bertram, Sergey Nizkorodov, *University of California, Irvine*

The photochemical aging of secondary organic aerosol (SOA) is important for changing their climate and human health-relevant properties. However, these photochemical processes are not well understood to date. One of these properties is viscosity, which is key to predicting lifetimes of particulate air pollutants and understanding their multiphase chemistry. Viscosity is also crucial to predicting the effects of particles on climate through cloud formation. We recently discovered that long-term photodegradation of SOA leads to the formation of a photo-recalcitrant fraction. Due to the unknown viscosity of this non-degrading fraction, considerable uncertainties exist regarding the impact of SOA on climate. To address this, we experimentally measured the humidity dependent viscosity and phase of the photo-recalcitrant fraction of biogenically derived SOA. Our high-resolution mass spectrometry results indicate that the average elemental oxygen-to carbon ratio and molecular weight of the photo-recalcitrant fraction increased by 15% and 10%, respectively, compared to the fresh particles. At the same time, photodegraded particles showed significantly increased viscosity and particle mixing times by as much as 5 orders of magnitude, compared to the fresh particles. The experimentally determined viscosities overlap well with those predicted by parameterizations based on the composition of the recalcitrant fraction, as determined by mass spectrometry. The global distributions of the aerosol mixing time and viscosity were calculated, and the results suggest that glassy aerosols formed at ~ 5 km in altitude for photodegraded particles, compared to ~ 10 km for fresh ones.

8AC.3

Evolution of the Molecular Composition and Physicochemical Properties of Sea Spray Aerosol in the Presence of OH Radicals. SAMANTHA KRUSE, Paul Tumminello, Allison Kawasaki, Kathryn Mayer, Jon Sauer, Christopher Cappa, Timothy Bertram, Vicki Grassian, Kimberly Prather, Jonathan Slade, *University of California, San Diego*

Sea spray aerosol (SSA) is the largest contributor by mass of aerosols to the atmosphere annually, with an average yearly flux of 6.8 billion metric tons. SSA particles can act as cloud condensation nuclei and ice nuclei, thereby affecting the hydrological cycle. However, this is heavily dependent on their composition and hygroscopicity, which may change due to atmospheric oxidation processes. In this work, we report on the molecular-level composition and transformations of nascent SSA (nSSA) in the presence of OH radicals and marine-derived gases generated from a phytoplankton bloom in a laboratory mesocosm with controlled wave breaking. We utilize an extractive electrospray ionization high-resolution time-of-flight mass spectrometer to study the evolving molecular composition of the extractable components of nSSA. This method enables real-time analysis of aerosol molecular composition by soft ionization with no detectable interference from inorganic salts. Our results compare well to more established ESI mass spectrometry of nSSA collected onto filters. Our analysis shows an apparent correlation between the average molar mass of the organic components in nSSA with biological activity in the water, while the average O:C ratio does not change as significantly with age of the bloom. With increasing OH exposure in the presence of marine-derived gases, the average molar mass of nSSA first increases at low levels of oxidation due to functionalization, then decreases significantly due to molecular fragmentation and volatilization at higher OH exposures. In comparison with particle bounce factor measurements, we demonstrate that the decrease in the average molar mass of aged SSA correlates with an increase in liquid-like particles resulting from smaller, more water-soluble organics present in the SSA. This work contributes to better understanding of the fundamental processes affecting the age and growth of SSA following emission from the ocean surface.

8AC.4

Aerosol Composition Measurements Using the Vocus Inlet for Aerosol (VIA): Applications in an Oil and Gas Production Region and an Indoor Cooking Event. DANIEL C. BLOMDAHL, Leif Jahn, Nirvan Bhattacharyya, Catherine Masoud, Kristi McPherson, Pearl Abue, Kanan Patel, Jordan Krechmer, Lea Hildebrandt Ruiz, Pawel K. Misztal, *University of Texas at Austin*

The Vocus Inlet for Aerosol (VIA; Aerodyne, Inc.) is a novel attachment to the Vocus PTR-ToF mass spectrometer to characterize the chemical composition of aerosols at high time resolution (1 Hz). The VIA thermally denudes particles into gas-phase compounds that the Vocus PTR-ToF then detects downstream. A honeycomb activated-carbon denuder removes gas-phase compounds upstream of the thermal denuder to ensure mass spectrum signals are solely from aerosol decomposition. The capabilities of the VIA will be discussed using laboratory results and results from two measurement occasions: (a) ambient aerosols from an active oil and gas extraction region and (b) an indoor oil cooking event. The VIA and Vocus PTR-ToF was used in a field campaign near Karnes City, a small town in south-central Texas surrounded by active oil and gas infrastructure. Temperature ramps of the VIA thermal denuder were completed in the field from 160 °C to 260 °C over 4 hours of measurements to elucidate the dependence of temperature on the desorption efficiency of compounds with semi- or low volatility. Real-time (1 Hz time resolution) measurements of aerosol composition with the VIA thermal denuder set at constant temperature over 5 days will also be reported. The chemical concentration data from an indoor cooking event involving olive, avocado, and canola oils—among other foods—will also be reported. Results from the ambient aerosol data from Karnes City and the rapid production of aerosols from cooking oils will showcase the wide range of applications of the VIA-Vocus system.

8AC.6

Iron(III)-Catalyzed Chemistry in Biomass Burning Organic Aerosol. KATHERINE HOPSTOCK, Hind Al-Abadleh, Sergey Nizkorodov, *University of California, Irvine*

Biomass burning organic aerosol (BBOA) is one of the largest sources of organics in the atmosphere. Mineral dust and biomass burning smoke frequently occur in the same atmospheric environment. Typical biomass burning compounds, such as dihydroxybenzenes and their derivatives, are capable forming light-absorbing, insoluble polymeric particles upon reaction with soluble iron under conditions characteristic of aerosol liquid water. Despite mechanistic advances in iron-catalyzed chemistry with isolated BBOA precursors, it is not well understood how this chemistry translates to secondary brown carbon (BrC) formation from real BBOA. In this study, BBOA was generated through the pyrolysis of various types of biomass fuels, and the water-soluble fractions were reacted with iron chloride under dark, acidic conditions. We utilized spectrophotometry to monitor changes in the mass absorption coefficient (MAC) of the dissolved organics. MAC measurably increased at visible wavelengths after several hours of reaction. Soluble and insoluble reaction products were separated, and dissolved in aqueous and organic solvents, respectively. Analysis was conducted with ultra-performance liquid chromatography coupled to a photodiode array spectrophotometer and a high-resolution mass spectrometer (UPLC-PDA-HRMS). Products absorbing at near-UV and visible wavelengths were tentatively assigned. In general, the insoluble products had higher molecular weights than the soluble products and starting BBOA compounds. The distribution of molecular formulas suggested that Fe(III) catalyzed oligomerization of phenols in solution. These results suggest that light-absorbing aerosol particles can be produced from Fe(III)-catalyzed reactions in aging BBOA plumes produced from smoldering combustion in the absence of any photochemistry. This chemistry has important implications for understanding the direct effect of BBOA/mixed dust aerosols on climate.

8AC.7

Secondary Organic Aerosol Formation from in situ Cl Oxidation of Ambient Air in an Oil and Gas Production Region Using an Oxidation Flow Reactor. NIRVAN BHATTACHARYYA, Catherine Masoud, Kristi McPherson, Kanan Patel, Leif Jahn, Pearl Abue, Daniel C. Blomdahl, Anita Avery, William Brune, Pawel K. Misztal, Andrew Lambe, Lea Hildebrandt Ruiz, *University of Texas at Austin*

Karnes City, TX lies in the middle of the Eagle Ford Shale play, an oil and gas region which significantly increased production in the past decade. Previous work in the region indicated high concentrations of alkanes, alkenes, and aromatic hydrocarbons and significant local concern about air quality impacts of well heads, hydraulic fracturing fluid, and flaring. Spring 2021 fieldwork was conducted in Karnes City to examine ambient particulate matter, gas phase emissions, and atmospheric processing of these emissions. A novel oxidation flow reactor (OFR) was deployed to study *in situ* Cl-initiated VOC oxidation and SOA formation. Cl generated by photolysis of oxalyl chloride with low pressure mercury lamps (λ = 254 or 313 nm) reacted with ambient gases and particles over a few minutes' OFR residence time. Ambient and post-OFR particle size distributions were assessed with a Scanning Electrical Mobility System and gas and particle phase compositions were analyzed by a variety of advanced mass spectrometry instruments including an aerosol chemical speciation monitor, a Filter Inlet for Gases and Aerosols coupled to an iodide-mode chemical ionization mass spectrometer, and a Vocus 2R proton transfer reaction mass spectrometer. During typical ambient conditions, Cl oxidation of ambient VOCs (including C_6-C_{10} hydrocarbons measured with Vocus) resulted in formation of oxygenated VOCs (OVOC) and a 5 to 10 fold enhancement in nucleation and Aitken mode particle number concentrations. During episodic pollution events with elevated hydrocarbon emissions (e.g. nighttime flares), OFR sampling resulted in 15 to 100 fold enhancements in particle number concentration and 5 to 30 fold enhancements in organic aerosol mass. These results highlight the potential impacts of Cl-initiated oxidative aging on OVOC and SOA formation in source regions influenced by chlorine chemistry.

8AC.8

Peroxy Radical Isomerization of a Model Organic Compound Under Laboratory Chamber Conditions.

MATTHEW GOSS, Victoria Barber, Yaowei Li, Alexander Zaytsev, Erik Helstrom, Francesca Majluf, Jordan Krechmer, Frank Keutsch, Jesse Kroll, *MIT*

Peroxy radical isomerization is an important reaction contributing to the formation of highly oxidized molecules, which influence secondary organic aerosol (SOA) formation. While rates are highly dependent on structure, isomerization rates for some systems are fast enough to compete with bimolecular peroxy radical reactions. Previous studies of these reactions have used carefully selected reaction conditions, such as extremely slow photochemistry, to enable measurement of isomerization rates. However, these methods do not allow one to examine the impact of isomerization on SOA formation or product distribution across multiple generations of oxidation. In this study, we identify a model compound, 1,6-heptadiene, predicted to undergo isomerization as a primary reaction pathway with an estimated rate fast enough to compete with bimolecular reactions under typical chamber conditions. We perform chamber oxidation experiments under different reaction conditions and identify multi-generational products consistent with a hypothesized mechanism. Finally, we compare experimentally-derived isomerization rate constants to theoretically-based estimates, and examine the impacts of isomerization under different chamber conditions on aerosol chemical composition.

8AC.9

The Impact of Temperature on Organic Peroxy Radical Isomerization and Aerosol Production.

NADIA TAHSINI, Matthew Goss, Jesse Kroll, *MIT*

Organic peroxy radicals (RO_2) are formed in the oxidation of nearly every hydrocarbon emitted into the atmosphere, and their subsequent chemistry plays a major role in radical cycling and the formation of secondary pollutants. While some RO_2 pathways are well known, in general their reactivity in low-NO_x conditions remains poorly constrained. Unimolecular RO_2 isomerization, which produces highly oxygenated organic molecules (HOMs), remains a particularly challenging pathway to elucidate due to competition with the bimolecular reactions. Here, we study the formation and transformation of products from the low-NO_x oxidation of large hydrocarbons in chamber experiments as a function of temperature. Product characterization is accomplished with mass spectrometric measurements, namely an Aerosol Mass Spectrometer (AMS) to characterize the amount and composition of aerosol formed under a given set of conditions. These results, coupled with simulations using the Master Chemical Mechanism (MCM) with the Framework for 0-D Atmospheric Modeling (F0AM), provide insight into the temperature sensitivity of RO_2 isomerization, and more generally to the role that isomerization plays in aerosol formation.

8AC.10

A Study on Elevated Concentration of Fine Particles at Urban and Agricultural Sites in Korea. JIHO JANG, Haebum Lee, Minhan Park, Joonwoo Kim, Nohhyeon Kwak, Taewoong Gong, Ilhwa Seo, Dahye Oh, Seunghye Lee, Kihong Park, *Gwangju Institute of Science and Technology*

Chemical components (ions, elements, organic carbon (OC), elemental carbon (EC)) of $PM_{2.5}$ were measured at urban Gwangju and agricultural Gimje sites in Korea to determine major factors for elevated $PM_{2.5}$ concentration ($PM_{2.5}$ event). The $PM_{2.5}$ event was defined when the daily $PM_{2.5}$ mass concentration was higher than 35 $\mu g/m^3$ in summer and 50 $\mu g/m^3$ in winter. Data suggest that the $PM_{2.5}$ event in summer at urban Gwangju site was mainly affected by secondary sulfate formation and vehicle emission, and that in winter secondary nitrate and sulfate formation and biomass burning under the stagnant condition played important roles in the $PM_{2.5}$ event. At agricultural Gimje site, the biomass burning and formation of secondary nitrate contributed to the elevated concentration of fine particles in summer. The ammonia rich environment at the agricultural site played important roles in the $PM_{2.5}$ event as well as new particle formation (NPF) event. More comparisons between two sites including source apportionment for $PM_{2.5}$ are being progressed and will be presented.

8AC.11

Significant Contrasts in Aerosol Acidity between China and the United States. BINGQING ZHANG, Huizhong Shen, Pengfei Liu, Hongyu Guo, Yongtao Hu, Yilin Chen, Shaodong Xie, Ziyan Xi, T. Nash Skipper, Armistead G. Russell, *Georgia Institute of Technology*

Aerosol acidity governs several key processes in aerosol physics and chemistry, thus affecting aerosol mass and composition, and ultimately climate and human health. Previous studies have reported aerosol pH values separately in China and the US, implying different aerosol acidity between these two countries. A full picture of the pH difference and the underlying mechanisms responsible is hindered by the scarcity of simultaneous measurements of particle composition and gaseous species, especially in China. Here we conduct a comprehensive assessment of aerosol acidity in China and the US using extended ground-level measurements and regional chemical transport model simulations. We show that aerosol in China is significantly less acidic than in the US, with pH values 1–2 units higher. Based on a proposed multivariable Taylor Series method and a series of sensitivity tests, we identify major factors leading to the pH difference. Compared to the US, China has much higher aerosol mass concentrations (gas + particle, by a factor of 8.4 on average) and a higher fraction of total ammonia (gas + particle) in the aerosol composition. Our assessment shows that the differences in mass concentrations and chemical composition play equally important roles in driving the aerosol pH difference between China and the US — increasing the aerosol mass concentrations, but keeping the relative component contributions the same, in the US to the level in China (by a factor of 8.4) increases the aerosol pH by ~1.0 unit, and further shifting the chemical composition from US conditions to China's that is richer in ammonia increases the aerosol pH by ~0.9 units. Therefore, both China being more polluted than the US and richer in ammonia together explain the aerosol pH difference. The difference in aerosol acidity highlighted implies potential differences in formation mechanisms, physicochemical properties, and toxicity of aerosol particles.

8AC.12

Chemical Composition of Submicron Organic Aerosol in Rural Environment: A Long-Term Study.

TOUQEER GILL, Julija Pauraite, Steigvilė Byčenkienė, Kristina Plauškaitė, *SRI Center for Physical Sciences and Technology*

Aerosol particles have a great impact on the climate based on their chemical composition, size, optical parameters and other. In addition, many parameters of atmospheric aerosol are depending on their origin. Therefore, it is essential to characterize the aerosols chemical composition and pathways of their formation.

This study focuses on the investigation of aerosol main chemical components in Rūgšteliškis (Lithuania) rural environment. Data were collected using Aerosol Chemical Speciation Monitor (ACSM), Aerodyne Inc. Three seasons (spring, summer and autumn) data from 2013, 2014, 2016, 2018 and 2019 were analysed. The time series and diurnal trends of organic and inorganic aerosols (OA and IA, respectively) were examined. OA was exhibiting higher contribution (60 – 80 %) to total submicron (less than 1 µm in diameter) particulate matter (PM1) over all seasons, whereas IA was showing a lower contribution which reached up to 20 – 40% (SO4 = 4 – 20%, NH4 = 3 – 21%, NO3 = 3 – 12% and Chl = 0.2 – 0.4%). Higher contribution of OA to PM1 observed in summers of years 2013, 2016 and 2018 compared to spring and autumn seasons. In addition to that, in the year 2014 and 2019 the highest contribution of OA was observed over the spring seasons.

A possible day and night aerosol chemistry were evaluated by OA and IA diurnal pattern analysis. Higher mass concentration of OA was observed in morning hours (5 – 7 h) and lower mass concentration in the second half of the day (13 – 19 h) (Fig. 1A). NO3 mass concentration showed similar pattern, which reached maximum between 5 – 7 h and minimum between 15 – 20 h (Fig. 1B), and likely indicates the nocturnal chemistry. SO4 and NH4 had lower mass concentration during daytime (10 – 19 h and 13 – 23 h, respectively) and higher mass concentration during the night time (1-6 h and 1-10 h, respectively) (Fig 1C, D). Significantly higher SO4 concentration was observed during the daytime. This is likely due to oxidation of gaseous precursor SO2 followed by the particle formation through nucleation and condensation processes, which triggers the formation of SO4 derived aerosol during the daytime. Neutralization of HNO3 and H2SO4 with NH3 likely formed ammonium derived aerosol in the form of NH4NO3 and (NH4)2SO4 [1]. Additionally, submicron aerosol particles acidity (H+Aer) and stoichiometric neutralization ratio were estimated and examined [2]. The outcomes of this investigation could provide a better understanding with respect to air chemistry on local and worldwide scales.

8HA.1

Characterizing Potash Rock Dust Generated from Full Scale Cutting Tests Performed with Three Different Radial Pick Wears.

SYD SLOUKA, Muhammad Ishaq, Jamal Rostami, Jürgen Brune, *Colorado School of Mines*

Respirable dusts pose serious long-term health issues to occupational workers where mechanized mining and tunneling machines are used in hard rock excavation. This is particularly true for the U.S. coal mining industry. Various mechanical excavation machines, such as longwall shearers, efficiently cut rock by striking the rock surface with hardened steel and tungsten carbide picks. Fine, breathable, rock dust is generated each time the pick tip contacts the rock surface and during the regrinding of the cuttings at the face by the loading process. In underground mines and tunnels, the respirable dust generated from cutting is also carried further down the production line by the ventilation air current or reintroduced into the air at transfer points, potentially exposing numerous miners.

This study characterizes and compares the respirable rock dust particles generated at the pick tip as a function of pick wear. Parameters studied include dust quantity, size distribution, mineralogy, and particle shape throughout the life-cycle of the pick. Results provide some insight to mine and tunnel operators for changing out picks to mitigate dust at the generation point related to the cutting process. Testing was performed on a linear cutting machine (LCM) which allows for full scale cutting tests in a laboratory environment. For this study, a dust collection system was designed and built to collect dust samples from LCM testing. Potash rock samples were used in these preliminary experiments with radial picks at new, moderately, and fully worn wear levels. Results show statistically significant effects of bit wear on dust parameters. Follow up testing is underway on other rock samples using different cutting tools.

8HA.2

Hygroscopicity and Shape Factor Measurements of Uric Acid Aerosol Towards the Treatment of Medical Conditions. DEWANSH RASTOGI, Kanishk Gohil, Chao Peng, Mingjin Tang, Akua Asa-Awuku, *University of Maryland College Park*

The growth of nanocrystalline (100-200 nm) uric acid deposits in joints and tissue can lead to gout and kidney failures. Uric acid stones constitute about 4-12% of all kidney stones worldwide and form in the human body during purine metabolism. Uric acid has low water solubility (6 mg/mL), and crystallization occurs when uric acid reaches saturated concentrations. Hence, quantifying the water uptake of ultra-fine uric acid particles may contribute to new medical treatments.

In this work, we measure the physical properties of uric acid aerosols. Aerosols generated by atomization are dried and then exposed to sub-saturated and supersaturated conditions. The aerosol electrical mobility and aerodynamic diameter size are measured using Scanning Mobility Particle Sizer and Aerodynamic Aerosol Classifier, respectively. These measurements are used to calculate the shape factor for the aerosol particles at different drying rates. A Thermogravimetric Analyzer (TGA) is used to measure the mass of water adsorbed on uric acid particles exposed to sub-saturated relative humidity conditions.

Results show that the shape factor decreases from 1.4 to 1 with the increase in either particle sizes or drying rates. These shape factor measurements are used to calculate the size-independent hygroscopicity parameter measured in the supersaturated regime. The overall hygroscopicity is found to be less than 0.001. Additionally, TGA measurements show negligible water uptake by uric acid crystals at low relative humidity. Hence, uric acid particles would likely crystallize from the surrounding media even when the concentration of uric acid is low in the body. Once formed, these crystals tend to be difficult to dissolve. The traditional nanoparticle water uptake theory (Köhler theory) cannot be applied to uric acid particles, and one needs to consider adsorption theory to understand the water uptake behavior of uric acid particles.

8HA.3

Particle and Toxin Filtration Efficiencies of Commercially Available Face Masks and Air Conditioning Filters to Reduce Exposure to and Health Impacts of Aerosolized Algal Toxins. CASSANDRA GASTON, Haley Royer, Raymond Leibensperger III, Michael Sheridan, Jiaming Hu, Kaycie Lanpher, Daniela Maizel, Helena Solo-Gabriele, Grace Zhai, Larry Brand, Alberto Caban-Martinez, Kimberly Popendorf, *University of Miami*

Harmful algal blooms (HABs) can generate toxins that can be aerosolized and negatively impact human health through inhalation. HABs are often found in waterways near residences, therefore, aerosolized HAB toxins can potentially affect both indoor and outdoor air quality. Given that HABs are predicted to increase worldwide, knowledge of the health impacts associated with the inhalation of aerosolized HAB toxins are needed in addition to effective mitigation strategies to prevent airborne exposure. In this work, we characterized both the particle filtration efficiency using particle sizing instruments as well as the mass concentration of different congeners of aerosolized microcystin (MC) toxins that penetrate through commercially available face masks and air conditioner (AC) filters. Particles were generated from cultures of the toxin-producing cyanobacteria Microcystis aeruginosa. Hydrophobic congeners of microcystin including MC-LF and MC-LW were enriched in aerosols compared to water, with MC-LR being the most abundant form, which has implications for the toxicity of inhalable particles generated from HAB-contaminated waters. Particle transmission efficiencies and toxin filtration efficiencies scaled with the manufacturer-provided filter performance ratings. Up to 80% of small, microcystin-containing aerosols were transmitted through AC filters with low filter performance ratings. In contrast, both face masks as well as AC filters with high filter performance ratings efficiently removed toxin-containing particles to below limits of quantification. Our findings suggest that face masks and commercially available AC filters with high filtration efficiency ratings are suitable mitigation strategies to avoid indoor and outdoor air exposure to aerosolized HAB toxins. This work also has relevance for reducing airborne exposure to other HAB toxins, non-HAB toxins, pathogens, and viruses, including SARS-CoV-2, the virus responsible for the COVID-19 pandemic.

8HA.4

Investigation of Microscreen System for Fiber Length Classification.

BON KI KU, Pramod Kulkarni, *Centers for Disease Control and Prevention, NIOSH*

Preparation of length classified fibers is critical for conducting toxicological studies that investigate health effects of fiber aerosols. Recent studies have shown that a fiber separation system using nylon mesh screens can be effective in reducing long tails on the fiber length distributions. However, this approach suffers from poor length resolution. To address this limitation, a high-throughput microscreen system (HMS) has been developed. The HMS induces fiber alignment perpendicular to the flow, through application of external electrical field, followed by separation using etched screens. Aerosolized test fibers in the laboratory were classified using HMS using a series of different nylon mesh screens (5, 10, 20, 30, 41 and 60 µm pore sizes), and the fibers collected on each screen were recovered by washing and their lengths were measured using a phase contrast microscope. The length distribution from each screen with electric field was compared to that from the screen without electric field. The results showed that the mean fiber lengths classified by the HMS without the electric field are 12.4, 11.7, 18.6, 20.9, 25.1 and 50.3 µm for screens corresponding to 5, 10, 20, 30, 41 and 60 µm pore size, respectively. In comparison, the mean length of test fibers was 28.6 µm. Operational characteristics and the data demonstrating the performance of the HMS system will be presented and discussed.

8HA.5

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

SUDHEER SALANA, Yixiang Wang, Joseph V Puthussery, Haoran Yu, Vishal Verma, *University of Illinois at 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 the 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 assessment of ROS activity as they incorporate the biological processes involved in the PM-induced ROS generation. Considering this need, we developed a first of its kind 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 is capable of analyzing a batch of six samples (including one negative and one positive control) in five hours and is equipped to operate continuously for 24-hours with minimal manual intervention after every batch of analysis, i.e., after every five hours. The instrument has a high analytical precision (CoV <20% for positive controls t-BOOH, Cu (II) and ambient PM sample). The results obtained from the instrument were in good agreement with manual measurements using t-BOOH (slope = 0.83 for automated vs. manual, $R^2 = 0.99$) and ambient samples (slope = 0.83, $R^2 = 0.71$). We further demonstrated the ability of this instrument to analyze a large number of both ambient and laboratory samples, and developed a dataset on the intrinsic cellular ROS activity of several compounds, such as metals, quinones, PAHs and inorganic salts, commonly known to be present in ambient PM. This dataset will help in apportioning the contribution of key chemical species in the overall cellular ROS activity of the ambient PM.

8HA.6

Assessing the Effectiveness of a Novel Negative-Pressure Particle Containment Device for Reducing Respiratory Particles during Intubation. MUCHUAN NIU, Liqiao Li, Haoxuan Chen, Peyton Tebon, John Shin, Tristan Grogan, Nir Hoftman, Yifang Zhu, *University of California, Los Angeles*

Health care workers (HCW) involved in respiratory droplet and aerosol generating procedures are at high risk of infection when treating the Coronavirus Disease 2019 (COVID-19) patients. The virus-laden respiratory particles can easily reach HCWs within a close proximity (~ 6 feet) through airborne transmission. Thus, the effectiveness of personal containment devices (PCD) applied to these high-risk procedures are critical to the safety of HCWs. However, current PCD designs usually lack a complete barrier between patient and HCW and the real-world particle removal efficiency is poorly understood. Here, we designed a suction-assisted local aerosol containment chamber (SLACC) and measured the particle number concentration (PNC) and size distribution simultaneously inside and outside of the SLACC at the head and side location of the surgical table, using saline nebulizer as the source of aerosol generation. We found that the SLACC device reduced > 97.7% of particles outside at either the head or the side location compared to inside SLACC. The aerosol source showed two size-modes at 0.6 µm and 2.4 µm, similar to the COVID-19 aerosol sizes measured in two Wuhan hospitals indoors; while no particle larger than 0.5 µm was observed outside of the SLACC. Our preliminary results showed that the SLACC device is highly effective in reducing PNC at outside locations, which could directly benefit the HCWs by reducing their exposures to airborne particles. In the future, we plan to recruit 100 patients and assess the real-world particle reducing abilities of the SLACC device during surgery. In addition to COVID-19, the SLACC device could be applied to any infectious diseases requiring isolation and airway management to protect HCWs.

8HA.7

Linkage between Multiple Cellular Responses with Reactive Oxygen Species Production from Exposure to Biogenic and Anthropogenic Secondary Organic Aerosols. FOBANG LIU, Tianchang Xu, Nga Lee Ng, Hang Lu, *Georgia Institute of Technology*

Atmospheric aerosol could cause a significant impact on human health. Many toxicological studies have suggested that the adverse health effects of aerosol exposure are linked to oxidative stress through the overproduction of reactive oxygen species (ROS). Meanwhile, some ROS-independent mechanisms have also been proposed to explain the biological effects upon aerosol exposure. It remains inconclusive as to whether the overproduction of ROS plays a central role in the impacts of biological effects/phenotypes caused by aerosol exposure. On the other hand, given the extraordinary chemical complexity and diversity of aerosol, the toxicity and the mechanisms of aerosol damage may also depend on the properties and chemical composition of the studied aerosol. Here, we employ the Georgia Tech Environmental Chamber (GTEC) facility to generate secondary organic aerosol (SOA) from the photooxidation of biogenic and anthropogenic precursors under different formation conditions. Alveolar macrophages are exposed to SOA and multiple cellular responses are measured, including caspase 3/7 activity, mitochondrial membrane potential, and cellular ROS (etc.). The caspase 3/7 activity plays a key role in apoptosis, and thus it serves as an important indicator of cell health. The mitochondrial membrane potential relates to mitochondrial activity, while mitochondria could be the main organelle in ROS production. Our preliminary results indicate that cellular ROS exhibits different relationships with caspase 3/7 activity and with mitochondrial membrane potential. The cellular response patterns from exposure to a variety of SOA samples and the linkage between multiple cellular responses to cellular ROS production will be discussed.

8HA.8

Aerosol Composition and Chemistry in Electronic Cigarettes in Response to Coil Temperature and E-liquid Formulation. Yichen Li, Belinda Ortega, Amanda Burns, Lillian Tran, Karizza Abellar, Morgan Poindexter, Xiaohan Li, Brian Brandley, George Hodgin, Amy Madl, Kent Pinkerton, TRAN NGUYEN, *University of California, Davis*

E-cigarette aerosol is a complex mixture of gases and particles whose composition is dependent on e-liquid formulation and puffing regimen. We present new insights into the balance of mass and chemical composition of mainstream aerosols from a 3rd generation e-cigarette device, as a function of on coil temperature and e-liquid composition. Two e-liquid systems were studied of varying composition (0:100 – 100:0): (A) mixtures of propylene glycol (PG) and vegetable glycerin (VG) that are relevant for nicotine-based e-cigarettes, and (B) mixtures of purified tetrahydrocannabinol (THC) oil and vitamin e acetate (VEA), which may be relevant for the onset of e-cigarette or vaping-associated lung injury (EVALI). The thermal degradation of these e-liquid compounds in the e-cigarette vessel produces a large variety of carbonyl and hydroxycarbonyls via heat-induced and radical-induced formation pathways. Coil temperature and e-liquid composition affect the total aerosol mass through modifying the aerosolization rates, but also the aerosol composition by modifying the efficiency and pathways of thermally-induced degradation. We discuss how heating the mixture of PG:VG and VEA:THC-oil with a coil impact aerosol composition compared to the pure substances. We demonstrate how the unequal aerosolization rates from PG and VG severely impact the emissions of toxic carbonyls such as acrolein during the lifecycle of the e-liquid tank or cartridge.

8HA.9

Cokriging With a Low-cost Air Sensor Network to Estimate Spatial Variation of Brake and Tire-wear Related Heavy Metals and Reactive Oxygen Species in Southern California, United States. JONATHAN LIU, Irish del Rosario, Jonah Lipsitt, Farzan Oroumiyeh, Jiaqi Shen, Suzanne E. Paulson, Beate Ritz, Jason Su, Scott Weichenthal, Yifang Zhu, Michael Jerrett, *University of California, Los Angeles*

Due to regulations and technological advancements reducing tailpipe emissions, there is an increased focus on non-exhaust automobile emissions, including break and tire wear particulate matter (PM) which contain heavy metals capable of generating oxidative stress in exposed organisms. Despite potential harms to human health, few studies have modeled the spatial variability of PM from brake and tire wear emissions.

Improvements in electrical engineering, internet connectivity, and an increased public concern over air pollution have led to a proliferation of low-cost air sensor networks such as the PurpleAir monitors, which primarily measure fine particulate matter (PM2.5). While unable to measure PM2.5 constituents, these networks are dense and cover a wide spatial area.

In this study, we model the concentrations of barium, zinc, 2-hour reactive oxygen species (ROS), and black carbon alongside DTT loss and OH formation. We use a cokriging approach, targeting fine particulate matter (PM2.5) constituents, measured across Southern California in two sampling campaigns and incorporating data from the PurpleAir network as a secondary predictor variable. Within the cokriging model, we create an external drift by incorporating a land-use regression (LUR) model. We obtained land-use variables such as traffic, business density, tree canopy cover, and impervious surfaces. We then used a deletion-substitution-addition (DSA) algorithm and K-fold cross-validation to select an optimal model for use within cokriging.

Our final LUR model exhibits good fit for predicting metal mass concentrations, black carbon, DTT loss, and 2-hour ROS (adjusted R2 = 0.50-0.68), and reasonable fit for OH and metal normalized mass concentration (adjusted R2 = 0.37-55). Additionally, we find that several of our LUR models exhibit statistically significant spatial autocorrelation (Moran’s I p: 0.01-0.80) and high correlation with collocated PurpleAir sensor PM2.5 measurements (R = 0.67). In this project we present an exposure surface of brake and tire wear in the Southern California meeting. We also present the results of an evaluation of the ability for a low-cost air sensor network to predict speciated PM2.5.

8HA.10

Health Risk Assessment and Chemical Characterization of Settling Dust Exposed to Children: A Case Study of Primary School at Karachi, Pakistan.

SAIYADA MASOOD, Sumayya Saied, Farheen Anwar, Azhar Siddique, Kamran Khan, Haider Khwaja, *Jinnah University for Women*

Primary school children are at high risk of pollution due to their frequent exposure with contaminants through various means and unawareness. Dust particles are heavier atmospheric aerosols of the range ≥ 100µm and retain in planetary boundary layer (PBL) and eventually settled on surface(s). The composition of particle depends on the origin of nucleation and track on which chemical species adhere and become the part before deposition. A preliminary study is designed to assess the dust particles with reference to the exposure of children in primary school at Karachi city. Indoor (classroom) and outdoor (playground) samples were collected for comparative study. Sample extracts were assessed for pH (6.15), anions (mg/kg) namely with average values F^- (426±136), Cl^- (13458±8161), Br^- (17.3±9.4), SO_4^{2-} (9331±3318), $C_2O_4^{2-}$ (79.7±58.2) through Ion chromatography and metal profile was obtained through XRF. Most prominent chemical species measured with distinctly high distribution in indoor and outdoor samples were the metal components (mg/kg) like Mo (6.5±1.6), Zr (55.1±3.5), Sr (219±3.97), Rb(19.3±1.75), Pb (117.2±6.55), Zn (799±17.9), Cu (190±13.8), Fe (12324±128), Mn (113±35.9), Ti (2134±75.9), Ca (126241±613) and K (11227±280), other metals were observed < LOD. Ca concentration was high due to the use of chalks in classrooms. Prominent concentration of sulfur in mg/kg (5988±482) was observed in indoor dust. Outdoor dust is associated with road dust. High levels of metals, like Cu, Pb and Zn are linked to high motor vehicle traffic in Karachi city. Health Risk was assessed by evaluating Average Daily Dose ADD(ingestion), ADD(inhalation) and ADD(dermal) for noncarcinogenic and carcinogenic metals vs reference values.

8HA.11

Association of Short-Term Exposure to Air Pollution and Heart Rate Variability for a Healthy Cohort in a Highly Polluted City of Delhi.

KASHISH JAIN, Gazala Habib, Nisar Ali Baig, Mohammad Yawar, Sandeep Singh, Siddharthan Deepti, *Indian Institute of Technology, Delhi*

The adverse effects of air pollution on respiratory and cardiovascular health have been established in a series of major observational studies. In rapidly developing countries like India where the mean pollutant levels are much higher than the health-based air quality guidelines, the risk increases even more. However, the extent of epidemiological cohort studies linking air pollution and health in India is still modest. The current study assessed the response of heart rate variability (HRV) parameters including ST-segment, a proxy to cardiovascular mortality, in a cohort of healthy individuals due to short-term exposure to pollutants like size segregated particulate mass (PM) and number (PN) concentrations and black carbon (BC). The cohort comprised of security guards working at the entrance gate of a college in the highly polluted city of Delhi. A questionnaire was administered for collecting baseline data on any background exposure or covariates including demography, smoking and drinking habits, etc. to establish the healthy status of participants which was a primary inclusion criterion. The real-time exposure to size segregated PM and PN was measured using Optical Particle Sizer along with gravimetric PM2.5 measurements. The BC measurements were made using an aethalometer. ECG holters were used to capture the real-time cardiac response along with activity trackers to adjust for variations in response due to any intensive activity. A linear mixed-effect model was used to examine the relationship between mean pollutant concentrations and HRV indices. Significant changes were observed in the HRV indices with the increase in pollutant concentrations. It indicates that even short-term exposures in a highly polluted environment can cause a significant decline in cardiovascular health for healthy individuals.

8IM.1

Excitation Emission Matrix Fluorescence Spectroscopy for Analysis of Reactive Oxygen Species from Particulate Matter Samples. ISHRAT SINGH, Jiayang He, Michael Paulsen, Igor Novosselov, Christopher Simpson, *University of Washington*

The presence of particulate matter (PM) in the environment can lead to adverse health impacts, like, cardiopulmonary diseases, neurological diseases, and lung cancer. While the epidemiological link between PM exposure and adverse health effects is clear, there is a lack of information regarding source-specific differences in PM toxicity. Thus, there is a clear need to quantify PM present in the environment and identify its sources and toxicity. Sources of combustion generated PM range from wildfires, residential wood burning, traffic emission, etc. Flame temperatures have been linked to changes in particle composition and hence the toxicity. Also, the capacity of combustion-generated PM to produce reactive oxygen species (ROS) has been proposed as one surrogate metric for the toxicity of PM. Currently, analysis of the composition of the organic fraction of PM is done using mass spectrometry (MS) methods, which are expensive and time-consuming. Excitation emission matrix (EEM) spectroscopy has been proposed as a low-cost, reliable method for analysis of the organic fraction of PM and for source apportionment. In this study, we investigate the correlation between EEM signature and ROS measurements. PM collected from laboratory flame, cookstove, and wildfire smoke are analyzed by EEM, GC-MS, and the dithiothreitol (DTT) assay for ROS. Using principal component regression (PCR) analysis of the EEM spectra, we drew the correlation between the EEM spectra and the DTT measurements. The results suggest that the total fluorescence measurement from EEM spectra is correlated with ROS, suggesting that EEM can be an alternative method to evaluate the ROS level in combustion-generated aerosols.

8IM.2

Development of an Inexpensive Spark-Induced Breakdown Spectroscopy Instrument for Measurements of Atmospheric Toxic Metals. HANYANG LI, Leonardo Mazzei, Christopher Wallis, Anthony S. Wexler, *University of California, Davis*

Atmospheric toxic metal particles are known or suspected to cause cancer and other serious health issues. To meet the demand for identifying and controlling toxic air contaminants in environmental justice communities, we have recently developed an inexpensive spark-induced breakdown spectroscopy (SIBS) instrument for detecting and quantifying toxic metal pollutants in the atmosphere. Compared to conventional instruments used to analyze elemental compositions (such as ICP-MS and XRF spectrometer), our instrument allows near real-time measurements and does not require complex sample preparation.

In this work, we nebulized standard solutions and used univariate calibration methods to obtain the limit of detection (LOD) and the relationship between spectral peak areas and ambient concentration. Furthermore, the plasma parameters affecting SIBS performance were optimized, such as the time delay to observation, the distance between electrodes, and the ablation voltage. Using the optimal parameters, the instrument successfully detected 10 metals (including Cr, Cu, Mn, Fe, Zn, Co, Al, K, Be, and Ni), with LOD ranged from 50 to 810 ng m-3 at a flow rate of 15 l min-1 and a 30 min sampling duration. Similar to other investigations using ion breakdown spectroscopy, we did not observe strong emissions lines for Hg, Pb, As, Sb, and Se, which were likely due to spectral overlap, matrix effects, and the limited detection range of the optical components. Overall, SIBS is a promising technique for field measurements of toxic metals in environmental justice, industrial and urban applications.

8IM.3

Enhanced Optical- and Atomic Force Microscopy-Photothermal Infrared and Raman Spectroscopy Enables Observation of Individual Ultrafine Aerosol Particles. YAO XIAO, Ziying Lei, Andrew Ault, *University of Michigan*

Atmospheric aerosol particles participate in multiphase reactions that impact their climate-relevant properties (i.e. absorbing or scattering solar radiation, and nucleating ice particle and cloud droplet formation). Measuring the chemical composition of individual aerosol particles is challenging, particularly for particles with aerodynamic sizes <1 µm. In previous studies, our group was the first to apply Optical Photothermal Infrared Spectroscopy (O-PTIR) and Atomic Force Microscope - Photothermal Infrared Spectroscopy (AFM-PTIR) to aerosol particle characterization, which has the advantage of analyzing particles at ambient temperature and pressure. However, the signal is still limited for the smallest individual due to insufficient sensitivity for key vibrational modes, which limits our ability to detect key species present in particles. In this study, we show the first use of gold substrates to improve the signal of trace organic and/or inorganic species in both laboratory and atmospheric particles compared to traditional silicon or quartz substrates. Organic and inorganic functional groups were characterized for lab-generated and ambient particles with the smallest sizes (500 nm to 1 µm and 50 nm to 500 nm for O-PTIR and AFM-PTIR, respectively). IR mapping was collected to further strengthen our understanding of the enhance mechanism and hyperspectral mapping shows the distribution of different groups in the multi-component particles like core-shell morphology. This novel approach method leads to enhanced detection limits and spatial resolution, allowing us to detect trace organic and inorganic species in aerosol particles in a smaller particle size range than previously possible.

8IM.4

High-Throughput Microfluidic Device to Study Ice Nucleation Behavior. MARGARET HOUSE, Priyatanu Roy, Cari Dutcher, *University of Minnesota*

Ice nucleating particles are any solid particles in the atmosphere that allow ice to freeze on their surface. They are important to weather and climate processes because they can cause clouds to partially or fully freeze, changing the optical properties of the clouds and how they contribute to the overall energy balance of the Earth. Studying ice nucleation in single particles on the nanoliter to picoliter scale is important for informing regional and global climate models that take aerosol activity into consideration. Recently, microfluidics has emerged as a novel technique by which single particles modeling atmospheric aerosols can be probed. Microfluidics offers the advantage of rapid and monodisperse droplet generation with precise temperature control and minimal solid-surface contact during experiments. We have utilized both a flow-through and static microfluidic device design to probe ice nucleation behavior of several aqueous-organic systems. We have found interesting relationships between ice nucleation temperature, morphology, and sample aging.

8IM.6

Measurement of the Rate and Controls of Small Particle Growth Using Ambient Air Captive Aerosol Chambers.

ZIHAN ZHU, Xuanlin Du, Candice Sirmollo, Diana Ibarra-Gomez, Don Collins, *University of California, Riverside*

New particle formation and growth plays a key role in controlling the concentration and distribution of cloud condensation nuclei (CCN), which influences the reflectivity and other properties of clouds. Uncertainties remain in quantifying particle growth rate and in characterizing aerosol behavior during real-world new particle formation events representative of a wide range of conditions and locations. In this work, two Captive Aerosol Growth and Evolution (CAGE) chambers were deployed at the DOE Atmospheric Radiation Measurement (ARM) Program's Southern Great Plains (SGP) site for a 2-month study in the spring and summer of 2021. Two identical chambers were used in parallel to study the sensitivity of particle growth to a series of additions and other changes by using one as the baseline or reference chamber and the other as the perturbation chamber. Particle growth rate and secondary aerosol properties in the two chambers were intermittently measured 24 h/day while conditions inside them mirrored those outside, with and without the controlled perturbations. The hygroscopicity, volatility, and CCN-activity characteristics of the secondary species added to the particles were characterized and related to the observed growth. The time-dependence of study-average growth rate is described using measurements from the baseline chamber. The temporal variation of particle size and properties is compared with predictions from a chemical box model. We will provide an overview of the experimental approach and will present preliminary results from the field study.

8IM.7

Design and Laboratory Evaluation of a New Flow Reactor to Study Aerosol Production and Processing through Gas- and Aqueous-phase Chemistry.

NINGJIN XU, Don Collins, *University of California, Riverside*

Cloud droplets serve as an important reaction medium for the formation and evolution of secondary aerosol formed through aqueous-phase reactions (aqSA). Large uncertainties remain in estimates of the production and chemical evolution of aqSA in dilute cloud droplets, which is partly due to the lack of available measurement tools and techniques. Recently, more attention has been directed to understand aqSA production in order to explain discrepancies between measured and modeled aerosol composition and concentrations. Unlike reported studies of secondary aerosol formed through gas-phase reactions (gasSA), laboratory investigations of aqSA mechanisms, products, and yields are usually performed in bulk aqueous solutions with high oxidant and precursor concentrations. The experimental concentrations and conditions often differ from those in the atmosphere and introduce uncertainty when results are implemented into multiphase models. Oxidation flow reactors (OFRs) are frequently used to study the formation and evolution of gasSA in the atmosphere, but few studies have reported the amount and properties of aqSA formed in aqueous aerosol and cloud droplets using an OFR.

Here we will describe a new OFR, the Accelerated Production and Processing of Aerosols (APPA) reactor, for measuring secondary aerosol formed from gas-phase chemistry and from aqueous-phase chemistry in aqueous aerosol and cloud droplets in both the laboratory and the field. For use in simulating in-cloud processes, droplets formed on monodisperse particles are introduced into the top of the flow cell, in which the relative humidity is controlled to 100%. We will describe the design and laboratory characterization of the APPA reactor, including the UV intensity distribution, OH exposure level, residence time distributions (RTD) for gases and particles, and transmission efficiencies of gases (SO_2 and CO_2) and particles. The droplet size distribution and transmission efficiency will also be presented. Aqueous-phase sulfate production from dissolution and reaction of SO_2 and O_3 in droplets was used as a test system. Results from those tests indicate that the observed aerosol growth is consistent with that predicted using first-order rate constants for the S(IV)-O_3 reaction for a dilute solution. We will present preliminary measurements of SA production from organic precursors and from ambient air.

8IM.8

New Insights into Complex Atmospheric Chromatograms Enabled by Advanced Data Processing Techniques. SUNGWOO KIM, Lindsay Yee, Allen Goldstein, Nathan Kreisberg, Susanne Hering, 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, a substantial fraction of data is never analyzed or interpreted. We have recently developed new methods to more comprehensively identify the full suite of analytes in a complex dataset by coupling positive matrix factorization (PMF) with a peak-filtering decision tree. In this presentation, we apply these methods to existing datasets collected by the Semi-Volatile Thermal Desorption Aerosol Gas chromatograph (SV-TAG) to identify new analytes and interpret their variability and transformations in the atmosphere. Comprehensive analysis of chromatograms collected in Manacapuru, Brazil in the wet season of 2014, finds roughly 1000 potential analytes of interest. We apply two matrix size reduction techniques, PMF and hierarchical cluster analysis (HCA) to yield new insights into the covariance and sources of previously overlooked analytes. In particular, we seek to understand the removal of these compounds through gas scavenging by precipitation. Comparison of analyte groups before, during, and after a precipitation event are used to qualitatively and quantitatively understand the impacts of this process on atmospheric composition.

8IM.9

Development and Performance Evaluation of "Chemspot" Instrument for the Characterization of Organic Aerosol. PURUSHOTTAM KUMAR, James Hurley, Nathan Kreisberg, Braden Stump, Susanne Hering, Pat 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 very limited chemical information of particulate matter. 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 an 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 moderate cost. Gas Chromatographic (GC) detectors including a Flame Ionization Detector (FID) and Flame Photometric Detector (FPD) are combined with a CO2 monitor to measure aerosol organic carbon, oxygen-to-carbon ratios, and total inorganic and organic sulfur. Automated calibration can be performed using a very small number of gas-phase calibrants (e.g. CO2, CH4, SF6) due to the usage of common and well-understood GC detectors. Particles are sampled by impaction onto a ~1 mm spot in a custom passivated quartz cell after passing through a condensational growth tube. The collected aerosol sample is thermally desorbed in a few controlled rapid temperature steps (for volatility binned composition) and the vaporized sample is passed through different detectors. We demonstrate here the efficient collection of particles between 10 nm and 1000 nm in diameter. Subsequent rapid thermal desorption at rates of 20 oC/s is shown to provide separation by volatility with a resolution of less than two orders of magnitude in vapor pressure. Results from the initial performance analysis of this instrument using the data obtained from organic aerosol environmental chamber experiments will be presented. Volatility-resolved carbon, oxygen, and sulfur concentrations in ambient aerosol will also be discussed.

8IM.10

Optimization Study of a Thermal Ambient Desorption Source to Improve Sensitivity for Fragile Heritage Objects and Conservation.

MICHAEL BUCHANAN, Xi Chen, Viraj Gandhi, Asher Newsome, Carlos Larriba-Andaluz, *IUPUI*

Ambient desorption/ionization may be combined with a variety of Ion Mobility Spectrometers (IMS) and Mass Spectrometer (MS) systems for analyzing surfaces at atmospheric pressure. A typical sampling system is direct analysis in real time (DART) which uses heated gas flow to thermally desorb analytes for ionization in the gas phase and collection by a vacuum inlet. In a collaboration with the Smithsonian Museum Conservation Institute, this project aims at improving the collection efficiency of particles in a similar system through the study of the thermo-fluid dynamic domain at the sample exposure position including inlet and outlet configurations. The system consists of the outflow tube (a heated capillary with a constant flow rate to extract molecules), sample plate and transfer inlet tube. The collection efficiency is one of the key factors that need improvement, which may be optimized by adjusting the distance and angle of the transfer tube to the sample plate as well as by modifying its geometry and shape. In this project, a series of simulations in nitrogen gas were implemented to study the sample particle trajectories aiming to improve transmission. The model was generated in a computational fluid dynamic (CFD) software SOLIDWORKS, and flow simulations were performed assuming laminar and turbulent flow. Many different configurations are sought by an iterative procedure to optimize the system’s collection efficiency looking at the stream tube that contains the analyte sample and directing it towards the sample inlet. The system is then verified through post-processing simulation of particle tracking. This must be done while meeting some real-life constraints such as keeping an appropriate distance between sample and heated capillary to avoid damage to cultural heritage objects.

8IM.12

Numerical Modeling of the Transport and Fate of Ice Nucleating Particles Inside a Continuous Flow Diffusion Chamber.

JORDAN SPENCER, Russell Perkins, Ezra Levin, Gavin McMeeking, Shantanu Jathar, *Colorado State University*

Ice nucleating particles (INPs) are important for the formation of ice clouds and, hence, INPs affect climate systems through variations in cloud precipitation and radiation balance. Laboratory measurements of INPs can be made using a continuous flow diffusion chamber (CFDC). Previously, numerical calculations including those for particle residence times in the CFDC have not matched experimental observations. In this study, we used a computational fluid dynamics software package (ANSYS Fluent) to model the transport, loss, and spatiotemporal distribution of 1 µm particles during normal operation in a CFDC. Predictions of the pressure, temperature, velocity, and saturation ratio across the annular space were consistent with those derived from analytical expressions, although we did observe differences in these profiles along the length of the CFDC column. Surprisingly, baseline results showed that nearly two-thirds of the particles were lost via turbulent eddies to the inner cold wall and only a third of the remaining particles were exposed to the maximum supersaturation ratio. Simulations were run to examine the sensitivity in the model results to sample and sheath flow rates (5 to 20 L min^{-1}), air and wall temperatures (237.15 to 300 K), particle size (0.3 to 30 µm), and modifications to the inlet geometry. We found that when the sample and sheath flows were cooled, changes were made to improve the inlet geometry, or flow was directed so as to push the particles away from the inner wall, the device performance improved. When compared to baseline results, loss rates were limited to a fifth of the total particles and three-quarters of those remaining were exposed to the maximum supersaturation ratio. Simulation results were found to be insensitive to the particle size range considered. Our findings are relevant to the future design and operation of CFDCs, providing new insights into how the device geometry and operating conditions relate to particle transport and fate.

8SS.1

CPMA-Electrometer Reference Mass Standard (CERMS): A Traceable Calibration Method for Aerosol Mass Concentration Instruments. GREGORY SMALLWOOD, Joel Corbin, Jason S. Olfert, Prem Lobo, *National Research Council Canada*

The mass concentration of aerosols is determined by a wide range of instruments employing a number of different measurement principles. The most significant gap in the calibration of these instruments is the lack of traceability. This limitation is avoided by using the centrifugal particle mass analyser (CPMA)–electrometer reference mass standard (CERMS) technique. All aspects of the CERMS technique are traceable to the SI, resulting in a traceable mass standard similar in principle to the calibration for CPCs. The CERMS is capable of classifying and measuring in-situ reference mass concentrations down to levels below 1 μg/m^3 and in real-time (~1 Hz). Additional advantages of the CERMS are its low uncertainty (~3 %) and its measurement of a well-defined quantity: total post-CPMA suspended PM mass. The CPMA in the CERMS system classifies all particles by mass-to charge ratio, independent of particle properties, including morphology and composition. Depending on the principles of the measurement instrument undergoing calibration, it may be important to select particles with similar properties to what the instrument is designed to measure. For instance, when presented with a nonvolatile black carbon (BC) aerosol for calibration, CERMS may be used to calibrate instruments for the measurement of BC mass concentration.

The presentation discusses the validation and characterization of the CERMS technique from a metrological perspective. We will also summarize recent applications of the CERMS, including the demonstration of a size-specific BC mass absorption cross section and the characterization of the lower limits of detection of the LII 300 and PAX. The results demonstrate the linearity of the CERMS system, and that it is independent of the CPMA setpoint. The sensitivity of the CERMS is shown by characterizing the limits of detection of the LII 300 and PAX instruments. The results support the use of CERMS with appropriate sources for the calibration of instruments measuring aerosol mass concentrations.

8SS.2

Optimized Sampling Settings and Reconstructions for Tandem Particle Mass Analyzer and Single Particle-Soot Photometer Measurements. Arash Naseri, Timothy Sipkens, Steven Rogak, JASON S. OLFERT, *University of Alberta*

Black carbon (BC) is one of the main contributors of the anthropogenic radiative forcing underlying climate change. The short life cycle of BC and its presence in compound forms (e.g., mixed with or coated by other volatile and organic materials) makes isolating BC contributions to climate change challenging. Resolving these uncertainties requires robust measurements of the distribution of refractory BC mass and non-refractory (e.g. organic) coatings of atmospheric particles. A tandem arrangement of a centrifugal particle mass analyzer (CPMA) and single-particle soot photometer (SP2) provides a measure of the non-refractory components of BC. Data inversion can then be employed to reconstruct the two-dimensional total particle-non-refractory black carbon (rBC) (m_p-m_{rBC}) distribution, mapping out the distribution of non-refractory material on rBC particles. In such a measurement, the CPMA is used to sort out particles by mass-to-charge ratio, while the SP2 measures the mass of rBC within each particle. This study derives the optimum sampling settings (*i.e.,* the number of CPMA setpoints per decade, the number of SP2 bins per decade, CPMA resolution, and the number of SP2 counts per CPMA setpoint) to accurately reconstruct m_p-m_{rBC} distributions, taking into account limitations in measurement duration (e.g., due to an unsteady aerosol source or the cost associated with drawn-out campaigns). Simulated measurements are combined with Monte Carlo sampling of the experimental settings to understand how experimental inputs contribute to reconstruction error. Optimized CPMA-SP2 settings are then presented for a typical atmospheric aerosol as a function of aerosol concentration and desired measurement time. Optimal sampling settings vary based on the concentration of the aerosol, the time available for the measurement, and the width of the distribution. Generally, we recommend: (i) large numbers of SP2 bins per decade (~ 50 to 100); (ii) a preference for higher SP2 sampling counts per CPMA setpoint (10^4); (iii) a moderate number of CPMA setpoints per decade (3 to 8); (iv) CPMA resolution around 1, and (v) a high CPMA flow rate (1.5 L/min), can be made to conduct the measurement in about an hour and achieve reconstruction accuracies below 3%.

8SS.3

Matrix-Based Inversion of Humidified Tandem DMA Data.

MARKUS PETTERS, *North Carolina State University*

Humidified tandem DMAs (HTDMAs) select a single particle mobility diameter, pass this quasi-monodisperse aerosol through a humidification system, and then measure the humidified mobility response function using a second DMA. The humidified mobility response function is influenced by the particle size distribution, aerosol charge distribution, and growth factor frequency distribution function of the upstream aerosol. Inversion from the humidified mobility response function to the growth factor frequency distribution is an ill-posed problem. Matrix-based inversion approaches are desirable because they make no prior assumption about the shape of the growth factor frequency distribution. However, prior attempts of matrix-based approaches sometimes produced oscillatory and negative solutions, thus limiting the utility of this approach. This work shows that constrained Tikhonov regularization is suitable to find the growth factor frequency distribution from raw HTDMA data, while also accounting for multiply charged particles. The proposed new methods are distributed via two freely available software packages: *RegularizationTools.jl*, a general-purpose software package to apply Tikhonov regularization to data and *DifferentialMobilityAnalyzers.jl*, which applies the regularization methods to the inversion of DMA and tandem DMA data. The inversion is applied to a multi-week HTDMA dataset collected at the U.S. Department of Energy observatory located at the Southern Great Plains site in Oklahoma, U.S.A. Results show that the proposed approaches are suitable for unsupervised, nonparametric inversion of large-scale datasets. The included software implementation of Tikhonov regularization is general and domain-independent, and thus can be applied to many other inverse problems arising in atmospheric measurement techniques and beyond.

8SS.4

The Particles We Don't Count Can Significantly Bias Optical Measurements.

CHUN-NING MAO, Akua Asa-Awuku, James Radney, Christopher Zangmeister, *University of Maryland*

A Cavity Ring Down Spectroscopy (CRDS) coupled with a Differential Mobility Analyzer (DMA) and a Condensational Particle Counter(CPC), is an experimental technique frequently used in lab to retrieve the aerosol extinction cross section. However, the extinction cross section is a size dependent parameter. It can be underestimated by the Mie Scattering theory when large, multiply charged particles exist in the CRDS measurement. Our experimental results show that even when an impactor was installed before the DMA, a low number density (~10 #/ccm) of large particles passed through the impactor and caused errors in extinction cross section measurement. Since the size of multiply charged particles are usually much larger than singly charged particles, 1% of the multiply charged particles can cause more than 5% relative errors in CRDS measurement. To obtain the correct extinction cross section, Tandem DMA measurement was applied to acquire the fraction of doubly charged and triply charged particles. Particles carrying more than three charges are usually out of the DMA size limitation, and their number density could be too low to measure. Since some multiply charging errors from DMA are inevitable, a theoretical method is developed to predict the fraction of the multiply charged particles in CRDS measurement. In this work, we test equations to predict the fraction of multiply charged particles and graphically identify the fraction of the multiply charged particles that would cause 5% relative errors in extinction cross section measurement. Results indicate that for 200nm size selected particles, 0.2% fraction of the particles carrying more than 3 charges could cause a 5% relative errors.

8SS.5

Calibration vs. Validation: Definitions, Best Practices, and Options in the Field. ANDREA J. TIWARI, Sebastian Schmitt, Torsten Tritscher, Juergen Spielvogel, Axel Zerrath, *TSI Incorporated*

As with any scientific or technical effort, data accuracy is important for researchers and others measuring aerosols. Terms like ‘calibration’ and ‘validation’ can be used in reference to judging instrument performance, but standard definitions for these are likely not uniformly accepted within the aerosol community. While the historical definition of ‘calibration’ has simply meant comparing two instruments to each other, in practice most people expect a ‘calibration’ to include any necessary adjustments to have been performed in order to ensure instrument performance (and thus data accuracy). Other terms like ‘validation’, ‘verification’ (and even potentially ‘sanity check’) may offer less in the way of quantitative criteria and ability to rectify any problems discovered, but these terms do not have widely-accepted definitions. This presentation proposes definitions for these terms from an aerosol instrumentation and service provider perspective.

Aerosol measurement-related applications vary widely, as do the approaches that users take to instrument performance and data accuracy. These approaches are informed in part by how desirable on-site instrument validation is for the application. In the interest of quality assurance, the European standardization committee (CEN) is introducing some standardization pertaining to ensuring instrument performance and accuracy (i.e. harmonization). We describe this range of quality-assurance approaches and applications, in order to illustrate the diversity of instrument validation needs within this community.

Performing certain checks and simple tests on a routine basis contributes significantly to ensuring proper instrument performance. This presentation will formalize some recommended routine checks (best practices) for ensuring particle measurement performance with a focus on Condensation Particle Counter (CPC) and Scanning Mobility Particle Sizer (SMPS), and will discuss other options users can consider using onsite within this ‘calibration / validation’ space.

8SS.6

Demonstration of a Calibration Standard for Aerosol Absorption Methods. CHRISTOPHER ZANGMEISTER, James Radney, *National Institute of Standards and Technology*

This study describes the characterization of a potential aerosol calibration standard for spectroscopic measurements. The material is a non-toxic, shelf-stable, H_2O-dispersible, highly absorbing carbonaceous nanomaterial. When atomized from aqueous suspension, the material forms particles with a collapsed morphology resembling aged soot or BC. The material is > 90 percent elemental carbon and has a mass absorption coefficient (MAC) and spectral dependence consistent with BC values published in the literature. The MAC at a wavelength of 532 nm decreased monotonically from 8.5 to 5.8 $m^2 g^{-1}$ for aerosol with mobility diameters between 150 nm and 500 nm. The single scatter albedo (SSA) at 405 nm and 660 nm wavelengths was a function of both wavelength and mobility diameter and increased from 0.1 to 0.4 between 150 nm to 500 nm, respectively. The absorption Ångström exponent (AAE) between $\lambda = 405$ nm and 780 nm decreased monotonically from 1.4 to 0.6 for aerosol with mobility diameters between 150 nm to 400 nm. We demonstrate that this material can be used for fast, efficient calibration of aerosol photoacoustic spectrometers and for evaluation of spectroscopic-based measurements of aerosol mass concentration using in-situ photoacoustic spectroscopy (PAS) and filter-based light attenuation measurements for up 50 $\mu g\ m^{-3}$, enabling inter-method and inter-laboratory instrument comparison.

8SS.7

A Comprehensive Test Standard for Indoor Air Quality Low-Cost PM2.5 Sensors. WILTON MUI, Xiaobi M. Kuang, Sahil Bhandari, Vasileios Papapostolou, Andrea Polidori, *South Coast Air Quality Management District*

Low-cost air sensors are a relatively new class of air pollutant monitoring devices that typically have characteristics of being compact, lightweight, portable, simple to operate, and roughly one to two orders of magnitude less expensive than research-grade or reference-grade instruments targeting the same pollutant. Despite these advantages, there are uncertainties about data quality and sensor performance. The Air Quality Sensor Performance Evaluation Center (AQ-SPEC) at the South Coast Air Quality Management District has previously published some of the few existing performance evaluation field and laboratory test methods for low-cost sensors targeting particulate matter smaller than 2.5 micrometers in diameter ($PM_{2.5}$). More recently, a new comprehensive test standard for indoor-specific low-cost $PM_{2.5}$ sensors has been developed in collaboration with ASTM International, and its relevance coincides with pandemic-related concerns of indoor particle concentrations. The new test standard is comprised of five phases conducted in an environmental test chamber with reference-grade monitors: 1) initial $PM_{2.5}$ concentration ramps using both an inorganic and an organic particle surrogate, 2) performance characterization across a range of temperature and relative humidity conditions, 3) investigating the effect of coarse particulate matter as an interferent, 4) repeated temperature cycles to simulate long-term operation, and 5) a final $PM_{2.5}$ concentration ramp using only the inorganic particle surrogate. Four sets of low-cost sensor models in triplicate were pilot-tested with this new $PM_{2.5}$ performance test standard. One sensor model tested accurately reported $PM_{2.5}$ values in the initial concentration ramp, while the other three models overestimated $PM_{2.5}$ values by about a factor of two; nonetheless all four models tested showed very high correlation with reference measurements ($R^2 > 0.99$). A variety of additional performance metrics to provide insights on other aspects of sensor performance are also deduced from the data, such as accuracy, precision, bias, climate susceptibility, interference, drift, and data recovery.

8SS.9

Performance of Correction Models for Accurate PM2.5 Estimation from Low-Cost Air Quality Sensor Data. DINUSHANI SENARATHNA, Vijay Kumar, Shantanu Sur, Suresh Dhaniyala, Supraja Gurajala, Sumona Mondal, *Clarkson University, Potsdam*

Environmental epidemiology requires accurate estimates of pollutant levels in ambient air to evaluate the health effects from long-term exposure. Among these pollutants, particulate matter smaller than 2.5 µm in diameter ($PM_{2.5}$) has been shown to be closely associated with various acute and chronic health problems. In the United States, Environmental Protection Agency (EPA) provides reliable measurements of $PM_{2.5}$ but the impact is limited by a sparse distribution of monitoring sites. Air quality measurements using low-cost sensors such as PurpleAir (PA) are currently being used to overcome this limitation. However, measurements from these sensors could be noisy, and an appropriate correction model will be required to get an accurate estimate of $PM_{2.5}$. In this work, we aim to evaluate and improve PA sensor-derived $PM_{2.5}$ using EPA data as a gold standard and determine the optimal distance between EPA and PA sites from a calibration perspective. We collected hourly $PM_{2.5}$ measurements from 14 PA sensors located in the Cook County of Chicago from August 2019 to July 2020 and developed a modeling approach that utilizes multiple regression techniques together with distance analysis. Interestingly, while considerable improvement was observed when multiple PA sensors were used in the model instead of a single PA sensor, the performance of the correction model did not depend on the relative distance of the PA sensors from the EPA sites. Additionally, our results suggest that temperature is a more influential ($R^2 = 0.60 \sim 0.80$) factor for the correction models compared with relative humidity ($R^2 = 0.50 \sim 0.60$). These correction models along with data pre-processing techniques implemented in this work could help extract accurate air quality prediction from the low-cost sensor networks.

8SS.10

Ammonium Sulfate: Good for Optical Diagnostics but Not Quite Good Enough for Calibration.

JAMES RADNEY, Christopher Zangmeister, Chun-Ning Mao, Akua Asa-Awuku, *National Institute of Standards and Technology*

Ammonium sulfate – (NH4)2SO4, AS – has seen significant use in the aerosol community as a test particle because of its ease of use, non-toxicity, nearly spherical morphology and well-known physical and chemical properties, e.g. thermal decomposition, hygroscopicity and refractive index to name a few. Historically, our lab used AS as a reference material for the co-calibration of extinction coefficient (αext) and number density (N) measurements by a cavity ring-down spectrometer and condensation particle counter, respectively, by comparing the derived extinction coefficients (Cext = αext/N) to those calculated using Mie theory and some form of effective medium approximation. Here we will present multiple years' worth of optical extinction data to highlight the variability in the measured Cext of AS. This variability demonstrates that AS can be used for diagnostic measurements with errors and uncertainties on the order of ± 10 %. To improve upon these errors and uncertainties, requires perfectly spherical nanomaterials with a better-defined refractive index, e.g. polystyrene nanospheres (PSL). Using PSL, we can co-calibrate the CRD and CPC to have precision and accuracy better than 2 %. While these values are still orders of magnitude higher than often found in gas-phase spectroscopy, it demonstrates that nanoscale heterogeneity may represent a physical limit for the use of aerosol as a calibrant.

8SS.11

Improvements to the Virkkula Filter Correction Algorithm for Measuring Carbonaceous Aerosol Optical Properties.

THEO PAIK, Patrick Sheridan, Rajan K. Chakrabarty, *Washington University in St. Louis*

Filter-based instruments, such as the particle soot absorption photometer (PSAP), are used to measure and constrain aerosol optical properties and related parameters at multiple sites worldwide. These filter-based optical measurements are subject to significant artifacts that depend on a given filter measurement system and aerosol optics. Resulting errors due to these artifacts could propagate into radiative transfer models that rely on filter-based optical data sets. Several correction algorithms have been proposed to align filter-based aerosol absorption data sets with standard reference particle-phase absorption measurements through process-based correction. Notably, Virkkula (2010) developed a simple correction scheme based on measurements of kerosene soot and “white” ammonium sulfate aerosol using a three-wavelength PSAP. Currently, the Virkkula correction algorithm is widely implemented for inferring particle-phase optical properties from filter-based measurements. It is, however, unclear how this algorithm performs for atmospherically relevant carbonaceous aerosol with spectrally-varying absorbing properties and single scattering albedo (SSA). Additionally, the applicability of this algorithm for newer filter-based optical instruments, such as the tricolor absorption photometer (TAP), has not been thoroughly evaluated. Here, we generated carbonaceous aerosol emissions with a wide range of spectrally-varying optical properties from laboratory biomass combustion. These aerosols were simultaneously sampled using a TAP, a tricolor PSAP, and integrated photoacoustic-nephelometer spectrometers at wavelengths comparable to the two filter-based photometers. First, we tested the validity of the original Virkkula's correction scheme. Next, we provide improved correction factors for the Virkkula algorithm as a function of absorbing aerosol type and SSA that could be readily implemented for analyzing archived datasets and future measurements.

Reference:

A. Virkkula, Aerosol Sci. Technol. 44, 706 (2010).

8UA.1

New Application of Gaussian Mixture Regression to Bias-Correct Low Cost PM2.5 Monitoring Data in sub-Saharan Africa.

Celeste McFarlane, DANIEL WESTERVELT, *Columbia University*

Reference grade PM2.5 monitors can serve as an important basis for the correction and calibration of low-cost sensors (LCS) for air quality monitoring. LCS, however, are affected by environmental factors such as temperature and relative humidity (RH), leaving a need for a correction factor to establish high quality data. LCS also have enormous potential for improvement in data coverage in resource-limited parts of the world such as sub-Saharan Africa. In March of 2020, a low-cost PurpleAir PM2.5 monitor was collocated for at least one year next to a Met One Beta Attenuation Monitor in Accra, Ghana which provided mediocre correlation and moderate bias between PurpleAir and BAM PM2.5 data (R^2 = 0.66, MAE = 6 μg m^{-3}). Both multiple linear and quadratic regression, which have previously been shown to reduce bias and increase correlation between PurpleAir and reference in many regions including sub-Saharan Africa, yielded minimal improvement in the correlation of the Accra collocation (R^2 = 0.71, R^2 = 0.83 respectively). Here, we develop a gaussian mixture regression (GMR) model, incorporating temperature and relative humidity, to improve the collocated PM2.5 correlation to R^2 = 0.90 and the bias to MAE = 2.5 μg m^{-3}. Gaussian mixture models (GMMs) are a clustering method with a characteristically high probabilistic nature that can help capture relationships between data and heterogenous variables for which we lack data. Using the probability distributions generated within each cluster, we use GMR to build a nonlinear regression model for the data. When coupled with time, temperature and RH, GMR can provide valuable insights towards understanding PurpleAir monitor limitations. We present the first ever application of GMR to geophysical data and demonstrate a substantial improvement over traditional methods without succumbing to overfitting.

8UA.2

Evaluating the Influence of Residential Wood Burning PM2.5 Emissions throughout the South Coast Air Basin.

XIANG LI, Melissa Maestas, Kyrstin Fornace, Scott A. Epstein, *South Coast Air Quality Management District*

The South Coast Air Basin (SCAB), which includes the greater Los Angeles metropolitan area, has had significant challenges meeting federal PM2.5 standards. As part of the fifth iteration of the Multiple Air Toxics Exposure Study (MATES V), levoglucosan measurements were conducted on over 900 filters at 10 monitoring stations over a 16-month period to serve as a marker of cellulose combustion. Extensive analysis of these measurements has provided critical insight into the spatial and temporal patterns of residential wood smoke, informing policy, PM2.5 forecasting, and outreach for the Check Before You Burn Program.

Levoglucosan measurements have also provided insight into the local influence of residential wood smoke at the Mira Loma monitoring station in Riverside County, the station with the highest annual 24-hour PM2.5 design value among all stations in the SCAB over the last decade. The monitoring station at Riverside is only about five miles away from Mira Loma. However, daily PM2.5 concentrations measured at Mira Loma were on average about 3-5 μg/m3 higher than Rubidoux from November to January.

To find out what contributes to this discrepancy, we analyzed hourly PM2.5 concentrations, levoglucosan concentrations, and meteorological data measured at both stations along with the PM2.5 speciation data (OC, EC, metals, inorganic ions) measured at the Rubidoux station over the past decade. In addition, we developed a model to predict the daily PM2.5 concentrations as a result of wood-burning based on PM2.5-to-levoglucosan ratios, meteorological conditions, and calendar parameters.

Preliminary results show that PM2.5 differences between stations are strongest in the winter months on days when the model predicted wood burning PM2.5 is elevated. This fact suggests that residential wood burning in direct proximity to the Mira Loma monitor may significantly influence the 24-hour PM2.5 design value for the SCAB. Additional levoglucosan measurements conducted simultaneously at Riverside and Mira Loma currently underway will provide further data to support or refute this hypothesis.

8UA.3

Investigating PM2.5 Composition and Sources in the San Joaquin Valley of California Using a ToF-ACSM with the Capture Vaporizer. Peng Sun, Ryan Farley, Lijuan Li, Deepchandra Srivastava, Christopher Niedek, Jianjun Li, Ningxin Wang, Christopher Cappa, Sally Pusede, Zhenhong Yu, Philip Croteau, QI ZHANG, *University of California, Davis*

The San Joaquin Valley (SJV) of California has suffered persistent particulate matter (PM) pollution despite many years of control efforts. To further understand the chemical drivers of this problem and to support state implementation plan (SIP) development for PM, a time-of-flight aerosol chemical speciation monitor (ToF-ACSM) outfitted with a PM2.5 lens and a new capture vaporizer has been deployed at the Fresno-Garland air monitoring site of the California Air Resource Board (CARB) since Oct. 2018. The instrument measured non-refractory (NR) species in PM2.5 continuously at 10 min time resolution. In this study, data acquired from Oct. 2018 to May 2019 were analyzed to investigate the chemical characteristics, sources and atmospheric processes of PM2.5 in the SJV. Comparisons of the ToF-ACSM measurement with various co-located aerosol instruments show good agreements. The inter-comparisons indicated that PM2.5 in Fresno was dominated by submicron particles during the winter whereas refractory species were found to account for a major fraction of PM2.5 mass during the autumn associated with elevated PM10 loadings. A rolling window positive matrix factorization (PMF) analysis of organic aerosol (OA) mass spectra was performed using the Multilinear Engine (ME-2) algorithm. Three distinct OA factors were resolved, including a hydrocarbon-like HOA, a biomass burning BBOA, and an oxygenated OOA. There were significant seasonal variations in PM2.5 composition and sources. During the winter, residential wood burning and oxidation of nitrogen oxides were major contributors to the occurrence of haze episodes with PM2.5 dominated by BBOA and nitrate. In autumn, agricultural activities and wildfires were found to be the main cause of PM pollution. PM2.5 concentrations decreased significantly after spring and were dominated by OOA during March to May. Our results highlight the importance of using seasonally dependent control strategies to mitigate PM pollution in the SJV.

8UA.5

Spatial Characterization of the Composition and Sources of Submicron Aerosols in the Corpus Christi - San Antonio Area Based on Mobile Measurements. SHAN ZHOU, Fangzhou Guo, James Flynn, Sascha Usenko, Subin Yoon, Sergio Alvarez, Sujan Shrestha, Rebecca J. Sheesley, Manisha Mehra, Meghan C. Guagenti, Chun-Ying Chao, Robert Griffin, *Rice University*

San Antonio is the seventh-most populous city in the US. However, in recent years, the air quality of San Antonio has worsened and aerosol mass concentrations have increased. There is a lack of characterization of the composition and chemistry of particulate matter pollution in this area. We investigated the spatial and temporal patterns in the concentration and composition of non-refractory submicron particulate matter (NR-PM_1) in Corpus Christi (upwind of San Antonio) and San Antonio using a high-resolution time-of-flight aerosol mass spectrometer deployed in a mobile laboratory from April 1 to May 19, 2021. The average mass concentration of NR-PM_1 in the Corpus Christi area was 8.2 ± 5.8 $\mu g\ m^{-3}$, comprising 45% sulfate and 38% organic matter. We observed particles that varied based on air mass origin and emission regime, including polluted oceanic air masses from the Gulf of Mexico enriched in ammonium sulfate, transported biomass burning plumes from within Texas and possible wildfire plumes from Mexico dominated by organic matter, vehicle emissions from city centers, anthropogenic emissions from refineries, and biogenic emissions between the two cities. In addition, we observed high spatial heterogeneity in aerosol concentration and composition. Sulfate was the dominant aerosol component in the airmass transported into Corpus Christi from the Gulf of Mexico; the mass concentration decreased from a peak level of 35 $\mu g\ m^{-3}$ to less than 2 $\mu g\ m^{-3}$ as the sampling location moved inland. Due to the influence of different sources, organic aerosol composition and the degree of oxidation varied substantially; organics were less oxidized as air was advected from the coast through Corpus Christi. Results from positive matrix factorization analysis that investigate the sources and processes of organic aerosol observed in this study will be discussed.

8UA.6

Elucidating Sources of Midday Ultrafine Particles in a Major City. HOSNA MOVAHHEDINIA, Nathan Hilker, Cheol H. Jeong, Greg J. Evans, *SOCAAR, University of Toronto*

Ultrafine particles (UFP; diameter less than 100 nm) can be emitted from anthropogenic sources or produced through atmospheric processes. Vehicular emissions are a major source of UFP in many urban areas. However, new particle formation (NPF) events can also make a significant contribution on some days. These events usually happen around midday and result in the formation of a large number of particles in the atmosphere which then grow and disappear through dispersion, coagulation, and condensation on the pre-existing particles. Many studies have identified these event days by looking at the total number concentration of UFP. However, our study showed that this method can result in incorrect classification of event days. In this study, we analyzed 13 years (2006-2019) of particle size distribution (PSD) data from downtown Toronto, Canada, and identified days that had a large number concentration of UFP around noon but were not NPF events. The average concentration of total UFP around midday on these days, known as midday pollution (MP) days, was about the same level as that for NPF days (MP: 34624 #/cm^3, NPF: 33623 #/cm^3), but the particle formation and growth were not evident on the PSD images of MP days. In general, MP days were ~4 times more frequent than the NPF days. The frequency of these days has decreased over the last decade (2006: 100 days, 2019: 33 days) while it has been almost constant for NPF days (2006: 10 days, 2019: 8 days). Analysis of other pollutant concentrations provides further evidence that the origin of UFP on these days differs from the NPF days.

8UA.7

Trends of Submicron Atmospheric Aerosol Number Concentrations - Effect of Legislative Regulations and Economic Transformations. Nadežda Zíková, PETRA POKORNá, Zdenek Wagner, Jakub Ondráček, Philip K. Hopke, *ICPF CAS, Prague, Czech Republic*

Atmospheric pollutant concentrations have mostly been decreasing in the last decades in the developed parts of the world, 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 aerosol 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, upgraded to ACTRIS project standards in 4/2012). Even earlier, in 2002, submicron measurements begun in Rochester, NY with a similar system.

In the over 12-years long dataset (2007 – 2019), the temporal trends in submicron aerosol concentrations (total and size-resolved) were analyzed, calculating the Mann Kendall test and the Sen slope [1]. Trends were compared to the legislative, economic, and source structure changes both in Prague and Rochester, as mitigation strategies and economic factors affecting the atmospheric aerosol concentrations differ at the two locations.

In Prague, no statistically significant trend was found with the exception of summer concentrations with an increasing trend. In Rochester, the concentrations of particles over 30 nm were decreasing ($p < 0.05$). The decrease could be connected to strategies of reducing emissions from light- and heavy-duty vehicles and electric power generation [2]. In seasonal data, the same trend was observed with the exception of autumn concentrations of particles below 300 nm showing statistically insignificant trend.

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[1] Collaud Coen et al., Atmos. Meas. Tech., 13:6945–6964, 2020.
[2] Squizzato et al., Atmos. Environ., 183, 209–224, 2018.

8UA.8

Concentrations of Atmospheric VOCs Emitted from Fireworks in Southwest Mexico City Measured by a Real-time Vocus PTR-TOF-MS. MARGARITA PALACIOS-ARREOLA, Maribel Hernández-Camarillo, Jessica Ortiz-Gutiérrez, Pawel K. Misztal, Omar Amador-Muñoz, *Universidad Nacional Autónoma de México*

Fireworks and bonfires are intensively used in New Year celebrations and various cultural and religious festivals, producing pollution plumes concentrated over short spatiotemporal scales. It is currently unknown what impact these sources have on air quality and health.

A Vocus proton transfer reaction time of flight mass spectrometer (Vocus PTR-TOF-MS) is a novel analytical technique allowing for continuous real-time measurements of volatile organic compounds (VOCs) with an ultralow detection limit (sub-ppt). Outdoor ambient air measurements were carried out at the southwest region of Mexico City, from December 7th to 14th, 2020 using a high resolution Vocus 2R PTR-TOF-MS (Tofwerk, Switzerland) operated in a positive ionization mode with H3O+ as a primary ion.

During December 12th festival (in celebrations of the Virgin of Guadalupe Day), intensive fireworks and bonfires were associated with large enhancements of numerous hydrocarbons and oxygenated VOCs. Aromatics were among the prominent compounds. Benzene reached 1,500 times higher concentration during the times of fireworks, than in the other days. Toluene and C10 aromatics rose up to 300- and 250-times higher baseline concentration, respectively. Those compounds are associated with industrial and vehicle emissions. Regarding oxygenated VOCs, the most enhanced compound was acetic acid, which increased approx. 200 times, while butanal/butanone exhibited an 80 times higher than typical concentration. In contrast, monoterpenes and sesquiterpenes retained a typical circadian behavior during the week, with a moderate spike, possibly associated to pine wood burning in bonfires, commonly burnt during this event. This is supported by the finding of increases in biomass burning tracers, such as furfural (10 times higher) and acetonitrile (3 times higher).

The VOC enhancements seem attributable to the festival based on an agreement between the time of the event, observed VOCs and also the higher concentrations of both PM10 and PM2.5 measured at the air quality monitoring station nearest to the event location.

This work aims to contribute with chemical fingerprinting of firework and bonfire plumes and discusses potential impacts of these episodic sources on urban air quality.

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8UA.9

Characterization of Urban Aerosol Sulfate Sources in Summer Using High-Resolution Aerosol Mass Spectrometry. FANGZHOU GUO, Alexander Bui, Benjamin Schulze, Henry Wallace, Matthew H. Erickson, Sergio Alvarez, Sujan Shrestha, Subin Yoon, Rebecca J. Sheesley, Sascha Usenko, James Flynn, Robert Griffin, *Rice University*

Currently the seventh most populous city in the United States and the second-most populous city in Texas, San Antonio has been one of the most rapidly growing large cities in the country over the past decade. To understand the sources of particulate matter that contributes to the degradation of San Antonio's air quality, a mobile air quality laboratory was deployed and operated in the southeast (Traveler's World RV Park) and northwest (University of Texas at San Antonio campus) of downtown San Antonio in May 2017. Chemical characterization of non-refractory submicron PM (NR-PM_1) was conducted using an Aerodyne high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS). Additional measurements included meteorological parameters and trace gas mixing ratios. Results from HR-ToF-AMS indicate large organic (2.96±1.74 $\mu g/m^3$, 54% of the total on average) and sulfate (1.78±1.23 $\mu g/m^3$, 33%) contributions at the Traveler's World site. By further categorizing the campaign into Oceanic, Near Inland, and Continental periods based on backward trajectory cluster analysis, it was observed that high sulfate concentrations were related primarily to air masses coming from the Gulf of Mexico. Utilizing empirical parameterizations from previous laboratory experiments and the ISORROPIA-II model, the contributions of methanesulfonic acid (MSA) and of organosulfates (conservative lower-bound estimate, OS_{min}) to the total sulfate signal were estimated, as were aerosol liquid water content (LWC) and inorganic aerosol pH values. The biogenic portion of the sulfate was largely influenced by the meteorological conditions, as inferred from a positive correlation between MSA concentration and LWC. However, no significant trends of OS_{min} with LWC or inorganic aerosol pH were observed. These results reveal the relative contributions of biogenic marine sources and regional anthropogenic activities to urban sulfate loadings.

8UA.10

Enhanced Aerosol Particle Growth Sustained by High Continental Chlorine Emission in India. Sachin S. Gunthe, PENGFEI LIU, Upasana Panda, Subha S. Raj, Amit Sharma, Eoghan Darbyshire, Ernesto Reyes Villegas, James Allan, Ying Chen, Xuan Wang, Shaojie Song, Mira L. Pöhlker, Liuhua Shi, Yu Wang, Snehitha M. Kommula, Tianjia Liu, R. Ravikrishna, Gordon McFiggans, Loretta Mickley, Scot T. Martin, Ulrich Pöschl, Meinrat O. Andreae, Hugh Coe, *Georgia Institute of Technology*

Many cities in India experience severe deterioration of air quality in winter. Particulate matter is a key atmospheric pollutant that impacts millions of people. In particular, the high mass concentration of particulate matter reduces visibility, which has severely damaged the economy and endangered human lives. But the underlying chemical mechanisms and physical processes responsible for initiating haze and fog formation remain poorly understood. Here we present the measurement results of the chemical composition of particulate matter in Delhi and Chennai. We find persistently high chloride in Delhi and episodically high chloride in Chennai. These measurements, combined with thermodynamic modeling, suggest that in the presence of excess ammonia in Delhi, high local emission of hydrochloric acid partitions into aerosol water. The highly water-absorbing and soluble chloride in the aqueous phase substantially enhances aerosol water uptake through co-condensation, which sustains particle growth, leading to haze and fog formation. We, therefore, suggest that the high local concentration of gas-phase hydrochloric acid, possibly emitted from plastic-contained waste burning and industry, causes some 50% of the reduced visibility. Our work implies that identifying and regulating gaseous hydrochloric acid emissions could be critical to improve visibility and human health in India.

8UA.11

Trends, Performance, and In-Field Calibration for Low Cost Particulate Matter Sensors in West Bengal, India. V. FAYE MCNEILL, Anindita Dutta, Sandhya Sethuraman, Siddharth Nobell, Rakhi Basu, Sarbani Palit, Daniel Westervelt, Debasis Dasgupta, Shairik Dasgupta, *Columbia University*

We present results from monitoring efforts using low-cost ambient particulate matter sensors (LCS) operating in West Bengal, India (Kolkata, Bandel, and environs). Two datasets are examined: a network of Purple Air sensors operating from August 2019-present and a deployment of locally developed sensors in 2020. LCS were co-located with reference-grade PM monitors (RGM) operated by the West Bengal Pollution Control Board for in-field calibration using random forest and multilinear regression. The Purple Air network performed well without additional correction for PM10 but exhibited a linear bias for PM2.5 which was corrected effectively using the calibration. After calibration, the network correctly diagnosed days as being in or out of attainment with India NAAQS 93% of the time (for both PM10 and PM2.5). Opportunities exist to complement existing government monitoring networks in India with LCS for increased spatial resolution and coverage.

8UA.12

Intra and Inter-Urban Variability in Chemical Characteristics of Fine Particulate Matter in Metropolitan Cities in India. PRINCE VIJAY, Shreya Dubey, Harish C Phuleria, *Indian Institute of Technology Bombay*

Fine particulate matter ($PM_{2.5}$) is the most critical criteria air pollutant in India and exceeds the regulatory limit in a majority of the metropolitan and class 1 cities across India and thus poses an important public health concern. In the present study, aim was to examine the seasonal variation of outdoor $PM_{2.5}$ and its chemical constituents in urban residential background locations in three metropolitan cities. Residential outdoor 24-hour averaged $PM_{2.5}$ was collected from three neighbourhoods, representing traffic, residential and industrial areas, in three metropolitan cities - Mumbai, Bengaluru and Delhi. The measurements were conducted at all locations for two weeks in two distinct seasons. Collected $PM_{2.5}$ samples were examined for trace metals and elements, elemental and organic carbon and inorganic ions using standard analytical methods. Average $PM_{2.5}$ during the winter was 121.6±31.1, 75.2±33.4 and 195.3±68.8 µg/m^3 for Mumbai, Bengaluru and Delhi, respectively, exhibiting significant differences among the cities ($p<<<0.05$). $PM_{2.5}$ levels in Mumbai were significantly lower (63.2±24.4 µg/m^3) during the summer ($p<0.05$). Weekday to weekend differences were not significant in Mumbai and Bangalore ($p>0.05$) but noticeable in Delhi ($p<0.05$). Black carbon (BC) was 1.9±0.3, 1.1±0.3 and 2.1±0.7 µg/m^3 for the three cities, respectively representing ~1% of mass. However, significant differences were not observed among the neighborhoods in the cities for both the pollutants. Water-soluble organic carbon (WSOC) was 8.5±2.3 during winter (6.5% of the $PM_{2.5}$) and 3.5±2.8 µg/m^3 during summer (2.7%) in Mumbai. Organic and elemental carbon concentrations in Mumbai during the summer were 11.2±2.7 and 1.3±0.4 µg/m^3, respectively. WSOC/OC ratios (0.1 for traffic, 0.2 for residential, and 0.6 for industrial locations) suggest the varying nature of OC at different locations in Mumbai and the differential impact of primary and secondary sources. Further chemical characterization of Delhi and Bengaluru samples and assessment of within city variation in chemical composition is underway.

9AC.1

Evidence that Halogen Bonding Catalyzes the Heterogeneous Chlorination of Alkene Aerosols.

MEIRONG ZENG, Kevin R. Wilson, *Lawrence Berkeley National Laboratory*

A key challenge in predicting the multiphase chemistry of aerosols is connecting the uptake coefficients, observed in an experiment, with the kinetics of individual elementary steps that control the chemistry that occurs across a gas/liquid interface. Here we report evidence that oxygenated molecules accelerate the heterogeneous reaction rate of chlorine gas with squalene (Sqe) aerosols. The effective uptake coefficient for Sqe is sensitive to both the aerosol composition and gas phase environment. In binary aerosol mixtures with 2-decyl-1-tetradecanol, linoleic acid and oleic acid, Sqe reacts 12-23x more rapidly than in a pure aerosol. In contrast, the reactivity of Sqe is diminished by 3x when mixed with an alkane. Additionally, small oxygenated molecules in the gas phase (water, ethanol, acetone, and acetic acid) also significantly enhance (up to 10x) the heterogeneous chlorination rate of Sqe. The formation kinetics of the chlorinated products suggest that overall reaction mechanism is not altered by the presence of these aerosol and gas phase additives, suggesting instead that they act as catalysts. Since the largest rate acceleration occurs in the presence of oxygenated molecules, we conclude that halogen bonding enhances reactivity by slowing the desorption kinetics of Cl_2 at the gas/aerosols interface, in a way that is analogous to decreasing temperature. These results highlight the importance of relatively weak interactions in controlling the multiphase reactions of aerosols in the atmosphere and indoor environments.

9AC.2

Volatile Organic Acid Formation from the Aqueous and Heterogeneous Oxidation of Isoprene-Derived Organic Aerosol Compounds.

James Cope, Karizza Abellar, Kelvin Bates, Xuan Fu, TRAN NGUYEN, *University of California, Davis*

Mixing ratios of formic acid (FA) and acetic acid (AA) are often underestimated in atmospheric models, particularly over areas with high biogenic influence. Although FA and AA formation has been suggested from the aging of biogenic organic aerosols, quantitative yields have remained elusive. This presentation discusses the FA and AA yields and formation pathways from the hydroxyl radical (OH) oxidation of major isoprene-derived organic aerosol compounds: 2-methyltetrols (2-MT) and 2-methytriolsulfates (2-MTS). We studied the aqueous OH radical oxidation of 2-MT and 2-MTS in bulk aqueous solution, as well as the heterogeneous OH oxidation of 2-MTS and a lower-volatility analog of 2-MT in suspended aerosol particles mixed with ammonium sulfate. 1H and 13C nuclear magnetic resonance (NMR) spectroscopy, high-performance liquid chromatography coupled with high-resolution mass spectrometry (HPLC-HRMS) were used to quantify organic acid yields. We demonstrate that the photochemical reactions of 2-MT, 2-MTS, and their chemical analogs are strong sources of small acids. Partitioning into the gas phase significantly effects aqueous yields. pH in the bulk aqueous phase, and aerosol water in the suspended particles, also have strong influence on the yields of organic acids. These related aerosol/bulk properties control the dissociation equilibria of organic acids, which affects both partitioning and oxidation chemistry. Kinetics, yields, product distribution, and reaction mechanisms will be discussed.

9AC.3

Acid-Catalyzed Aging of Secondary Organic Aerosols.

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

Secondary organic aerosols (SOA), formed through the gas-phase oxidation of volatile organic compounds (VOCs), can reside in the atmosphere anywhere between days to weeks. The formation of SOA takes place rapidly within hours after VOCs emissions, but they can undergo much slower physical and chemical processes throughout its lifetime in the atmosphere. The acidity of atmospheric aerosols spans a wide range, with the most acidic particles having negative pH values. The impact of highly acidic conditions on aerosol chemical composition remains uncertain. The goal of this work is to elucidate mechanisms and rates of acid-catalyzed aging of mixtures of reprehensive SOA compounds. SOA samples were generated in a continuous flow reactor and then collected using a foil substrate. Samples were extracted and aged by exposure to varying concentrations of aqueous sulfuric acid for 1-2 days. Analysis of fresh and aged samples was conducted using an ultra-liquid chromatography coupled with a photodiode array spectrophotometer and a higher resolution mass spectrometer to examine the chemical composition of SOA before and after aging. At the time of writing this abstract, we observe that SOA aged in moderately acidic conditions (pH 1) lead to small changes in the composition, while SOA aged in a highly acidic environment (pH -1) resulted in significant changes in the chemical composition. The prevailing mechanism of aging appears to be dehydration and condensation resulting in light-absorbing unsaturated products. The findings from this study will improve our understanding of SOA aging processes.

9AC.4

Evolving Toxicity Of Heterogeneously Oxidized Benzo[a]pyrene Aerosol Particles.

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 degrades PAHs, it may also lead to the formation of toxic secondary products, modulating their health impacts in important but poorly understood ways. To better elucidate the products formed from these degradation reactions, environmental chamber studies were conducted on the heterogeneous oxidation of particle-phase benzo[a]pyrene (BaP). BaP-coated ammonium sulfate aerosol particles (BaP-AS) were exposed to two common atmospheric oxidants, ozone (O_3) and OH. Reaction products and kinetics were investigated by measuring the evolving particle-phase composition with an Aerosol Mass Spectrometer (AMS). The major products observed in both reaction systems include BaP-dione isomers ($C_{20}H_{12}O_2$), BaP-lactone ($C_{19}H_{10}O_2$), and BaP-epoxide or diol ($C_{20}H_{12}O$). The reaction with OH yielded more oxygenated compounds than the reaction with O_3, suggesting OH reacts with both first- and second-generation products. Toxicity studies of BaP-AS collected from chamber experiments were examined using the high-throughput 'CometChip' assay to quantify DNA damage. Preliminary results show exposure to untreated BaP-AS exhibited increased DNA damage with increased dosage, similar to the BaP control standard. The change in toxicity of oxidized BaP-AS was measured as a function of oxidant exposure. Differences in DNA damage was related to observed changes in aerosol particle composition.

9AC.5

Chemical Modification of Protein Exposed to Urban Air.

RACHEL L. DAVEY, Erick Mattson, J. Alex Huffman, *University of Denver*

Ozone (O_3) and nitrogen dioxide (NO_2) have been shown to react with pollen proteins to induce chemical modifications like the formation of nitrotyrosine (NTyr). Proteins with these modifications have been shown to induce an immune response in animal models and could promote adverse human health effects including respiratory, cardiopulmonary, or ocular diseases. It has been hypothesized that proteinaceous material suspended in the atmosphere as particulate matter, e.g. on the surface of airborne bioparticles like pollen or spores, could undergo heterogenous reactions to produce chemically modified proteins. Nitrated proteins in and on bioparticles could thus have a negative impact on human health, especially in urban areas. As a way to investigate the protein modification process under ambient reaction conditions, bovine serum albumin (BSA) and ragweed pollen protein (Amb) samples were loaded onto filters and exposed to urban air in Denver, Colorado. Ambient air was drawn through protein-loaded filters for 1-21 days each. The nitration degree was measured via high-performance liquid chromatography (HPLC) using existing literature methods. Losses and measurement artifacts were characterized to support the experimental procedure. O_3 loss was quantified from across three commonly used particulate matter (PM) filters (Kynar, HEPA, PP). The PM filters reduced O_3 concentrations by 5-80%, with Kynar filters performing with the lowest O_3 reduction. Protein mass extraction efficiency as a function of substrate filter material and protein loading mass using both native and nitrated protein is also shown. Finally, preliminary results correlating NTyr formation in BSA and Amb exposed to various concentrations of O_3 and NO_2 in urban air are shown.

9AC.6

Quantitative Analysis on the Relationship between Aerosol Optical Properties and Chemical Composition in Urban Areas.

PAULO ARTAXO, Djacinto Monteiro dos Santos, Bruno Backes Meller, Milena Ponczek, *University of Sao Paulo*

The urban and regional climate is strongly affected by aerosol optical properties. Aerosol composition and size distribution influence the optical properties significantly. Studies have been focused on looking at aerosol source apportionment or the physical properties of particles. We intend with this study to look at the integration between aerosol composition and physicochemical properties. Measurements were performed at three urban areas: São Paulo, Manaus, and Rio Branco. São Paulo has an unusual fuel mixture. Manaus links biogenic VOCs and urban emissions leading to rapid aerosol formation, and Rio Branco is loaded with biomass-burning aerosols. The properties measured include submicron particle number size distributions (PNSD), using SMPS, Mass absorption efficiency (MAE) derived from equivalent black carbon, with Multi-Angle Absorption Photometer (MAPS) and AE33 Aethalometer, light scattering using TSI and Ecotech nephelometers. The aerosol non-refractory chemical composition was determined using a Quadrupole Aerosol Chemical Speciation Monitor (ACSM). Multiple linear regression models between PMF results from ACSM and size distribution plus optical properties reveal the association between mechanisms that control the aerosol size, optical properties, and submicron particles' composition.

For Rio Branco, the most efficient in terms of scattering was the BBOA (12.77 ± 0.63 m² g^{-1} at 532 nm), while the least efficient was the HOA (1.95 ± 0.56 m² g^{-1} at 532 nm). Regarding MAE, strong spectral dependence was detected both for black carbon and organics. For São Paulo, where 60% of PM1 mass loading was attributed to SOA and secondary inorganic aerosol, accumulation mode was mainly associated with highly oxidized OOA and traffic-related emissions. In contrast, Aitken mode shows strong contributions of sulfate and nitrate aerosols. Also, high AAE values (>2) and strong contribution of organics to the absorption coefficients were observed in São Paulo, especially under regional biomass burning influence.

9AC.7

Observations of Oxidized and Reduced Nitrogen-Containing Gases and Particles via Liquid Chromatography at a Coastal Downwind Site Demonstrate the Prevalence of Reduced Nitrogen Molecular Features.

DREW GENTNER, Jenna Ditto, Jo Machesky, *Yale University*

Reactive nitrogen compounds play key roles in atmospheric organic chemistry through reactions of organic compounds (e.g. volatile organic compounds) with NO_X (NO and NO_2), nitrate radicals (NO_3), and other oxidized nitrogen species, yielding a wide range of products with oxidized nitrogen-containing functional groups (i.e. NO_Z). Additionally, compounds containing reduced nitrogen are emitted from anthropogenic and biogenic sources (incl. biomass burning) and their secondary formation has been observed via reactions with ammonia (or small amines). Using multi-season measurements from a coastal site downwind from several major urban areas on the Long Island Sound in Connecticut, we observe a diverse array of multifunctional nitrogen-containing organic compounds in the gas and particle phase, and elevated levels of nitrogen-containing organic aerosols compared to other sites.

The functional groups comprising these nitrogenated organic aerosols were determined via offline liquid chromatography with electrospray ionization (LC-ESI) and high-resolution tandem mass spectrometry, and included reduced nitrogen groups (e.g. amines, imines, nitriles) present in both acyclic and cyclic structures, as well as functional groups commonly found in NO_Z species (e.g. organonitrates). While these nitrogenated compounds very often included oxygen atoms, the oxygen atoms were frequently independent of the reduced nitrogen functional groups and instead part of other oxygen-containing structures (hydroxyls, etc.). In the particle phase LC-ESI measurements, the prevalence of reduced nitrogen functional groups often rivaled that of oxidized nitrogen groups. In the summer, reduced nitrogen groups contributed to half of compounds with an O/N ratio < 3 and two-thirds of compounds with an O/N ratio ≥ 3, and in the winter they contributed to half and only one-eighth, respectively. Supplemental gas-phase measurements via LC-ESI indicates the presence of gas-phase reduced nitrogen compounds as possible precursors to particle-phase compounds containing nitrogen and oxygen. In all, this work highlights the prevalence of reduced nitrogen molecular features in oxygen- and nitrogen-containing compounds beyond typical NO_Z species, including those that may be the result of aqueous-phase chemistry (e.g. azoles), and provides a detailed molecular-level analysis of functionalized organic compounds in the less-studied Northeastern U.S.

9AC.8

Synergistic Multiphase Chemistry of Isoprene Hydroxy Hydroperoxides (ISOPOOH) with Sulfur Dioxide in Acidic Sulfate Aerosols Leading to Secondary Inorganic and Organic Aerosol Formation.

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. 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 and ISOPOOH play important roles in the formation of inorganic sulfate in cloud water mimics. However, there is limited information on the role of ISOPOOH in SOA and sulfate formation in wet aerosol oxidation of dissolved reduced sulfur species such as sulfur dioxide and inorganic sulfite.

In order to examine the reaction products, kinetics, and implications of ISOPOOH with aqueous sulfite, ammonium bisulfate particles were injected into the UNC 10-m3 indoor environmental chamber under humid (i.e., 72% RH) and dark conditions. After the inorganic sulfate concentration stabilized, selected concentrations of gas-phase 1,2-ISOPOOH were injected into the chamber, and aerosols showed a minimal mass increase. Gaseous SO_2 was subsequently injected into the chamber and a significant amount of aerosol mass was produced. 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), a particle-into-liquid sampler (PILS) for analysis by ion chromatography analysis (IC), and filter samples were analyzed by an ultra-performance liquid chromatography coupled to an electrospray ionization high-resolution quadrupole time-of-flight mass spectrometry (UPLC-ESI-HR-QTOFMS) to obtain offline molecular-level information. Results show that a significant amount of inorganic sulfate and organosulfates were formed rapidly after injecting SO_2, altering the chemical and physical properties of the particles including phase state, pH, reactivity, and composition. Multifunctional C_5-organic species that were previously measured in atmospheric fine aerosol samples were also reported here as reaction products, including 2-methyletrols and 2-methyltetrol sulfates that were previously thought to be only produced from the reactive uptake of isoprene-derived epoxydiols (IEPOX). Such results indicate that the multiphase reactions of ISOPOOH could have significant impacts on the atmospheric lifecycle of organic aerosols and sulfur, as well as the physicochemical properties of ambient particles.

9AC.9

Secondary Organic Aerosol Formation and Chemical Composition from Biogenic Oxygenated Terpenes.

FARZANEH KHALAJ, Véronique Perraud, Shan Gu, Celia Faiola, *University of California, Irvine*

Biogenic volatile organic compounds (BVOCs) released primarily from terrestrial vegetation contribute up to 90% of total atmospheric volatile organic compounds (VOCs) and up to 50% of the production of secondary organic aerosol (SOA) worldwide. SOA formation and composition influence aerosol climate effects and atmospheric radiative properties, but many BVOCs have not been the subject of previous laboratory SOA studies. For example, oxygenated monoterpenes are commonly emitted from plant species in Southern California's coastal sage ecosystem, but their SOA chemistry is not well understood. This study investigates SOA formation and composition from oxygenated terpenes that have been identified in sage shrub emissions, such as camphor, eucalyptol, borneol, and bornyl acetate. SOA was generated via photooxidation in an oxidation flow reactor (OFR). Continuous monitoring of ozone and particle size distributions was conducted using an ozone monitor and a scanning mobility particle sizer (SMPS), respectively. For the SOA chemical composition, samples were collected on Teflon filters and analyzed offline using an ultra high performance liquid chromatography system equipped with a heated electrospray ionization source and a high resolution Q Exactive Plus orbitrap mass analyzer (UPLC-HESI-HRMS). VOC samples were collected at the OFR inlet and outlet on absorbent cartridges and analyzed offline with a thermo-desorption gas chromatograph mass spectrometer (TD-GC-MS). SOA mass yield curves, impact of OH exposure on SOA mass yield, and high-resolution chemical composition of the SOA particles generated from these oxygenated terpenes reactions will be compared. This study sheds light on the potential role of these less-studied oxygenated terpenes in SOA formation and will help improve predictions of SOA production in a future climate where sage shrubs are expected to exhibit range expansion.

9AC.10

Low Secondary Organic Aerosol Production from Oxygenated Volatile Chemical Products.

MACKENZIE HUMES, Mingyi Wang, Sunhye Kim, Jo Machesky, Drew Gentner, Allen Robinson, Neil Donahue, Albert A. Presto, *Carnegie Mellon University*

Traditional anthropogenic Secondary Organic Aerosol (SOA) research has focused on emissions from combustion sources, including components of 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 due to their large emission factors. Current models under-predict SOA formation and the oxidation products of I/VCPs are likely an overlooked source. Various I/VCPs containing oxygen groups such as glycol ethers, esters, and oxygenated-aromatics have SOA formation potentials which have not been previously studied. 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 both molecular weight and polarity, the addition of these groups may prevent SOA formation. In this study, we oxidized common I/VCPs containing oxygen groups under high and low-NO_x conditions in an oxidation flow reactor to determine their potential as SOA precursors.

We oxidized four glycol ether I/VCPs, two oxygenated-aromatic VCPs, and two ester VCPs at 50% RH with and without NO_x present. The two aromatic ring-containing compounds (2-phenoxyethanol and 1-phenoxy-2-propanol) had SOA mass yields of approximately 15%. CIMS data demonstrated this was due to the formation of lower volatility products from the aromatics. SOA composition varied with NO_x level despite similar mass yields. Higher oxidation occurred under low-NO_x, though nitrogen content remained low under high-NO_x. All non-aromatic species had SOA mass yields below the detection limit. Overall, this supports the idea that oxygen groups can inhibit SOA formation in non-aromatic compounds and that some oxygenated VCPs may be used in consumer products without resulting in SOA production.

9AC.11

Comprehensive Product Characterization in the OH Oxidation of Dimethyl Sulfide: Effects of RO2 Fates on Sulfur Distribution.

QING YE, Matthew Goss, Jordan Krechmer, Yaowei Li, Francesca Majluf, Alexander Zaytsev, Joseph Roscioli, Manjula Canagaratna, Frank Keutsch, Colette L. Heald, Jesse Kroll, *MIT*

The atmospheric oxidation of dimethyl sulfide (DMS) from the oceans is the major source of natural sulfate aerosol globally. However, many details of the oxidation mechanism remain poorly constrained, largely due to limitations in measuring the full suite of oxidation products.

Here, chamber experiments were performed to measure product formation from OH-initiated oxidation of DMS using a suite of advanced online instruments that measured a broad suite of gas-and aerosol-phase sulfur-containing compounds. Specifically, hydroperoxymethyl thioformate (HOOCH2SCHO, HPMTF), the recently discovered compound formed from the isomerization of methylthiomethylperoxy radical (CH3SCH2OO•), was identified and quantified. The isomerization rate constant of the methylthiomethylperoxy radical is estimated to be ~ 0.1 s-1. Experiments were conducted under high and low NO level and under different temperatures to explore the fates of RO2 on the distribution of sulfur products. Over the course of 18 h atmospheric-equivalent oxidation under low NO condition (sub-ppb level NO), HPMTF is the dominant S species followed by SO2. Under high NO conditions (~50 ppb NO) and after 2 h oxidation, HPMTF does not form and the S budget is dominated by particle-phase products namely sulfate and methane sulfonic acid. Under low NO conditions and lower temperature (10 C), HPMTF is still the major product formed from the abstraction channel while there is an increased fraction of products from the addition channel including DMSO and DMSO2. Lastly, the effective reaction rate coefficients of HPMTF and methyl thioformate with OH were also estimated.

9IM.1

A Photothermal Sensor Concept for Black Carbon Mass Concentration Measurement.

ULRICH RADESCHNIG, Markus Knoll, Benjamin Lang, Alexander Bergmann, *Graz University of Technology*

The impact of black carbon (BC) on human health and its role as potential accelerator of climate change place it among major scientific and policy concerns. Quantifying BC with adequate sensitivity and selectivity is challenging and yet requires expensive and heavy equipment. A highly promising concept for reliable, low-prized and miniaturized sensing devices resides in the concept of photothermal spectroscopy (PTS). To demonstrate this, we have developed a sensor concept for BC mass concentration by exploiting a fiber-coupled Fabry-Pérot interferometer (FPI) combined with a low-cost laser diode as excitation source. Here, periodic irradiation of the BC particles caused a periodic change in temperature and thus in the refractive index, monitored with the FPI. The FPI featured a 1 x 2 mm (width x length) air spaced etalon, through which an air flux with a specified BC mass concentration was guided. The excitation was realized by focusing a laser beam with a wavelength of 860 nm and an optical peak-to-peak power of 1.5 W onto the particles upstream of the etalon. A modulation frequency of 300 Hz and a gas flow of 0.34 l/min was chosen, offering a favorable signal-to-noise ratio while providing a good balance between flow noise and gas exchange time. BC particles were generated with a commercially available soot generator and the adjusted mass concentration in each case was compared to a reference instrument. The concentrations were quantified up to 1.2 mg/m^3, and the background corrected signal amplitude yielded a linear correlation to the reference instrument. A limit of detection of approximately 15 µg/m^3 (3σ) was determined. BC particles that were not thermally excited (= excitation beam off) did not exhibit a detectable signal in the FPI etalon. Our results provide a promising sensing method for monitoring BC mass concentrations that impresses through its ability of miniaturization.

9IM.2

Performance of Black Carbon Instruments for Extractive Remote Emission Sensing. MARKUS KNOLL, Benjamin Lang, Alexander Bergmann, *Graz University of Technology*

Black carbon (BC) is well known for having an impact on health and our environment, whereby combustion-based vehicles are one of the main contributors. Studies have shown that comparatively few vehicles are responsible for a large fraction of the overall particulate emissions. However, current enforcement strategies are ineffective in identifying these high emitting in-use vehicles. Remote emission sensing (RES) is a promising approach for identifying these high emitters. Commercial RES systems are delivering accurate emission factors for gaseous species but lack accuracy for particulates. Extractive point sampling (PS) is one potential approach for measuring particulates remotely. Due to the transient nature of emission events caused by passing vehicles and exhaust dilution by ambient air, instruments must be able to capture those events and resolve small concentrations. In studies examining such extractive approaches, laboratory-grade instruments like the Aethalometer AE33 (Magee Scientific) have been used.

In this work, a custom-designed photoacoustic BC sensor (PA-BCS) optimized for RES is compared to two state-of-the-art BC instruments for their applicability in PS. These are an AE33 and a Microsoot Sensor Plus (MSSPlus, AVL List GmbH). The instruments are compared concerning their limit of detection (LOD), sensitivity, and response time, which are essential factors for RES.

A comparable LOD (~1 µg/m^3 at 1 s averaging time) could be reached for all instruments. Measurements with varying BC concentrations showed high correlations (R^2 > 0.98) between the instruments. Response time measurements revealed that the PA-BCS and MSSPlus feature significant shorter rise and fall times than the AE33. Comparing the deviations between the responses, considerable differences could be observed between the two photoacoustic instruments (PA-BCS, MSSPlus) and the AE33. These investigations bring along more insights into the applicability of these instruments in point sampling RES.

9IM.3

Performance Assessment and Field Operation of a Portable Optical Particle Spectrometer (POPS). FAN MEI, Mikhail Pekour, Jason Tomlinson, Beat Schmid, Darielle Dexheimer, Casey Michael Longbottom, *Pacific Northwest National Laboratory*

Given that the aerosol population distributes heterogeneously in the vertical and horizontal dimensions, accurate representation of atmospheric aerosol properties is a long-standing problem in atmospheric research. This study focuses on determining the operational envelope of a POPS for in-situ airborne measurements. It suggests a POPS can maintain its performance under different environmental conditions as long as the laser temperature remains above 25 C and the aerosol flow temperature inside the optical chamber is 15 C higher than the ambient temperature. The comparison between POPS and an Ultra-High Sensitivity Aerosol Spectrometer (UHSAS) suggests that the coincidence error is less than 25% when the measured number concentration is less than 4000 cm-3. The measured size accuracy by both instruments remained unaffected up to 15,000 cm-3. While both instruments' sizing accuracy is affected by the aerosol chemical composition and morphology, the influence is more profound on the POPS.

9IM.4

A Simulated Respiratory System for Secondhand Smoke Generation and Aerosol Toxicological Studies. WEIXING HAO, Kapiamba Kashala Fabrice, Huang Yue-Wern, Yang Wang, *Missouri University of Science and Technology*

Secondhand smoke endangers both the environment and the health of non-smokers. Exposure to secondhand smoke from tobacco products can cause both acute and chronic health impacts. However, secondhand smoke generated from Electronic Nicotine Delivery Systems (ENDS) has not been thoroughly studied. Due to the scarcity of repeatable data generated by volunteers, a simulated respiratory system that generates representative secondhand smoke will be significant for studying the physical, chemical, and toxicological properties of the smoke. In order to generate representative secondhand smoke aerosols, the simulated respiratory system needs to mimic the particle deposition of smoke particles. To capture the size-dependent deposition efficiency, the International Commission on Radiological Protection (ICRP) developed the human respiratory tract model for radiological protection that describes the deposition efficiencies in extrathoracic, bronchi, and alveoli regions of the respiratory system.

Enlightened by our recent study on characterizing size-dependent filtration efficiency of common household fabric materials, we identified three filter media that generate nearly identical filtration efficiencies compared to three regions of the human respiratory system over a wide submicron size range. It is therefore feasible to combine these filter materials to construct a simulated human respiratory system in aerosol deposition and the generation of representative secondhand smoke. In this study, we demonstrated the performance of the proposed respiratory system under various sampling flow rates and relative humidities. The difference of aerosol deposition efficiencies between the simulated respiratory system and the ICRP model was below 10% in the size range of 30 to 500 nm. Additionally, we compared the properties of tobacco cigarettes and ENDS secondhand smoke particles to those of primary smoke particles. Such a system can facilitate the laboratory studies of secondhand smoke due to its simple structure, high repeatability, ease of control, and free of human subjects.

9IM.5

Using Soft Aerosolization and Sampling Techniques for the Conservation of Virus Infectivity during Airborne Exposure Experiments. GHISLAIN MOTOS, Kalliopi Violaki, Aline Schaub, Shannon David, Tamar Kohn, Athanasios Nenes, *EPFL, LAPI, Lausanne*

Recurrent epidemic outbreaks such as the seasonal flu and the ongoing COVID-19 are disastrous events to our societies both in terms of fatalities, social and educational structures, and financial losses.

Further scientific research thus needs to be conducted to better understand the mechanistic processes that lead to airborne virus inactivation as well as the environmental conditions favourable to these processes. In addition to modelling and epidemiological studies, chamber experiments offer to simulate everyday life conditions for virus transmission. However, the current standard instrumental solutions for virus aerosolization to the chamber and sampling from it use high fluid forces and recirculation which can be highly damaging to the biological material (Alsved et al., 2020) and also do not represent the most relevant production of airborne aerosol in the respiratory tract.

In this study, we utilized two of the softest aerosolization and sampling techniques: the sparging liquid aerosol generator (SLAG, CH Technologies Inc., Westwood, NJ, USA), which forms aerosol from a liquid suspension by bubble bursting, thus mimicking natural aerosol formation in wet environments (e.g. the respiratory system but also lakes, sea, toilets, etc…); and the viable virus aerosol sampler (BioSpot-VIVAS, Aerosol Devices Inc., Fort Collins, CO, USA), which uses condensational growth to gently collect particles down to a few nanometres in size. We characterize these systems with particle sizers and biological analysers using non-pathogenic viruses such as phages suspended in surrogate lung fluid and artificial saliva. We compare the size distribution of produced aerosol from these suspensions against similar distributions generated with standard nebulizers, and assess the ability of these devices to produce aerosol that much more resembles that produced in human exhaled air. We also assess the conservation of viral infectivity with the VIVAS vs. conventional biosamplers.

9IM.6

Size Distribution and Electrostatic Charge Measurements for Disinfectant Droplets of Electrosprays. QINGFENG CAO, Seong Chan Kim, Qisheng Ou, Chenxing Pei, David Y. H. Pui, *University of Minnesota*

The COVID-19 disease has caused significant harm to the societies of many countries worldwide. Thus, it is crucial to conduct proper indoor cleaning with disinfectant to reduce the possibility of transmission of the coronavirus. This study is aimed to evaluate the droplet size distributions and mean charge level of two electrosprays that are commonly used for spraying disinfectant on indoor surfaces. One sprayer has three nozzle settings with the nominal droplet size being 40 µm, 80 µm and 110 µm, respectively, while the other sprayer has only one nozzle setting with a finer droplet size distribution. Two different disinfectant solutions were tested during our measurements. The Global Sizing Velocimeter (GSV) system (TSI Model GSV-1000) was applied to characterize the droplet size distributions generated by the two sprayers, which is a global imaging technique for simultaneous size and velocity measurement of transparent and spherical particles over a two-dimensional measurement region. The deflection velocity method was then applied to determine the droplet charge, where two parallel metal plates with an electric field intensity of 1 kV/cm was installed at the measurement area, deflecting the charged droplets in between. The GSV system was then applied to track the deflection velocity in the horizontal direction for each detected droplet, based on which the corresponding electrostatic charge was calculated. This investigation provides an effective approach for measuring the size distribution and electrostatic charge for disinfectant droplets of electrosprays.

9IM.7

Using CFD Method to Study the Particle Transportation Characteristics through a Critical Orifice. DA YANG, Suresh Dhaniyala, Pedro Campuzano-Jost, Jose-Luis Jimenez, Dongwook Kim, Hongyu Guo, *Clarkson University*

Low-pressure aerosol measurements often require sample flows to pass through a critical orifice and the fate of particles through the orifice determines the accuracy of these measurements. Despite the fact that orifice systems are integral to many aerosol measurements, we have limited knowledge of the aerosol transport efficiency through them. Modeling the transport of aerosol particles through a critical orifice is complicated by the interaction of super-sonic flow structures, turbulence, non-continuum effects, and strong gradients in flow velocities. In this study, we use computational fluid dynamics (CFD) software, FLUENT 18.1, to model flow through an orifice under different orifice sizes, downstream pressures, and downstream geometries and compare our simulation results to experimental data. We demonstrate the importance of orifice downstream geometry and associated flow features in critically determining size-dependent particle penetration curves.

9IM.8

Evaluation of Electro-sprayer Performance by Using Fluorescent Tracer. DONGBIN KWAK, Seong Chan Kim, Thomas H. Kuehn, David Y. H. Pui, *University of Minnesota*

Due to the ongoing COVID-19 pandemic situation, evaluation to mitigate the risk of transmission of the SARS-CoV-2 virus in an indoor environment are urgently required. Among the various types of disinfectant methods, electro-spraying is often applied to decontamination in public places due to its unique characteristics. Monomodal distribution with a peak size of ~100 µm occurred for the uncharged droplets, but if there is an electrostatic charge on the droplets, a bimodal distribution with peak sizes of ~10 and ~100 µm was found. As a result, the increase of effective contact area due to small progeny droplets was determined as 30-50% for the same sprayed amount of solution. The wraparound effect was examined on two different cylinders: copper (Cu) and polyvinyl chloride (PVC) pipe. When the target surface was not charged (Cu 0 kV and PVC 0 kV), the average normalized concentrations on the back side of the cylinder (????=180°) was increased by around 67% for charged droplets. However, when the target surface was highly charged (PVC –19 kV), the average normalized concentrations at ????=180° was increased more than two times for charged droplets.

9IM.10

Characterization and Application of a Novel Wide-Range SMPS. Sebastian Schmitt, AXEL ZERRATH, Torsten Tritscher, Jacob Scheckman, Amine Koched, Juergen Spielvogel, Thomas Krinke, Oliver F. Bischof, *TSI Incorporated*

Characterization and continuous monitoring of ambient ultrafine particles (UFP) has been a topic in aerosol research for the last three decades. Various particle counters and sizers have been used to study number concentrations and size distributions, along with particulate matter and gas measurements. With much experience gained during this time, Europe is even making the next step and harmonizes these measurements with two European standards: The CEN/TS 16976:2016 guideline on “Ambient air – Determination of the particle number concentration of atmospheric aerosol”, and the CEN/TS 17434:2020 on “Ambient air - Determination of the particle size spectra of atmospheric aerosol using a Mobility Particle Size Spectrometer (MPSS)”.

This study will introduce a newly developed wide-range Scanning Mobility Particle Sizer (model 3938W50, TSI Inc., USA). This system includes the well-known Classifier platform (model 3082, TSI Inc.) as well as the CEN 16976-compliant Condensation Particle Counter (CPC model 3750-CEN, TSI Inc.). A new Differential Mobility Analyzer (DMA, model 3083, TSI Inc.) is introduced to cover the entire required size range from 10 to 800 nm in one scan. It is a commercial version of the Vienna DMA (Winklmayr et al. 1991) with a custom-design licensed from TROPOS Leipzig. Existing SMPS systems can be upgraded with it, together with a dedicated relative humidity and temperature sensor (model RHT3000, TSI Inc.) as well as a new version of the Aerosol Instrument Manager software.

We will present first results from calibration measurements and an instrument comparison with atmospheric aerosol following the recommendations given in the CEN technical specifications. We show a thorough evaluation of the first units of this novel wide-range SMPS using both laboratory-generated as well as ambient aerosol sampled from an urban location. Total integrated number concentration data are compared to a stand-alone CPC used as concentration reference.

First results display an excellent agreement in total number concentrations from two SMPS systems equipped with DMA models 3083 and 3081, and the reference CPC. Finally, measurements of an atmospheric aerosol using a novel, fully integrated measurement setup including an ambient sampling system for UFP will be presented.

9IM.11

Development of a Humidified Single Scattering Albedometer (H-CAPS-PMssa).

CHRISTIAN CARRICO, Tyler Capek, Kyle Gorkowski, Allison Aiken, Claudio Mazzoleni, Manvendra Dubey, *New Mexico Institute of Mining and Technology*

We report the development and validation of a new humidified aerosol single scattering albedometer to quantify the effects of water uptake on submicrometer particle optical properties. The instrument simultaneously measures in-situ aerosol light extinction (σ_{ep}) and scattering (σ_{sp}) using a cavity-attenuated phase shift-single scattering albedo particulate matter (PM) monitor (CAPS-PM_{SSA}, Aerodyne Research, Inc.). It retrieves by difference aerosol light absorption (σ_{ap}) and directly quantifies aerosol single scattering albedo (SSA), the aerosol 'brightness.' We custom built a relative humidity (RH) control system using a water vapor-permeable membrane humidifier and coupled it to the CAPS-PMSSA to enable humidified aerosol observations. Our humidified instrument (H-CAPS-PM_{SSA}) overcomes problems with noise caused by mirror purge-flow humidification, heating, and characterizing cell RH. Careful angular truncation corrections in scattering, particularly for larger particles, were combined with empirical observations. Results show that the optimal operational size to be Dp < 400 nm. The H-CAPS-PM_{SSA} was evaluated with several pure single-component aerosols including ammonium sulfate ($(NH_4)_2SO_4$), absorbing nigrosin, and levoglucosan, an organic biomass smoke tracer. The measured σ_{ep}, σ_{sp}, and the derived optical hygroscopicity parameter (κ) for size-selected ammonium sulfate are in good agreement with literature values. For dry size-selected nigrosin in the $100 < D_p < 400$ nm range, SSA values increased from ~0.3 to 0.65 with increasing D_p. The enhancement in nigrosin σap at RH = 80% was a factor of 1.05 to 1.20 relative to dry conditions, with the larger particles showing greater enhancement. SSA increased with RH with the largest fractional enhancement measured for the smallest particles. For polydisperse levoglucosan, we measured an optical κ of 0.26 for both light extinction and scattering and negligible absorption. Our new instrument enables reliable observations of the effects of ambient humidity on mixed aerosol optical properties, particularly for light-absorbing aerosols whose climate forcing is uncertain due to measurement gaps. Companion work will examine the hygroscopic behavior of brown carbon surrogates and absorbing mixtures.

9IM.12

A Laminar Gas Inlet for High-speed Aircraft Sampling.

DA YANG, Suresh Dhaniyala, Rainer Volkamer, Roy Lee III Mauldin, *Clarkson University*

Aircraft sampling of aerosol and gas samples is complicated by the interaction of samples with inlet walls. The impact of wall-contact on gas-sampling is well recognized but poorly quantified. Here, we study an inlet designed to operate on the NCAR GV aircraft to sample gas phase constituents at high accuracy under laminar flow condition. We evaluate the connections between inlet geometry parameters and operating conditions to turbulence in the sample flow and establish ideal design parameters and flow conditions for wall-contact free sampling. We use computational fluid dynamics (CFD) modeling to simulate flow in and around the inlet and integrate these simulations with gas-phase diffusion modeling for this study. The modeling predictions will be compared with high-speed wind-tunnel measurements that are being planned for summer.

9SS.1

Improving Quantitative Analysis of Spark-Induced Breakdown Spectroscopy: Multivariate Calibration of Toxic Metal Particles Using Machine Learning.

HANYANG LI, Leonardo Mazzei, Christopher Wallis, Anthony S. Wexler, *University of California, Davis*

We have recently developed a low-cost spark-induced breakdown spectroscopy (SIBS) instrument for *in-situ* analysis of heavy metal particles nebulized from aqueous solutions. In this work, we investigated the application of machine learning methods to improve the quantitative analysis of elemental mass concentrations measured by this instrument.

Compared to the classical univariate calibration approach used in spectral analysis, multivariate calibration approaches have been found to be beneficial to eliminate matrix effects and enhance analytical sensitivity. In this context, we applied the machine learning methods of least absolute shrinkage and selection operator (LASSO), partial least squares (PLS) regression, principal component regression (PCR), and support vector regression (SVR) to develop multivariate calibration models for 13 types of toxic metals, some of which are included on the US EPA hazardous air pollutants (HAPS) list (e.g., Cr, Cu, Mn, Fe, Zn, Co, Al, K, Be, Hg, Cd, Pb, and Ni). The performance of the proposed models was compared to that of univariate calibration models for each analyte, using coefficient of determination (R2) and root mean square error. By computing the limit of detection (LOD) derived by the proposed models, we found that multivariate models tend to have lower LOD than univariate models.

Furthermore, we assessed the applicability of the proposed models for quantifying elemental concentrations in mixtures of toxic metals, serving as independent validation datasets. Among the various models, the mass concentration predicted by the LASSO model shows the best agreement with known concentrations of each analyte. In contrast, SVR performs relatively poorly. Ultimately, the LASSO model developed in this work is a very promising machine learning approach to quantify mass concentration of toxic metals using our recently-developed SIBS instrument.

9SS.2

Characterising the Silver Particle Generator: The New Silver Standard.

MARTIN IRWIN, Jacob Swanson, Vincius Berger, Umesh Sonkamble, Adam M Boies, Hans-Joachim Schulz, *Catalytic Instruments*

There currently exist few commercial options for the generation of solid aerosol particles in the 1-100 nm size range. These options include spark generators, tube furnaces, electrosprays, and gas burners utilizing diffusion flames. Thus, there is a need for additional options for a simple-to-use, particle generator capable of producing sufficiently high concentrations of small, solid aerosol particles. Uses for such a device include the calibration of condensation particle counters, measuring filtration efficiencies, and the calibration and complex measurements made possible with specialist aerosol equipment. Silver particles can be used as a proxy for soot particles but given their single elemental composition this approach may offer reduced uncertainties to other generation techniques.

Tube furnaces can be used to generate silver nanoparticles for calibrated CPCs, but aside from the size, cost, and inconvenience of a tube furnace, it is challenging to generate repeatable concentrations and size distributions from a typical tube furnace.

Here we present the characterisation of a new Silver Particle Generator, capable of producing sufficiently high concentrations of particles in the 1 - 50 nm size range. Data presented includes CPC calibration and repeatability measurements across its operational range. This novel Silver Particle 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 greatly enhanced compared to a typical tube furnace. Further, day-to-day variability is greatly reduced, in both concentration and size domains. Thermal cycling has been optimised, and the device is operational from standby in under 10 minutes. Importantly, our novel and patented design allows for a more compact device that allows for lower energy consumption.

9SS.3

Developing Particle Standards to Improve Measurement and Model Performance. JAMES SMITH, Nicole Riemer, Chongai Kuang, Manjula Canagaratna, Philip Croteau, Cassandra Gaston, Jose-Luis Jimenez, Murray Johnston, Arthur J. Sedlacek, Ernie R. Lewis, Christopher Cappa, Yan Feng, Rajan K. Chakrabarty, Markus Petters, Paul DeMott, *University of California, Irvine*

This poster provides an overview of a recent effort within the Department of Energy’s Atmospheric Systems Research Program to bring together theorists, modelers and experimentalists in order to identify improvements to existing aerosol standards or articulate needs for new types of standards that will both aid in interpreting lab and field measurements as well as assure that aerosol measurements address modeling needs. We highlight methods for generating aerosol standards and the application of those standards to instrument calibration. We focus on methods that could be employed in the near term with established technologies, as well as improvements needed to address current needs in their respective research areas that represent “unsolved challenges” in their field. We cover a broad range of disciplines within aerosol science, including the measurement of aerosol size distribution and composition, optical properties, cloud condensation nuclei (CCN), and ice nucleating particles (INPs).

9SS.4

Characterization and Quantification of Novel Ambient Organic Aerosol Compounds using Machine Learning and the UCB-GLOBES Mass Spectral Database. EMILY FRANKLIN, Lindsay Yee, Robert Weber, Paul Grigas, Allen Goldstein, *University of California, Berkeley*

The chemical composition of ambient organic aerosols plays a critical role in driving their climate relevant properties and holds important clues to their sources and the formation mechanisms of secondary aerosol material. In most environments, this composition remains incompletely characterized. Mass spectral analysis of organic aerosol material collected during several recent ambient sampling campaigns consistently shows that >80% of individually catalogued compounds lack definitive mass spectral matches in the literature or NIST/NIH/EPA mass spectral databases. This creates significant challenges in utilizing the full analytical capabilities of techniques which separate and generate mass spectra for complex environmental samples. In particular, TD-GCxGC-MS achieves advanced separation of complex organic samples with two GC columns in sequence, with each individual species characterized by its 1st (volatility) and 2nd (polarity) dimension retention times and 70 ev EI mass spectrum. Typically, high hundreds to low thousands of individual organics are isolated from any given sampling medium, yet the majority cannot be identified or quantified by traditional means. In this work, we develop the use of machine learning techniques and further update the Goldstein Library of Biogenic and Environmental Spectra (UCB-GLOBES) to quantify and characterize novel organic material. A random forest model trained and tested on a known 135 component custom representative external standard predicts the quantification factors of novel environmental organics based on position in volatility-polarity space and mass spectrum, enabling reproducible, efficient, and optimized quantification of novel environmental species. Intercomparison between mass spectra, both known and novel, identified across a wide range of ambient conditions as well as from single precursor oxidation experiments through UCB-GLOBES database enables the identification of new tracers of specific atmospherically relevant oxidation mechanisms. Finally, clustering of novel environmental spectra based on chemical similarity provides insight into the true chemical complexity of organic aerosol.

9SS.5

Optical and Physical Properties of Manufactured Carbon Black Particles. TIMOTHY ONASCH, Brian Heffernan, Richard Miake-Lye, Andrew Freedman, *Aerodyne Research, Inc.*

To date, there are no black carbon or soot particle-based absorption standards to establish traceable calibrations for instruments that measure these combustion-generated particle types. Here we report on the optical and physical properties of six select manufactured carbon black particles to assess their applicability as potential absorbing particle standards. Samples of commercially available surface-modified carbon black particles were generated by water-based atomization and diffusion drying. Monodisperse distributions were selected with a Cambustion Aerodynamic Aerosol Classifier. Particle mass and size (i.e., electrical mobility) were measured. Mobility-measured effective densities of these particles varied between particle types, but all decreased as a function of size. Optical properties were measured using a Cavity Attenuated Phase Shift (CAPS) Single Scatter Albedo (SSA) monitor operating at 630 nm. Measured mass absorption coefficients (MAC) varied between particle types and typically exhibited a maximum value between 100-400 nm, where the measured SSA values were increasing rapidly with size. These results will be discussed in the context of potential absorbing particles standards.

9SS.6

Evaluating the Consistency of All Submicron Aerosol Mass Measurements (Total and Speciated) for the NASA Atmospheric Tomography Aircraft Mission (ATom). HONGYU GUO, Pedro Campuzano-Jost, Benjamin A. Nault, Douglas Day, Jason Schroder, Jack Dibb, Eric Scheuer, Maximilian Dollner, Bernadett Weinzierl, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

Aerosol intercomparisons are inherently complex, as they convolve instrument-dependent detection efficiencies vs. size and variations of the sampled aerosol population, in addition to differences in detection principles. The NASA ATom mission sampled the remote marine troposphere 86S-82N and 0-12.5km in four aircraft deployments, carrying an advanced and well-calibrated aerosol payload. This provides a unique opportunity to explore the agreement of the different instruments over a large range of conditions and improve our understanding of the various instrumental uncertainties, including the overall Aerosol Mass Spectrometer (AMS) calibration uncertainties. During ATom, special attention was paid to characterize the AMS size-dependent transmission, which is critical for accurate comparisons across instruments with inevitably different size cuts. Good agreement was found between the AMS calculated volume (including the black carbon from an SP2 instrument) and Aerosol Microphysical Properties (AMP) after applying the AMS inlet transmission (regression slope = 0.949 and 1.083 for ATom-1&2, respectively; SD = 0.003). The comparisons for sulfate, OA, and seasalt (the three main components of the remote PM1 aerosol) measured by AMS with the PALMS showed similar consistency once differences in particle detection at different sizes were accounted for. Similarly, comparisons with sulfate from SAGA (IC) filters showed good consistency once episodes with large supermicron mass were filtered out. Comparisons of the AMS with the SAGA mist chamber IC sulfate were affected by the variable time response of the latter instrument but were overall consistent. Overall, no evidence for AMS calibration artifacts or unknown sources of error was found for the mostly aged air masses encountered in ATom. A comprehensive evaluation of the different sources of uncertainty and their impact on the comparisons was performed, and factors to be considered for performing such intercomparisons and improving the reliability of submicron mass quantification in the future are discussed.

9SS.8

Is It Possible to Overcome the Lack of Authentic Standards in Quantification of Biogenic Secondary Organic Aerosol Tracers? DANIEL BRYANT, Alfred Mayhew, Sri Hapsari Budisulistiorini, David Topping, Andrew Rickard, Jacqueline Hamilton, *University of York*

Biogenic secondary organic aerosol (BSOA) is a key contributor to organic aerosol and analysis at a molecular level allows a greater understanding of formation pathways and individual compound contributions. Liquid chromatography (LC)/high-resolution mass spectrometry (HRMS) is a powerful technique for targeted and non-targeted analysis of SOA. However, accurate quantification is reliant on authentic standards for which subsets of SOA such as BSOA are limited. Recent studies synthesising authentic BSOA standards show large differences in the ionisation efficiencies of BSOA tracers when using electrospray ionisation. This highlights an important issue with MS aerosol measurements, where direct-injection studies often assume equal ionisation efficiencies for identified species, while some LC-MS studies use proxy standards for different compound classes. Both could lead to significant under/overestimation of the contributions of individual BSOA tracers to aerosol metrics or average BSOA composition. This study aims to establish a method for more reliable quantification of BSOA species without the need for authentic standards.

This study proposes quantification based on the prediction of relative ionisation efficiency (RIE) factors established on chemical structure and properties. RIE's were determined for 90 authentic standards across a broad range of functionalities, relative to pinonic acid. The RIE's were coupled to structural descriptors and a random forest model developed to predict the RIE's of BSOA compounds without authentic standards. BSOA species were then quantified using the predicted RIE factors in samples collected in Beijing. This resulted in a large reduction in the BSOA concentrations measured when compared to using cis-pinonic acid to calibrate the BSOA, with the impacts on common aerosol metrics (O:C, H:C, OSc) discussed. This study provides initial evidence that the structures of BSOA tracers can cause large variability in their ionisation efficiencies, and that future work is needed to develop alternative, synthesis free strategies.

9SS.9

Predicting Glass Transition Temperature and Viscosity of Organic Molecules via Machine Learning and Molecular Embeddings. TOMMASO GALEAZZO, Manabu Shiraiwa, *University of California, Irvine*

Modeling secondary organic aerosols (SOA) rely on accurate representation of physical properties of semi-volatile organic species composing atmospheric particles. Notably, partitioning of SOA species between the gas and particle phases is highly influenced by particle phase state and viscosity. SOA viscosity can be estimated from the glass transition temperature (T_g) of the constituting compounds, which can be predicted from the elemental composition of individual organic molecules. For accurate predictions, information on molecular structure and functional groups would need to be considered for modeling of complex SOA mixtures.

Here, we introduce a new T_g prediction method powered by a machine learning (ML) model and by "molecular embeddings", recently developed high-dimensional descriptors of chemical species. Molecular embeddings are developed from word2vec and Morgan algorithm representations of chemical species extracted from SMILES (i.e. mol2vec). We have trained state-of-the-art ML models on a large database of experimental T_g data of pure organic species and their corresponding molecular embeddings. Different algorithms have been explored for accuracy in predicting T_g. The final T_g prediction method is built on top of an Extreme Gradient Boosting (XGB) model and it largely outperforms previous T_g parametrizations. The new ML powered model has a mean absolute error of 19.0 K and a R^2 of 0.97, it accounts for atom connectivity within molecules and it can predict different T_g for compositional isomers. The new ML model can also reproduce experimental viscosity data and quantify the influence of number and location of functional groups within a molecule on pure compounds viscosity. This new ML powered T_g model can be exploited to predict viscosity in numerical models involving organic species, with future applications that go beyond aerosol chemistry and extend to modeling of organic molecules.

9SW.1

Examination of Smoke Marker Ratios from Wildfires.

AMY P. SULLIVAN, Sonia Kreidenweis, Emily Fischer, Bret Schichtel, Jeffrey Collett, *Colorado State University*

One of the main sources of organic carbon (OC) and water-soluble organic carbon (WSOC) aerosols is biomass burning. Therefore, it is important to be able to determine the contribution of biomass burning to the total OC or WSOC concentration. Smoke marker measurements provide one of the most common methods to make this determination. The key to using the smoke marker approach is knowing the smoke marker to OC or WSOC ratio at the source. However, there is still much uncertainty in these smoke marker ratios, especially for biomass burning emissions from wildfires. Therefore, in this work, we aim to try to better understand the constraints and variability that should be placed on smoke marker ratios when attempting to determine the contribution of smoke from wildfires. Comparisons between source samples collected at the Fire Science Lab in Missoula, MT from the FLAME (Fire Science at Missoula Experiment) studies and samples collected from ground-based and airborne sampling of various wildfires across the U.S. will be made. Results for smoke markers such as potassium and levoglucosan will be presented. How parameters such as fuel type and aging might play a role on smoke marker ratios will also be discussed.

9SW.2

Photolysis of Biomass Burning Organic Aerosol, Chemical Transformations and Photo-Bleaching.

RACHEL O'BRIEN, Hongmin Yu, Natalie Warren, Marley Adamek, Aron Jaffe, Christopher Lim, Christopher Cappa, Jesse Kroll, Carolyn Jordan, Bruce Anderson, *William & Mary*

Brown carbon (BrC) in aerosol particles and cloud droplets can contribute to climate warming by absorbing solar radiation in the visible region of the solar spectrum. Large uncertainties remain in our parameterization of this warming, in part due to a lack of knowledge about atmospheric lifetimes for the chromophores (the light absorbing structures in BrC molecules). An important removal pathway includes chemical transformations that fragment the chromophore, thus removing its ability to absorb visible light. However, the photochemical loss rates measured in the laboratory often do not match what is observed in ambient measurements. There are also different amounts of photo-resistant BrC, which is a fraction of the mixture that does not rapidly bleach. An important BrC source in the atmosphere is biomass burning and the overall photochemical decay rates for these emissions are important to quantify to improve our parameterizations of their radiative effects. Here we show results for laboratory studies of FIREX filter samples probing the role of water vapor for aerosol particles irradiated on a filter. Kinetic analysis of photobleaching in aqueous solutions demonstrates that an intermediate photolysis rate should be included to improve predictions for BrC lifetimes in the atmosphere.

9SW.3

Dilution and Photooxidation Driven Processes Explain the Evolution of Organic Aerosol in Wildfire Plumes. ALI AKHERATI, Charles He, Lauren A. Garofalo, Anna Hodshire, Delphine K. Farmer, Sonia Kreidenweis, Wade Permar, Lu Hu, Emily Fischer, Coty Jen, Allen Goldstein, Teresa Campos, Mike Reeves, Darin Toohey, Jeffrey R. Pierce, Shantanu Jathar, *Colorado State University*

Wildfires are an important atmospheric source of primary organic aerosol (POA) and precursors for secondary organic aerosol (SOA). However, there are large uncertainties surrounding the emissions and physicochemical processes that control the transformation, evolution, and properties of POA and SOA in large wildfire plumes. In this work, we develop a plume version of a state-of-the-science model to simulate the dilution, oxidation chemistry, thermodynamic properties, and microphysics of organic aerosol (OA) in wildfire smoke. The model is applied to study the in-plume OA in four large wildfire smoke plumes intercepted during an aircraft-based field campaign in summer 2018 in the western US. Based on estimates of dilution and oxidant concentrations before the aircraft first intercepted the plumes, we simulate the OA evolution from very close to the fire to several hours downwind. Our model results and sensitivity simulations suggest that dilution-driven evaporation of POA and simultaneous photochemical production of SOA are likely to explain the observed evolution in OA mass and composition with physical age. In addition, we show that the rapid chemical transformation within the first hour after emission is driven by higher-than-ambient OH concentrations (3×10^{6}-10^{7} molecules cm^{-3}) and the slower evolution over the next several hours is a result of lower-than-ambient OH concentrations ($<10^{6}$ molecules cm^{-3}) and depleted SOA precursors. Model predictions indicate that the OA measured several hours downwind of the fire is still dominated by POA but with an oxidized POA and SOA fraction that varies between 20% and 50% of the total OA. Semivolatile, heterocyclic, and oxygenated aromatic compounds, in that order, contribute substantially to SOA formation. This modeling work is a step forward in bridging laboratory and field observations of wildfire smoke aerosol.

9SW.4

Using Low-Cost Sensors to Trace Biomass Burning Aerosol Plumes from Wildfires in Southern California. DANIELLE ROCCO, Esther Morales, Jaebin Ju, Linh Luu, Daniel B. Curtis, *California State University, Fullerton*

Wildfires are a major source of particulate matter in the atmosphere and have important implications for air quality, especially if they occur near highly populated areas. Additionally, due to climate change and other factors, wildfire frequency and size are expected to increase in certain areas such as the Western United States. PurpleAir sensors are low-cost air quality monitors that provide real time measurements of PM2.5 concentration, among other quantities. They have become increasingly popular due to their affordability, user-friendly operation, and low maintenance. Although questions remain about the accuracy of low-cost sensors, as a result of their low-cost and ease of use, there are now thousands of these sensors located across California (and other areas) that can be viewed publicly in real time on an interactive map and the data compared to better understand regional air quality.

The unique traits of low-cost sensors, especially the ability to have provided a new and affordable technique to potentially track biomass burning aerosol plumes from wildfires in the area. In this study, multiple local PurpleAir Sensors were used to analyze and track plumes from two fires located in Southern California, the Silverado Fire and the Blue Ridge Fire. Both fires ignited on October 26th, 2020 and were fully extinguished on November 7th, 2020. Preliminary results reveal that PurpleAir Sensors are efficient in detecting fires. Particle concentrations were observed for each sensor and a trend for the Silverado Fire was observed with concentration decreasing as distance away from the fire increases. The results from the Blue Ridge fire appear to be more complex. Further comparisons were conducted using the NOAA Hysplit Model to take meteorological conditions into consideration and the model shows agreement with the PurpleAir sensors.

9SW.5

Using Low-Cost Air Sensors to Assess Community Level PM Exposure from California Wildfires. AMBER KRAMER, Jonathan Liu, Liqiao Li, Yifang Zhu, *University of California, Los Angeles*

The use of low-cost air sensors has become a vital key to understanding air quality at the community level. In this study we demonstrate the efficacy of using publicly available PurpleAir sensor data to assess community exposures to wildfire-induced fine particulate matter ($PM_{2.5}$, $d_a < 2.5$ µm). We sourced publicly available sensor data within 25 miles of ten wildfires in the state of California in 2020, one in 2019, and one in 2018, and paired the indoor PurpleAir sensors with nearby outdoor PurpleAir sensors (within 5 km). We observed that the average outdoor $PM_{2.5}$ concentrations could increase up to 100-fold during the early stages of nearby wildfires compared to pre-fire levels. Indoor $PM_{2.5}$ concentrations peaked up to 40-fold over pre-fire averages between 80 and 350 minutes after the observed outdoor PM peak. The peaks and troughs of indoor $PM_{2.5}$ concentrations followed the observed outdoor $PM_{2.5}$ levels in a similar and delayed pattern throughout the time of wildfire, indicating that wildfire-induced $PM_{2.5}$ could infiltrate into the indoor environments. In addition, we found that indoor $PM_{2.5}$ concentrations returned to pre-fire averages within the period of time it takes to contain fires, while outdoor $PM_{2.5}$ concentrations can stay upwards of two weeks before returning to pre-fire averages. This study demonstrates the efficacy to use low-cost air sensor data to better understand the community level impacts of wildfires. Our results suggest indoor $PM_{2.5}$ concentrations could reach dramatically higher levels during wildfire events and the Public Health warnings to remain indoors during nearby wildfires may not be sufficient to protect community health.

9SW.6

Use of a Low-Cost PM Sensor Network to Characterize the Impact of 2020 Washington Wildfire on Indoor Air Quality and Personal Exposure. CHING-HSUAN HUANG, Nanhsun Yuan, Jiayang He, Mei-Yu Liao, Selina Teng, Igor Novosselov, *University of Washington*

Exposure to wildfire smoke has been linked to an increased risk of cancer and cardiorespiratory mortality. Recently, low-cost air quality sensor networks have been widely implemented in different scenarios to identify pollution sources and hotspots given their capability of capturing high spatiotemporal resolution data. In 2020, a series of large wildfire events occurred in Oregon, California, and Washington State in the United States, making public more aware of the impact of wildfire on air quality. This study utilizes a low-cost particulate matter (PM) sensor network to quantify the PM concentration indoor/outdoor (I/O) ratios and the personal exposure to PM during a wildfire episode in Seattle, Washington. During September 2020, seven pairs of indoor and outdoor PM sensors were deployed in the seven households located in the urban Seattle area along with a personal exposure monitor worn by a subject. The results showed that households equipped with high-efficiency particulate air (HEPA) filters had lower I/O ratios compared to those without air filtration; median I/O ratio of 0.38 vs. 0.80, respectively. The distributed sensor network had high correlations of outdoor $PM_{2.5}$ concentration measurements with a nearby Puget Sound Clean Air Agency monitor ($R^2 = 0.93$). The wearable monitor showed high variance as the subject spent time in different microenvironments. When the daily personal exposure was proportionally attributed to each location, the wearable sensor data agreed with stationary monitors for the same microenvironment. The findings have implications in developing intervention strategies in reducing $PM_{2.5}$ exposures and the associated health effects of wildfire smoke. Future studies with controlled environments and larger sample sizes are warranted to investigate the roles of other factors such as air exchange rate in mitigating the impact of wildfire smoke on indoor air quality.

9SW.7

Effects of Wildfires on Outdoor Black Carbon Level to Indoor Air Quality. DARIA PASHNEVA, Julija Pauraite, Agnė Minderytė, Inga Garbarienė, Vadimas Dudoitis, Kristina Plauškaitė, Simonas Kecorius, Gediminas Mainelis, Jurgita Ovadnevaite, Steigvilė Byčenkienė, *SRI Center for Physical Sciences and Technology*

Wildfires are significant source of fine airborne particulate matter ($PM_{2.5}$), but little is known how indoor air filtering systems are performing under intensive smoke conditions. For this aim, black carbon equivalent mass concentration (eBC) was measured in a modern office with a mechanical ventilation system. Measurements took place from 30th September to 6th October 2020 in the urban background environment in Lithuania. Aethalometer (Magee Scientific, AE31) and Aerodynamic Particle Sizer (TSI 3321) spectrometer used in this study were connected to the sampling system which automatically switches sampling from one environment to another every 30 minutes. During measurement campaign an intensive pollution episode, related to long-range transport wildfire smoke, was observed. The results indicated that smoke event increased both indoor and outdoor eBC mass concentrations twice. Air filtering efficiency was found to be highly dependent on particles size. Particle number size distribution and particle mass-weighted size distribution in indoor and outdoor air together with their averages for the event and non-event days will be presented. Acknowledgment: This research was funded by a grant (No. S-MIP-20-28) from the Research Council of Lithuania.

9SW.8

Quantifying the Impacts of Traffic-Related Air Pollution (TRAP) and Wildfire Smoke on Indoor and Outdoor Air Quality in Daycare Settings: A Pilot Study. Melanie MacArthur, Emily Peterson, Linda Dix-Cooper, NAOMI ZIMMERMAN, *University of British Columbia*

This study assesses the impact of traffic-related air pollution (TRAP) and wildfire events on indoor and outdoor air quality at daycares in Vancouver, Canada. Pre-school age children are a vulnerable population to the negative health impacts of poor air quality (e.g. elevated risks of asthma, child acute bronchitis). While several studies have explored indoor and outdoor air quality of public and private schools, gaps for daycare air quality still remain. During wildfires as recent as 2018, carbon monoxide (CO), nitrogen oxides (NO_x) and particulate matter less than 2.5 µm ($PM_{2.5}$) concentrations exceeded provincial regulatory limits, emphasizing the importance of communicating and understanding best practices for minimizing air pollution exposure at the community level.

To understand indoor and outdoor air quality during wildfire episodes and typical periods, continuous measurements were conducted at 14 daycares for two weeks in September-October 2020. Site-selection was stratified across variables hypothesized to affect air quality including proximity to roadways, proximity to recreational and green space, facility size and height above ground.

Indoor and outdoor concentrations were measured with Real-time Affordable Multi-Pollutant (RAMP, SENSIT Technologies) monitors which measure CO, CO_2, NO, NO_2, O_3, $PM_{2.5}$ and meteorological parameters at 15 s resolution. Additionally, environmental features were recorded for each site, with emphasis on vegetative and physical barriers surrounding play areas. Assessment metrics focused on hourly average concentrations, indoor-to-outdoor pollutant ratios, and diurnal patterns.

Communicating the findings was a key objective of this study. A detailed report of individual results was developed, with simple behavioural and schedule adjustment suggestions for managers to implement at the daycare level. A de-identified aggregate report summarizing all sites was also received by all daycares, including relationships between air quality and environmental justice identifiers.

9SW.9

Toxic Emissions from Fires at the Wildland Urban Interface: Laboratory Measurement of Formaldehyde and Aerosol from Building Materials. KATHERINE BENEDICT, James E. Lee, Kyle Gorkowski, Manvendra Dubey, Allison Aiken, *Los Alamos National Laboratory*

Emissions from burning urban fuels including home building materials and plastics has not received much attention, yet are likely to release greater amounts of toxics into the atmosphere. Fires regularly occur in populated areas and are spreading across the wildland urban interface (WUI) threatening neighborhoods with increasing severity due to drought and land use changes. In order characterize the toxicity of urban fires we report on laboratory measurements aerosol and trace gas emissions from burning of targeted building materials. Emissions from plywood, melamine particle board, pressure treated lumber, and MDF, all with known composition are quantified and contrasted with traditional natural hardwood fuels. We report significant emission of formaldehyde, a toxic EPA regulated gas, from plywood in an open wood-stove burner. We also measure the size distribution, soot and metal content of the smoke aerosols and interpret it using the composition of the fuel and the combustion phase. Finally, we will report detailed chemical results of emissions using a new closed-system tube furnace. In these burning experiment temperatures will be slowly ramped up and trace gas emissions from pyrolysis, smoldering and flaming phases are resolved. Our gas phase analysis focuses on formaldehyde (HCHO), CO, and CO_2 while aerosol are characterized for their optical properties, organic, inorganic , and black carbon content, and size distribution. While our preliminary analysis did not detect a significant presence of metals in smoke this issue will be explored further with our soot particle aerosol mass spectrometer. Finally, smoke emissions from urban and natural fuels will be contrasted to better attribute their toxicity.

9SW.10

Quantifying the Health Benefits of Respirators and Face Coverings to Mitigate Exposure to Wildfire Air Pollution. JACK KODROS, Kate O'Dell, Jon Samet, Christian L'Orange, Jeffrey R. Pierce, John Volckens, *Colorado State University*

Public familiarity with the use of face coverings to reduce the risk of respiratory disease has increased during the coronavirus pandemic; however, recommendations for their use outside of the pandemic (in non-occupational settings) remains limited. As wildfire smoke events continue to become an increasing public health concern, recommendations for personal intervention strategies to limit exposure to wildfire smoke are essential. Here, we develop a framework to quantify the potential health benefits of wearing respirators or face coverings to mitigate exposure to wildfire smoke. This modeling framework considers variation in the type, fit, and wearing compliance of a given mask (cotton-fiber masks, synthetic-fiber masks, N95 respirators), aerosol characteristics, and exposure-response data. We find that N95 respirators offer robust protection against wildfire smoke, reducing particulate exposure by more than a factor of 16 when worn with a leakage rate of 5%. Synthetic-fiber masks offer less protection with a strong dependence on aerosol size distribution (exposure reduction factors ranging from 8 to 2). Cotton-fiber masks offer only 20% reductions in exposure. To assess the ability of face coverings to provide population-level health benefits to wildfire smoke, we perform a case study for the 2012 Washington state fire season where daily wildfire smoke $PM_{2.5}$ ranged from 10-120 $\mu g\ m^{-3}$. After accounting for assumptions on mask-wearing compliance, our modeling framework suggests that while cotton-fiber masks offer minor reductions in respiratory hospitalizations (a 2-7% reduction in smoke-attributable hospital admissions) due to limited filtration efficiency and poor fit, N95 respirators and synthetic-fiber masks may lead to notable reductions in hospitalizations (19-35% and 7-18%, respectively). For all masks, the bypass rate of air around the filtering piece is a key factor governing potential exposure reduction and health benefits during severe wildfire events.

9SW.11

2020 California Wildfire Smoke in New Mexico: Characterization and Toxicological Studies Reveal Signs of Neurological Aging and Inflammation. David Scieszka, Russell Hunter, Jessica Begay, Marsha Bitsui, Yan Lin, Joseph Galewsky, Masako Morishita, Zachary Klaver, James Wagner, Jack Harkema, Guy Herbert, Selita Lucas, Charlotte McVeigh, Alicia Bolt, Barry Bleske, Andrew Ottens, Haiwei Gu, Shahani Noor, MATTHEW CAMPEN, *University of New Mexico*

Wildfire smoke originating from California routinely spread across the western states throughout the summer and fall of 2020. Using a mobile laboratory with a particle concentrating system located on the Laguna Pueblo, approximately 1h west of Albuquerque, we conducted a 20-day, 4h/d whole body exposure in C57BL/6 male mice and examined pulmonary and systemic, especially neurological inflammatory consequences. The mobile laboratory-based concentration of PM2.5 led to exposure levels averaging 104 µg/m3, with high levels of 209 and 191 µg/m3 seen on the first 2 days of exposure, during the peak of wildfire PM2.5 transport to this region. We also measured the overall content of levoglucosan, a specific marker for wood smoke, in pooled PM filter samples, which revealed that the first 3 days of exposure had a high contribution of wood burning in the PM2.5. Days 13-16 of the exposure also contained modestly elevated levoglucosan. Inflammation was evident in the lung of PM-exposed mice, with elevated numbers of macrophages in bronchoalveolar lavage and several cytokines (MIP1, MIP2, IP10 increased relative to filtered air control mice. Wildfire PM exposure also led to signs of inflammation in the bone marrow (MIP2, IP10). Flow cytometry conduct in brains reveal substantial increases in numbers of activated microglia, infiltration of peripheral leukocytes, and increased expression of adhesion molecules on cerebrovascular endothelial cells. Metabolomics of the cerebellum revealed reduced NAD+, succinate, and taurine in PM-exposed mice, consistent with metabolic shifts associated with aging. These outcomes, from PM traveling across the continent, suggest broad-scale public health neurological impacts may arise from wildfires.

9SW.12

Assessing the Impact of Wildfire PM2.5 on Indoor Air Quality with Crowdsourced PurpleAir Sensor Data in California. YUTONG LIANG, Deep Sengupta, Mark Campmier, Joshua S. Apte, Allen Goldstein, *University of California, Berkeley*

Driven by fire suppression and climate change, the number and severity of large wildfires have been increasing for decades in western United States. Many studies have connected wildfire smoke exposure to elevated risk of respiratory morbidity. In previous studies, the exposure to wildfire smoke $PM_{2.5}$ (particles with < 2.5 µm aerodynamic diameter) was typically estimated from ambient (outdoor) concentrations. However, because people in the US on average stay indoors for 87% of the time, the protection against outdoor wildfire smoke particles provided by buildings should not be overlooked in exposure assessments.

The fast-growing PurpleAir sensor network allows us to assess how indoor air quality is moderated by the buildings and occupants' behavior during wildfire events. Using observations outside and inside over 1400 buildings from the PurpleAir sensor network in California during 2020 and 2018 wildfires, we found that infiltration ratios (indoor $PM_{2.5}$ of outdoor origin/outdoor $PM_{2.5}$) were reduced on average by ~50% on smoky days compared with non-smoky days, which was related to reduced ventilation and enhanced indoor filtration. Newer buildings and buildings utilizing air conditioning or filtration had lower infiltration ratios. Even with such protective measures, mean indoor concentration of $PM_{2.5}$ was on average more than doubled by wildfire events.

9UA.1

Using Rain Washoff to Estimate Dry Deposition of Atmospheric Aerosols to Horizontal Urban Surfaces. ALEXANDER JOHNSON, Cliff Davidson, *Syracuse University*

Building roofs comprise a major fraction of the overall horizontal urban surface area and are receptors of dry deposited aerosols. During a storm, rainwater will wash the dry deposited material from a building roof into stormwater runoff. Measuring the concentrations of certain chemical species in runoff from a building roof and the amount of runoff could therefore be used to estimate dry deposition to that surface during the antecedent dry period.

The goals of this study were to measure dry deposition to horizontal urban surfaces and to measure rain washoff of dry deposited material from the surfaces. In each experiment, two flat Teflon coated disks and two bowl-shaped disks of similar size were exposed to the atmosphere on the roof of Hinds Hall at Syracuse University to collect dry deposition. Airborne concentrations were simultaneously measured. Shortly before a rainstorm, samples were collected from the flat disks. In the subsequent storm, fresh rain and runoff from the bowl-shaped disks were collected. All samples were analyzed to determine the dry deposition fluxes and dry deposition velocities of fluoride, chloride, nitrate, sulfate, ammonium, sodium, magnesium, potassium, and calcium to the disks.

Dry deposition fluxes measured to the flat disks and to the bowl-shaped disks show reasonable agreement, suggesting the reliability of using the bowl-shaped disks to assess rain washoff. Nearly complete washoff of the dry deposited material from the bowl-shaped disks is possible under a steady rain.

Additional experiments are underway to measure dry deposition to a green roof by washing the leaves of vegetation after lengthy dry periods. In future experiments, concentrations of chemical species in rain runoff from building roofs and from vegetation will be used to estimate dry deposition of these species in urban areas.

9UA.2

Impact of Forest Belts on Reducing Desert Dust Concentration in Urban and Suburban Areas. OFIR VADAS, 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. Applying of planted forest belts (windbreaks) reduces airborne dust during dust storms, resulting to healthier atmosphere in urban and suburban environments. This study investigated the impact of forest belts 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 windbreak, and windbreak aerodynamics. The two-dimensional model is based on the application of theory of turbulent diffusion in conjunction with model of dust particles deposition on vegetation elements. The initial wind velocity profiles, used in the simulations were fitted from data obtained in field measurements in the studied region. Numerical simulations are performed for windbreaks, which consists of planting pine trees (pinus halepensis) typical for northern Negev region, Israel. Using the developed model, a numerical simulation of the dust transport through windbreaks of various porosities and widths was carried out. In particular, numerical analysis was performed for highly porous windbreaks with widths 1.25H and 2.5H, where H is the average height of the windbreaks. Results of calculations showed that during high-level dust storms at the leeward side of the windbreaks PM_{10} concentrations are reduced by 14% and 20% correspondingly. It has also been shown that the use of windbreak strips can reduce the PM_{10} concentration by 6-8% even at a considerable distance (about 1 km) from the windbreak. The results of this study emphasize the importance of planted semi-arid forest belts for controlling air pollution in the adjacent urban areas by reducing PM concentration in the atmosphere during dust events.

9UA.3

The Impact of Sea Breeze and Precipitation on Particulate Matter Concentrations in Houston. CHUN-YING CHAO, Marina Karki, Wei Li, Yuxuan Wang, Robert Griffin, *Rice University*

Along with emissions and atmospheric chemistry, meteorological parameters such as recirculation (i.e., a land-sea breeze pattern) and precipitation determine concentrations of air pollutants. In coastal areas, the land-sea breeze circulation has been found to play an important role in determining air quality because the pattern recirculates polluted air back and forth across the urban coastal boundary. Precipitation impacts air quality predominantly through enhancing wet deposition processes. To understand how these weather patterns affect particulate matter (PM) levels, historical monitoring data are used for Houston, which is the fourth most populous city in the United States, is home to many industrial activities, and is located near the Gulf of Mexico. This study uses fine PM concentration and precipitation data from Texas Commission on Environmental Quality (TCEQ) monitors during summers from 2010 to 2019. Land-sea breeze patterns were quantified using a recirculation pattern metric. First, hourly meteorological data and calculated recirculation metrics from coastal TCEQ monitors were used to categorize sea breeze and other weather patterns. Second, fine PM concentrations at two TCEQ monitors near the Houston area – Clinton and Deer Park– were quantified and compared for the identified weather patterns. Third, the importance of inland distance on the strength of the sea breeze was considered. The statistical relationships between fine PM concentrations, summer precipitation, and land-sea breeze circulation metrics determined in this work will be discussed.

9UA.5

The Relative Influence of Roadway and Harbor Particle Sources before and during COVID-19 Related Lockdown in Charleston, South Carolina. ROBY GREENWALD, Eleanor Clarke, *Georgia State University*

We PM2.5 number and mass concentration and black carbon (BC) mass concentration at a waterfront site in downtown Charleston, South Carolina during the time period surrounding the COVID-19 related lockdown in February-March 2020. In addition to particle and meteorological measurements, we collected roadway traffic data from the South Carolina Department of Transportation and ship transponder data from the Marine Traffic company. Similar to other regions of the world, we observed sharp reductions in motor vehicle traffic following stay-at-orders associated with the pandemic response. Roadway traffic decreased 50% as assessed by the number of vehicles crossing the Cooper River approximately 2 km from the sample site. Ship traffic in Charleston harbor during this time period however did not follow the same pattern as roadway traffic. Some types of ship traffic were temporarily reduced or ceased altogether. For example, cruise ship operations were discontinued, and passenger boats for tourism purposes operated on a reduced schedule. On the other hand, commercial and cargo ship traffic continued operations. We constructed a simple model to identify plumes from ships moving in the harbor based on wind direction and speed and ship GPS data. PM2.5 data collected at the sample site typically showed temporal trends consistent with regional ambient air quality monitors with notable exceptions. BC concentrations was temporally inconsistent with PM2.5 trends but frequently corresponded to wind direction blowing from local sources, including harbor traffic. Occasional increases in BC concentration were observed to occur when wind direction was from the largest highway in the immediate vicinity; however, more frequent increases in BC were observed when wind direction was from nearby ship traffic, including large vehicle carriers and smaller tour boats. Numerous increases in BC did not temporally correspond to any known source near the sample site. These results are consistent with both roadway and harbor traffic influencing BC concentration in downtown Charleston.

9UA.6

Ultrafine Particle Ground-Level Impacts during Aircraft Approach and Climb Out Operations at a Major Cargo Hub.

MARYSSA LOEHR, Jay R. Turner, *Washington University in St. Louis*

Ultrafine particles (UFP) contribute to adverse health outcomes such as asthma, obstructive pulmonary disease, cardiovascular disease, and lung cancer. Recent studies have drawn attention to elevated ground-level UFP number concentrations from aircraft and airport operations emissions. In this study, we aim to quantify ground level impacts of individual aircraft during climb out and approach operations at a commercial airport with a large air cargo hub. Ground level UFP concentrations are measured along public roads near the airport at one-second resolution using mixing particle condensation counters (MCPC, Brechtel, Hayward, CA) on mobile platforms. Measurements are conducted during late evening and early morning hours corresponding to air cargo arrivals and departures, respectively. These times of day tend to have low atmospheric mixing layer heights which suppress the vertical dispersion of emissions and exacerbate ground level concentrations. Aircraft typically approach the airport into the wind and UFP during the arrivals period features contributions from individual approaching aircraft superposed on a rising baseline because of increased airport operations to process the cargo. UFP concentrations reaching 160,000 #/cc were observed ~0.7 km downwind of the airport at locations underneath or immediately downwind of the arrival flight path. In contrast, aircraft typically depart into the wind and UFP measurements upwind of the airport to characterize climb out emissions were not confounded by airport operations impacts. Ground-level UFP during climb out operations rarely exceed 50,000 #/cc at locations ~0.5 km from the airport even though the climb out phase uses more engine thrust, likely because the aircraft rapidly ascend above the mixed layer. Nighttime UFP in a low-income residential area ~1.3 km downwind of the airport consistently exceeded 50,000 #/cc during periods of peak flight activity and rose to >90,000 #/cc because of the corresponding increase in airport operations to support air cargo handling.

9UA.7

Effect of the COVID-19 Pandemic on Aerosol Composition in Atlanta, GA.

JEAN RIVERA-RIOS, Taekyu Joo, Tianchang Xu, Masayuki Takeuchi, Chris Peng, Leah Williams, Philip Croteau, John Jayne, Jennifer Kaiser, Nga Lee Ng, *Georgia Institute of Technology*

The COVID-19 pandemic led to drastic changes in human behavior across the United States. Lockdowns caused reductions in anthropogenic activities, including reduced traffic and the closure of businesses like bars and restaurants. Atlanta, GA, is an urban environment surrounded by sources of biogenic emissions. Air quality in Atlanta is modulated by the interplay between anthropogenic and biogenic emissions. We performed field measurements during the summer and fall/winter of 2020 in order to evaluate the effects of the COVID-19 pandemic related behavioral changes on air quality in Atlanta. Measurements include, O_3, nitrogen oxides (NO, NO_2), volatile organic compounds (VOCs), PM_1 volume and number concentration and non-refractory PM1 particle composition. The organic aerosol (OA) composition, using data from a High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS) and a Time-of-Flight Aerosol Chemical Speciation Monitor (TOF-ACSM), was source apportioned with positive matrix factorization (PMF). The resolved factors have been previously observed in Atlanta. Secondary factors include more-oxidized oxygenated organic aerosol (MO-OOA), less-oxidized OOA (LO-OOA), and isoprene aerosol (Isop-OA). Primary/anthropogenic factors include hydrocarbon-like OA (HOA), cooking OA (COA) and biomass-burning OA (BBOA). The months of April and May had the lowest amount of traffic relative to previous years. Changes to O3 during those months include higher overall overnight concentrations and lower daily maximums. Changes to secondary OA (SOA) composition include reductions in the mass fraction of MO-OOA. This aerosol subtype is replaced by a different one, a LO-OOA-like factor (LO-OOA2) that behaves differently from the one we typically observe in Atlanta, LO-OOA1, which is also observed. Other changes include reductions in the frequency and intensity of COA enhancements during the low-traffic months, indicating that other types of anthropogenic activities were also impacted and had effects on SOA composition. Measurements in Atlanta allow us to examine the effects of anthropogenic emission reductions on SOA from biogenic sources.

9UA.8

Assessing the Impact of Industrial Activities on Ambient Air Particulate Matter in East Java, Indonesia.

MUHAYATUN SANTOSO, Philip K. Hopke, Diah Dwiana Lestiani, Endah Damastuti, Syukria Kurniawati, Didin Agustian Permadi, Arie Dipareza Syafei, *Center for Applied Nuclear Science and Technology, BATAN*

The impact of industrial activities on air quality has been assessed by collecting APM samples using a Gent stacked filter unit sampler from 2018-2020. Monitoring was conducted in three locations around industrial sites in East Java Province, Indonesia. Industrial impacts were identified from the PM2.5, BC and elemental concentrations, especially heavy metals such as Pb, Fe, and Zn, which were higher than in other cities in Java. The comparison of PM2.5 and PM10 in the industrial areas of other cities will also be presented. Black carbon concentrations showed that BC in industrial areas was higher than in cities in other parts of Java because of coal use as a major fuel. Characterization results show that the main elements in APM were S, K, crustal elements (Al, Si, and Ca), and heavy metals (such as Fe, Zn and Pb). Comparison of heavy metals in industrial sites and in other cities in Java showing the levels of heavy metal pollution will also be discussed. The results of several APM samples at industrial sites showed high Pb concentrations (exceeding 1 $\mu g/m^3$), as well as Fe and Zn concentrations that were at a higher level than other cities in Java. These results agree with source apportionment results where the source profiles show the presence of a Cu metal industry, a Pb smelter, a Zn industry, and a steel industry. These results illustrate the contribution of the activities of various types of metal industries around the sampling locations. The results obtained indicate the importance of detecting pollution early so that the results can be used as a reference in formulating appropriate policies and avoid greater impacts later.

9UA.9

Contrasting the Impact of Traffic Changes on Air Quality During the COVID-19 Lockdowns in Maryland and Florida.

KIARA MEGGITT-GOFF, Mariel Judd, Tate Grant, Scott Parr, Marwa El-Sayed, *Embry-Riddle Aeronautical University*

In 2020, the COVID-19 pandemic caused lockdowns worldwide, which in turn lead to dramatic reductions in traffic patterns and consequently resulted in changes in the concentrations of several atmospheric criteria pollutants. The purpose of this study is to investigate the impact of the changes in traffic patterns during the pandemic lockdowns on air quality across two diverse regions in the eastern United States, namely the states of Florida and Maryland. Four criteria pollutants are considered in this study including nitrogen dioxide (NO_2), carbon monoxide (CO), ozone (O_3), and particulate matter with aerodynamic diameter less than 2.5 micron ($PM_{2.5}$). Hourly pollutant concentrations during 2015-2020 is acquired from the Maryland Department of the Environment and Florida Department of Environmental Protection in Maryland and Florida, respectively. Vehicle classified traffic data in 2019 and 2020 were retrieved from the Florida and Maryland Departments of Transportation, for Florida and Maryland, respectively. To characterize the impact of the lockdowns on traffic and air quality, data from 30 (Florida) and 21 (Maryland) monitoring sites pertaining to 2020 is compared to historic data in three periods, namely pre-lockdown, lockdown, and post-lockdown. Statistical correlations are tested to determine relationships between traffic patterns and air quality in the two studied regions. Results herein will provide insight into the impact of vehicular emissions on air quality and has implications for future policies on emissions related to different classes of vehicles.

9UA.10

Multi-dimensional Characterization of Particulate Matter Low-cost Sensors in Florida. Jasper Bowles, Marc Compere, Kevin Adkins, MARWA EL-SAYED, *Embry-Riddle Aeronautical University*

Current attempts to measure ground-based atmospheric particulate matter (PM) by the Environmental Protection Agency (US EPA) in its federal reference and federal equivalent methods (FRM and FEM, respectively) are not only cumbersome and costly but also lack high spatiotemporal resolution. Due to their stationary nature, the EPA's methods are limited in measuring the concentrations of PM at the ground-level, lacking the ability of monitoring concentrations at multiple altitudes. This, hence, hinders our ability to accurately characterize the origin and the sources responsible for the formation of these atmospheric pollutants. Recently, the development of low-cost sensors (LCSs) has been used to address the economic, practical, and technological shortcomings associated with obtaining PM measurements at high spatial and temporal scales. The aim of this study is to characterize the horizontal and vertical profiles of atmospheric PM using LCSs at Daytona Beach, Florida, a site characterized by its diverse atmospheric pollution. To achieve this, we place commercial LCSs in two varying operational modes: stationary, and mobile on unmanned vehicles (UVs) flying up to 400 ft altitude. Two commercial LCSs which rely on light scattering techniques and optical particle counters, namely: PurpleAir and OPC-N3, respectively, are compared in this study and their performance is evaluated across varying environmental and meteorological conditions in summer 2021. At the stationary position, validation of PM concentrations is established by collocating LCSs with an FEM monitor. Validation of the sensors on UVs is conducted by mounting a Vaisala AQT 420 sensor to a tethered balloon collocated with the LCSs on the UVs. This work has implications for the detection of atmospheric pollutants in congested, remote, and endangered areas at fine temporal and spatial resolutions.

9UA.11

Discovery of Atmospheric Microplastic Particles in Urban Emissions. ANA MORALES, Jay Tomlin, Christopher West, 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 are also deemed as 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 unrecognized, 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 operation process 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. Chemical imaging of the dry aerosol particles generated from the steam water showed abundant presence of small MNP particles in the size range of 100-500 nm, where smaller particles showed a higher degree of oxygenation. We use a combination of mass spectrometry techniques to enable molecular characterization of the MNP constituents and spectro-microscopy techniques to elucidate size distributions, morphology, and internal structures of MNP at the nanometer scale. 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.

9UA.12

Identifying Patterns and Sources of Urban Ultrafine Particulate Matter Using Mobile Measurements of Lung-Deposited Surface Area. RISHABH SHAH, Lauren Padilla, Daniel Peters, Megan Dupuy-Todd, Elizabeth Fonseca, Geoff Ma, Rod Jones, Jim Mills, Nick Martin, Ramon Alvarez, *Environmental Defense Fund*

Scientific literature increasingly suggests that among $PM_{2.5}$ components, health effects of ultrafine particles (UFP; diameter < 100 nm) are concerning because of deeper penetration in the respiratory tract and blood-borne translocation to vital organs. Further, UFP surface area has important implications for adsorptive chemistry in the lung tissue.

Within 500 m of sources (e.g., highways), UFP concentrations decline rapidly due to dilution and coagulation. These sharp spatial gradients are difficult to detect with $PM_{2.5}$ mass measurements due to the small mass contribution from UFP and, in case of optical sensors, size cut-off. However, number and surface area concentrations within the UFP size range can capture near-source gradients and aid in identifying hyperlocal UFP sources.

We present mobile, high spatio-temporal resolution measurements of lung-deposited surface area (LDSA) concentrations with a medium-cost aerosol dosimeter (Naneos Partector, measuring surface area of 20-400 nm particles via diffusion charging). We equipped two Google Street View vehicles in London to perform 1 Hz measurements of LDSA, black carbon (BC), optical $PM_{2.5}$ mass, and NO_2 from September 2018 to October 2019. Our findings show that variations in mobile time series of $PM_{2.5}$ mass in London are small (3-5× background; often confounded with temporal variability), compared to those in LDSA and BC (10-20×), which we associate with sources e.g., higher concentrations on high-volume roadways during morning and afternoon traffic. Further, we examine the applicability of ratios of LDSA to BC, NO_2, and CO_2 to distinguish source types (e.g., low LDSA:BC may indicate diesel exhaust, while high LDSA:BC may indicate other sources such as gasoline exhaust and/or cooking). Our rich dataset enables us to perform high spatio-temporal resolution mapping of LDSA, assessing patterns that may go unnoticed with $PM_{2.5}$ mass measured by optical particle counters.

10BA.2

Tracking Antimicrobial Resistance Genes across Canada: Coast-to-Coast-to-Coast. PAUL GEORGE, Marc Veillette, Amélia Bélanger Cayouette, Mahsa Baghdadi, Maosheng Yao, Nathalie Turgeon, Jacques Corbeil, Caroline Duchaine, *Université Laval*

The spread of antimicrobial resistance genes throughout the environment is of great concern to public health and policymakers. Antibiotic-resistant bacteria can spread throughout the wider environment through the air in bioaerosols originating from anthropogenic sources, such as agriculture, wastewater treatment, or hospitals, and pass resistance genes to other bacteria via horizontal gene transfer. Resistance genes may differ depending on the source, so understanding the diversity of resistance genes in the environment is necessary to make actionable policy to combat their spread. Here, we apply a recently developed method using passenger vehicle air filters as passive monitors of airborne bacteria and antimicrobial resistance genes across Canada. We have collected 317 cabin pollen filters from individuals, city governments, and vehicle service departments from 27 locations in 9 provinces. Approximately 20 g of filter material was removed from each filter. The subsample was processed using a stomacher Mix 1 homogenizer in saline and 0.05% tween 20 solution to collect dust and bacteria. Large particles were removed with differential centrifugation and 3 mL aliquots were collected after high-speed centrifugation. We extracted DNA from these aliquots and quantified copy numbers of 16S and the ratio of resistance genes using qPCR. There is evidence of a widespread distribution of various tetracycline resistance genes, including tet32, tetlL, tetM, and tetW, which appear in large cities and smaller well-connected population centres across Canada. However, most tetracycline resistance genes were not detected in filters from remote locations. We also detected widespread sulphonamide resistance, namely sul1, in these samples. There is little evidence of aminoglycoside resistance genes and unclear trends in the colistin resistance gene mcr-1. We are working on expanding our resistance panel and identifying the sources of resistance genes is ongoing.

10BA.3

Investigating the Effects of Environmental Factors on the Spread of Antibiotic Resistant Bacteria in a Dairy Facility. HYOUNGMOOK PAK, Maria King, *Texas A&M University*

Widespread use and availability of antibiotics has led to infectious and pathogenic bacteria developing antibiotic resistance. Various environmental factors, such as temperature, relative humidity, and wind, can also induce stress in bacterial cells, activating antibiotic resistance genes to increase their survivability against harsh and extreme conditions. These bacteria can survive for a longer time and travel further distances if they become airborne, which is the case in many livestock facilities. Computational fluid dynamics (CFD) was utilized to examine the movement of bioaerosols within and around the dairy facility. CFD simulation results were compared with experimental results, such as air velocity measurements and microbiome data, to confirm and validate their accuracies. In this research, aerosol and manure samples were collected from multiple locations throughout an open stall dairy facility in summer and winter. Temperature, relative humidity, and air velocity measurements at each sampling location were also recorded. In both summer and winter, antibiotic resistance mapping revealed that bacteria showed strong resistance against different antibiotics in the southwestern and northeastern sides of the facility. This was due to wind blowing towards the east-northeast direction and 36 axial fans in the facility generating wind towards the northern side of the dairy facility. Air flow streamlines and air velocities calculated by the CFD simulations using ANSYS closely matched with experimental measurements. Microbiome analysis and principal coordinate analysis revealed that relative abundance of bacteria sequences was correlated with sampling locations, temperature, and relative humidity. These experimental and simulation results indicate that environmental factors do affect the spread of antibiotic resistant bacteria in a dairy facility and CFD can be used to track their movement.

10BA.5

Passive Bioaerosol Samplers: Efficient Tools for Long-Term and Spatially Distributed Sampling.

SYDONIA MANIBUSAN, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Bioaerosols consist of airborne particles of biological origin and may cause negative health effects, including the transmission of various diseases, such as COVID-19. Therefore, bioaerosol sampling and samplers are increasingly important for understanding the transmission of infectious diseases and the biological composition of our air. In addition to active samplers, passive bioaerosol samplers are useful tools to determine the presence of and exposures to airborne biological particles. Owing to their low cost and ease of use, passive bioaerosol samplers and their application see increased interest and application. This presentation will overview different types of passive bioaerosol samplers, their collection mechanisms, advantages and disadvantages, applicability in different environments, and available methods of sample analysis. Passive samplers include gravitational settling devices (such as the agar settle plates, dustfall collectors, and settling filters), electrostatic samplers, including electrostatic dust cloths (EDC), the Rutgers Electrostatic Passive Sampler (REPS), and other technologies. Settled dust has also been used as a surrogate for studying previously aerosolized biota. Passive bioaerosol sampling technology can sample over extended durations and can be distributed over large areas, a task that is not easily or affordably accomplished by active sampling devices. Although passive bioaerosol samplers are limited in their ability to quantify the volume of air sampled and have variable collection efficiencies, these devices could be complementary tools in the overall sampling strategy. They can aid in informing researchers of the biological component of our airborne environment.

10BA.6

Rapid Detection of Single Bioaerosol Particles Using Circular Intensity Differential Scattering (CIDS).

YONG-LE PAN, Aimable Kalume, Jessica Arnold, Chuji Wang, Joshua Santarpia, *U.S. Army Research Laboratory*

It is highly desirable to detect life-threatening bioaerosols from atmospheric aerosols, in situ, rapidly and continuously. Single particle diagnostic techniques can obtain signatures of individual particles, rapid time variations of species, and information of low concentration particles that are generally obscured by other dominant particles in collected samples/ensembles. Currently early-warning biosensors are based on fluorescence and elastic scattering from single aerosol particle with high-false-alarm rate, while particles are successively drawn through the interrogation volume of sensors. It was reported that DNA helical structures in biological molecules have non-zero circular intensity differential scattering (CIDS, normalized Mueller scattering-matrix element S14) than that from isotropic particles. However, CIDS measurements were only carried out on suspension samples with a polarization modulator and rotating detector due to its ultra-weak signals (10^{-3}-10^{-6}). Such complex laboratory instrumentation is not readily deployable as field biosensor.

Here, we report an advanced design for measuring CIDS from single aerosol particles without any moving parts and modulator. The scattering phase function was obtained using a reflector to project scattering light at different angles onto a 1-D/2-D detector instead of rotating the detector. The differential signals were measured from a particle interacting with two illuminating laser beams with left- and right-circular polarizations, which were produced by fixed optical components without any modulator. This innovative setup shortens the measurements from tens of minutes to tens of microseconds. Primary measurements showed that 3 micron diameter bioaerosol [DNA-tagged polystyrene latex (PSL) microsphere and aggregate of B. subtilis spores] have at least 3 times stronger CIDS signals than non-bioaerosol particles (PSL and tryptophan molecules). This gives great promise for developing new early-warning biosensor with a potential to lower false alarm rate.

Acknowledgements
Thank DTRA CB10745 support.

10BA.8

Environmental Effects Triggering Antibiotic Resistance in Bacteria.

BROOKE SMITH, Maria King, *Texas A&M University*

Antibiotic resistance is a threat globally to public health, safety and agriculture. Recent research has found that bioaerosols change physically, chemically and biologically in different environmental conditions. The goal of this research was to explore how gram-negative and gram-positive bacteria react to different environmental conditions, including temperature, relative humidity, airflow and duration of aerosolization. Fresh vegetative Escherichia coli (E. coli) cells and Bacillus globigii (B. globigii) spores were aerosolized at different durations and collected using a 100 L/min wetted wall cyclone (WWC) bioaerosol collector and a 300 L/min low-cutpoint WWC collector. The response of each bioaerosol to environmental conditions was analyzed by susceptibility and genetic testing. The Kirby Bauer susceptibility test indicated the strongest resistance response to cephalothin, gentamicin, and ciprofloxacin, which are cell wall or DNA replication inhibitors respectively. Significantly more resistance was detected in E. coli aerosolized for 5 min versus 45 min, however, similar resistance was detected in the 5 minute and 30 min aerosolizations which indicated that aerosolization over 30 min causes increased amount of stress that the bacteria cannot alleviate. Interestingly, no resistance was detected in bacteria aerosolized for 10 min, potentially due to a transient response of the cells to compensate for the osmotic and other stresses during aerosolization. However, high susceptibility was maintained in all durations to imipenem and cefoperazone, both cell wall synthesis inhibitors, albeit with a contrasting mechanism to other beta lactams. The culturability of archived spores increased significantly compared to E. coli aerosols. Fresh E. coli collected with the low-cutpoint sampler exhibited a dormant duration of viability but recovered after 2 days at room temperature. The knowledge gained from this study may help in designing environmental conditions to attenuate the development of ARGs and antibiotic resistance in bioaerosols.

10BA.9

Exposure to Bacterial Aerosols with Antimicrobial Resistance Surrounding 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 1.5 m 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. Two different systems were tested in this study, consisting of an industrial and a residential septic system. From each system bioaerosols were collected in the winter and summer to observe the effect of different environmental conditions on bioaerosol emission and viability. Wastewater and sprinkler water from the industrial and residential septic systems, respectively, were also collected to compare the bacteria concentration and composition. Results from microbial and molecular analysis indicate lower concentrations of bacteria in the aerosols compared to the water samples. Antibiotic test results from the industrial system indicate that aerosolized bacteria from the winter are more resistant to the antibiotics used compared to aerosolized bacteria from the summer. Antimicrobial resistance (AMR) from the industrial septic system tests are comparable to residential testing, with both resulting in higher percentages of resistance in the bioaerosols during the winter seasons. The occurrence of aerosolized bacteria depends on operational conditions and discharge methods, and AMR development is related to seasonal changes, humidity, temperature, and air velocity. The results indicate that different mechanisms may be involved in the development of antibiotic resistance in the aerosolized bacteria compared to factors triggering resistance in the effluent microbiota.

10BA.10

Estimating SARS-CoV-2 Infection Risk in University Residence Halls Using CO2 Pulse Injections. Daniel Amparo, RYAN MORAVEC, Barbara Turpin, Glenn Morrison, *UNC-Chapel Hill*

Exploring the dynamics air movement in buildings can provide insight into SARS-CoV-2 transmission risk. This study focused on better understanding SARS-CoV-2 transmission risk within three university residence halls that had experienced outbreaks of COVID-19. Each residence hall differed in room and suite layout, HVAC system, and volume. We repeatedly released pulses of CO2 into a source (infectious person) room and measured the dynamic CO2 concentration in the source room and receptor rooms which were above, below, and adjacent to the source room. Air change rates in the source room were calculated from the decay rate of CO2. The proportion of shared air was determined by comparing the integrated dynamic CO2 concentration in the source and receptor rooms. The mean transport time between rooms was determined by applying a residence time distribution analysis to the same data. The middle 80% of results ranged from 1.1/h to 7.8/h for source room air change rates, 0.02 to 0.3 proportion of shared air and 0.3 to 1.9h mean transport time. Applying a Wells-Riley analysis using these results, the risk of SARS-CoV-2 infection in adjacent rooms ranged from 0.02 to 0.5 assuming an average quanta emission rate of 5 quanta per hour and exposure duration of 3.5 days. Door position (e.g. ajar or closed) both increased and decreased risk, depending on the location of the receptor room. Strategies to reduce risk of transmission in an occupied residence hall include improved filtration, increased ventilation, and reduced contact time. The magnitude of room-to-room deposition losses, SARS-CoV-2 deactivation rates, and quanta emission rates introduce the greatest variability into our estimates.

10BA.11

SARS-CoV-2 in Residential Rooms of Two Self-Isolating Young Persons with COVID-19. SRIPRIYA NANNU SHANKAR, Chiran Witanachchi, Alyssa Morrea, John Lednicky, Julia Loeb, Md. Mahbubul Alam, Z. Hugh Fan, Arantzazu Eiguren-Fernandez, Chang-Yu Wu, *University of Florida*

Individuals with COVID-19 have generally been advised to self-isolate at their residences, unless they need medical attention. Epidemiological data and contact tracing suggest that airborne transmission of SARS-CoV-2 leads to outbreaks in residential settings. However, environmental monitoring for the detection of virus in such settings are limited. We present a pilot study on environmental sampling for SARS-CoV-2 virions in the residential rooms of two self-quarantined volunteers with COVID-19. Apart from standard surface swab sampling, different air samplers positioned 0.3-2.2 m from the volunteers were used: inline air samplers with polytetrafluoroethylene (PTFE) filters, VIable Virus Aerosol Sampler, NIOSH 2-stage cyclone sampler, and Sioutas personal cascade impactor sampler. SARS-CoV-2 RNA was detected in one air sample from volunteer A’s room with a rRT-qPCR quantitation cycle (Cq) of 38.21 for the SARS-CoV-2 N-gene, indicating a low amount of airborne virus. In contrast, the samples collected from volunteer B’s room yielded Cq values ranging from 14.58 to 31.13 in various air and surface samples, indicating that this volunteer was actively shedding relatively high amounts of SARS-CoV-2. Despite Cq values of 34-37 in rRT-qPCR analyses of vRNA purified from the cell culture medium inoculated with samples from volunteer B’s room, attempts to isolate SARS-CoV-2 in cell culture were unsuccessful, due to out-competition by a co-infecting Human adenovirus B3 (HAdVB3) that killed the Vero E6 cell cultures within 4 days of their inoculation. The size distribution of SARS-CoV-2 containing particles collected from the air of volunteer B's room was in the range <0.25 µm to >4.4 µm, suggesting a risk of aerosol transmission. The detection of virus in surface samples also underscores the potential for fomite transmission of SARS-CoV-2 in indoor settings. Following CDC guidelines for hygienic practices and limiting contact with an infected individual are recommended for reducing infection risks in residential settings.

10CC.1

How Do Measurements of Single Particle Composition Constrain Gas-Particle Exchange? DANIEL MURPHY, Karl D. Froyd, Charles Brock, Agnieszka Kupc, Gregory Schill, Christina Williamson, *NOAA CSL*

We will used data from the Atmospheric Tomography (ATom) and earlier missions to show how measurements of single particle composition can offer insights into gas-particle exchange processes that are not available from bulk measurements. Primary and secondary sources can often be distinguished. If a low-volatility species such as sulfuric acid or organics is condensing onto pre-existing particles, it will generally be present on almost all particles. In contrast, a primary source of sulfate or organics will usually lead to a distinct population with different concentrations on different particles. We will show examples of these processes.

A second way single particle composition can constrain gas-particle exchange is by measuring the evolution of distinct types of particles in the same air. A good example is in the lower stratosphere, where stratospheric sulfuric acid particles with and without meteoric metals coexist with mixed organic-sulfate particles that originated in the troposphere. That these particles remain distinct has important implications for aerosol chemistry and the concentrations of several gas-phase species. Neither semi-volatile organics nor ammonia can be in equilibrium with the gas phase. The gas-phase concentrations of semi-volatile organics and ammonia must be very low, or else the sulfuric acid particles would not stay so pure. Yet the sulfuric acid particles in the Northern Hemisphere show a very small but measurable uptake of organics, indicating non-zero gas-phase concentrations of those species. Finally, the organic-sulfate particles must be resistant to photochemical loss, or else they would no longer retain their organic content.

10CC.2

Estimation of Aerosol Direct Radiative Effect through CATCH-derived Aerosol Types. BETHANY SUTHERLAND, Nicholas Meskhidze, *NC State University*

The ability to remotely assign aerosol types (i.e. Dust, Urban, Smoke, Fresh Smoke, and Maritime) from the High Spectral Resolution Lidar (HSRL) retrievals presents a promising opportunity for narrowing the uncertainty in global calculations of the Direct Radiative Effect (DRE) of aerosols. Here we present the results of using type-specific values of single scattering albedo (SSA) and asymmetry parameter (g) in DRE calculations over North America. Since spatiotemporal distributions of aerosol types are not currently available, aerosol types analogous to HSRL are determined using the CATCH (Creating Aerosol Types from Chemistry) algorithm (Dawson et al., 2017). Type-specific values are chosen using the GEOS-Chem chemical transport model. The CATCH-derived type specific values of SSA and g are compared with AERONET retrievals for locations and times where a single type contributed the majority of the extinction. DRE uncertainty calculations is estimated based on the spread in GEOS-Chem-derived SSA and g values due to intra-type variability in aerosol chemical composition. This spread in SSA and g is then compared to the range of values derived using aerosol microphysics from AEROCOM III models. Preliminary results from July of 2014 show that the CATCH/GEOS-Chem derived type-specific SSA and g are comparable with AERONET retrievals. Additionally intra-type variability of SSA and g, having mean inter-quartile ranges less than 0.01 and 0.032 respectively (due to variability in the chemical composition for aerosols of a single type), is generally lower than the spread in values derived from the AEROCOM models. This study indicates that using type-specific aerosol optical properties in conjunction with HSRL retrieved aerosol types could lead to DRE estimates with lower uncertainty than is currently achieved. Results spanning the entire year of 2014 will be presented, as well as an analysis of seasonal trends in type-specific optical properties.

References

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10CC.4

Characterizing the Vertical Transport of Aerosols During Deep Convective Events. CHANAKYA BAGYA RAMESH, Dié Wang, Scott Giangrande, Jian Wang, Yang Wang, *Missouri University of Science and Technology*

Atmospheric aerosols affect the global energy budget by scattering and absorbing sunlight (direct effects) and by changing the microphysical structure, lifetime, and coverage of clouds (indirect effects). Globally, new particle formation in free troposphere is a major source of nucleation- and Aitken-mode aerosols. Recent studies showed that deep convective systems can transport these aerosols from free troposphere to boundary layer by strong convective downdrafts. These vertically transported aerosols can grow into cloud condensation nuclei (CCN) and significantly influence the subsequent cloud formation. Compared to entrainment and mixing, deep convective downdraft processes may be more rapid and efficient in the vertical transport of aerosols. However, most climate models do not include the downdraft induced aerosol vertical transport as a source of CCN, mainly because the frequency of deep convective events varies significantly with geographic location, and thus their contributions to CCN are unpredictable.

In this study, we analyze vertical transport of aerosols during Holistic Interactions of Shallow Clouds, Aerosols and Land Ecosystems (HI-SCALE) campaign. This vertical transport mechanism is characterized by an abrupt emergence of nucleation- or Aitken-mode aerosols with sizes below 50 nm, a decrease of equivalent potential temperature, and a change of carbon monoxide concentration measured at the ground site. Using this criterion, we identified eight deep convective transport events with various intensities during the HI-SCALE intense operation periods (51 days). Measurements onboard the G-1 aircraft before the transport events support the finding that aerosols and carbon monoxide were transported from the free troposphere. The size of the transported Aitken-mode aerosols was found to be negatively correlated with the decrease of the equivalent potential temperature, probably resulting from the different altitudes of the source of the downdraft. The relationship between the downdraft intensity and properties of the vertically transported aerosols (size and number concentration) will be further discussed.

10CC.5

Turbulent Flux Measurements of the Near-surface and Residual-layer Nucleation Particles. NICHOLAS MESKHIDZE, Markus Petters, Mohammad Maksimul Islam, *North Carolina State University*

New particle formation (NPF) events have been observed at various locations over the world. The main objective of the field campaign that was conducted at the DOE ARM SGP site in Oklahoma from 15 Oct. to 15 Nov. 2020, was to examine the feasibility to use the eddy-covariance flux measurement of >3 and >10 nm particles to distinguish between ground-level and residual-layer NPF events. Equipment deployed include a 10-m telescopic tower, multiple condensation particle counters, a sonic anemometer, an SMPS and POPS (for aerosol number size distribution from 10 to 300 nm and 180 nm to 3 mm, respectively), an HTDMA (for 15, 20, 30, 40, and 50 nm-sized particle hygroscopicity), and a mini SODAR (for wind profiles between 15 and 500 m).

Here we report results showing data of eddy-covariance particle flux superimposed with observed small particle events. Seven small particle events (defined as periods where 3 to 10 nm-sized particle number concentrations increased by greater than one order of magnitude above the background) were observed. Downward vertical turbulent fluxes of sub-10 nm-sized particles generally coincided with the small particle events, suggesting that the majority of the new sub-10 nm particles observed at the surface during the event originated aloft and were brought to the surface by convective mixing during the daytime evolution of the planetary boundary layer. Hygroscopic growth factor measurements indicated growth factors much smaller than those of ammonium sulfate, suggesting that organic compounds dominated the sub-50 nm sized particle chemical composition. Results of our study show that eddy covariance vertical turbulent flux measurements of 3 to 10 nm sized particles can provide an important constraint and help to understand the formation, origin, and evolution of nucleation mode particle number concentration and size distributions during ground-based observational campaigns.

10CC.7

Aircraft Measurements of Single Particle Size and Composition Reveals Real-world Mixing State Necessary to Explain Activation Fraction during HI-SCALE.

GEORGES SALIBA, David Bell, Kaitlyn J. Suski, John Shilling, Fan Mei, Gourihar Kulkarni, Adam Varble, Johannes Muelmenstaedt, Jian Wang, Jason Tomlinson, Jerome Fast, Alla Zelenyuk, *Pacific Northwest National Laboratory*

Shallow convective clouds are ubiquitous in many regions of the world. Currently, aerosol-cloud parameterizations for convective clouds are a large source of radiative uncertainty in global climate models, highlighting the need for in-situ characterization of the size, composition, and mixing-state of activated particles and their more accurate model representation. Here we present aircraft measurements performed over the Atmospheric Radiation Measurements, Southern Great Plains climate facility in Oklahoma during the spring and summer of 2016, which were characterized by contrasting aerosol composition. These measurements quantified the properties of below-cloud aerosol, cloud droplet residuals, interstitial particles, and above-cloud aerosol of continental shallow cumuli. Organic-rich particles accounted for a larger number fraction of below-cloud particles in the summer compared to spring, consistent with higher emissions of biogenic volatile organic compounds, i.e. isoprene. We also present single-particle measurements that provide evidence of a strong influence of the size, composition, and mixing state of below-cloud aerosol on the activation fraction for shallow cumuli. The data indicate that cloud droplet residuals were larger and more hygroscopic compared to below-cloud aerosols, consistent with the efficient activation of these particles and aqueous formation of sulfate components in cloud droplets that increase the size and hygroscopicity of residuals. Using below-cloud measurements of aerosol composition, size distributions, and mixing-state, we calculated the effective cloud supersaturations between 0.06% and 0.24% (median = 0.1%). Moreover, we show that commonly used assumption of an internally mixed aerosol yielded calculated supersaturations that are significantly larger than measured, highlighting the importance of accurately describing the aerosol mixing state in models.

10CC.8

Measurements of Hygroscopic and Optical Properties of Size Selected Gray Carbon Aerosols: A New Empirical Function to Estimate Radiative Forcing.

TYLER CAPEK, Christian Carrico, Kyle Gorkowski, James E. Lee, Katherine Benedict, Claudio Mazzoleni, Allison Aiken, Manvendra Dubey, *Michigan Technological University*

Water vapor can significantly affect the physical and optical properties of atmospheric aerosol leading to changes in atmospheric radiative forcing. Water can condense onto the particles, increasing their size and altering their morphology. Absorbing particles range from hydrophobic to hydrophilic, the latter leading to water uptake and enhancements in absorption and scattering. To demonstrate water uptake for internally mixed absorbing particles, we measured the optical response to humidification of ammonium sulfate (non-absorbing), nigrosin (absorbing), and two darker and lighter ammonium sulfate and nigrosin mixtures. The molar ratio of ammonium sulfate to nigrosin of the two mixtures were 1:1 and 4.7:1, respectively. We used a novel humidified cavity attenuated phase shift albedometer (H-CAPS-PM_{SSA}) at 450 nm by Carrico, Capek et al. (Aerosol Science & Technology, 2021). This instrument measures extinction and scattering at well-controlled relative humidity values ranging from 30 ± 2% – 90% ± 3%. These measurements enable for the quantification of absorption and single scattering albedo at high relative humidity, with high precision. We found absorption enhancements due to humidification to be as high as 1.08 for pure nigrosin, and 1.15 for the mixtures. Enhancements in single scattering albedo were dependent on the amount of nigrosin within the dry aerosol. Furthermore, the enhancement at a certain relative humidity value could be empirically fit using a quadratic function, with nigrosin volume fraction as the independent variable. For each size and composition investigated, this relation was dependent on a single fitting parameter that is related to dry aerosol size and relative humidity. It is likely that this parameterization can be extended to phase separated absorbing and non-absorbing components. Our parameterization can be used to predict changes in aerosol optical properties with humidity in cloud-resolving and/or climate models to better predict their radiative forcing.

10CC.9

Comparing Online and Offline Measurements of Ice-Nucleating Particles from Two Autumn Field Campaigns.

ELISE WILBOURN, Larissa Lacher, Hemanth Sandeep Kumar Vepuri, Jens Nadolny, Ottmar Möhler, Naruki Hiranuma, *West Texas A&M University*

Atmospheric ice-nucleating particle (INP) concentrations are a source of uncertainties in current climate models, partially due to a lack of global-scale INP measurements. INPs were traditionally measured using either offline or in-situ measurements, both involving large quantities of time and labor. Advancements using the Portable Ice Nucleating Experiment (PINE) chamber, a remotely operated expansion chamber working continuously, allow for longer INP measurement periods at time scales of 8-15 minutes per measurement. Recently, PINE was deployed on two field campaigns, first from October 1 – November 15, 2019 in Oklahoma, USA (referred to as southern great plains, SGP), and second from October 1, 2020 – March 28, 2021 on Graciosa Island, Azores, Portugal (referred to as eastern north Atlantic, ENA). These sites have drastically different aerosol concentrations and sources. PINE measured INP concentrations relevant for mixed-phase cloud formation, but the chamber is limited by statistical accuracy to temperatures below -15 °C with current methods, limiting information on higher-temperature INPs during these campaigns. To address this limitation, aerosol particles were also collected on filters at a several-day time scale for offline analysis using a droplet freezing assay to assess associated INP concentrations. Here we compare measurements taken with PINE and those measured with offline techniques. Although SGP and ENA measurements were taken during the same season, the filter measurements and PINE measurements indicate that the terrestrial SGP site has a consistently higher INP concentration, potentially driven in part by higher overall particle concentration. This is in line with previous studies indicating INP concentrations at terrestrial sites tend to be one to two orders of magnitude higher than concentrations at marine sites like ENA. Our preliminary results suggest good agreement between online and offline techniques, validating the use of a multi-instrument technique to measure INP concentrations.

10CC.10

Dynamic Mixing State Effects on the Hygroscopicity of Ammonium Sulfate – Water Soluble Organic Compound Mixtures.

PATRICIA RAZAFINDRAMBININA, Kotiba A. Malek, Kristin DiMonte, Tim Raymond, Dabrina Dutcher, Miriam Freedman, Akua Asa-Awuku, *University of Maryland*

In the atmosphere, hygroscopic aerosol particles can uptake water and form clouds that will in turn reflect or absorb solar radiation, indirectly affecting the Earth’s climate and net radiative forcing. Submicron organic species compose ~50% of tropospheric aerosol particles by mass, which includes a subset of water-soluble organic compounds (WSOC) that are known to readily mix with ammonium sulfate. However, knowledge of the mixing state and its effect on hygroscopicity is limited. In this research, internal and external mixtures of ammonium sulfate with sucrose, levoglucosan, and adipic acid were able to be produced, and a laminar flow mixing tube facilitated the mixing state evolution of the mixtures. A cloud condensation nuclei counter (CCNC) and a humidified tandem differential mobility analyzer (H-TDMA) measured the water uptake of mixtures at subsaturated and supersaturated conditions. Here, we present the changes in experimental water uptake and cloud condensation nuclei activity with mixing states as a single hygroscopicity parameter (κ), and compare it to a predicted value derived from the Zdanovskii-Stokes-Robinson (ZSR) model. This work shows the complexity of binary internal and external mixtures and results imply that: (1) Organic-inorganic mixtures can produce non-ideal solutions that modify droplet solution. (2) Mixing state can be observed and defined by a function of the organic-inorganic composition ratio, which can aid the improvement of global climate models.

10CC.11

Phase Behaviour of Mixtures of Primary and Secondary Organic Aerosols.

FABIAN MAHRT, Elli Newman, Yuanzhou Huang, Julia Zaks, Yiming Qin, Paul Ohno, Scot T. Martin, Markus Ammann, Allan Bertram, *University of British Columbia*

Atmospheric aerosol particles play an important role for air quality and climate. Primary organic aerosol (POA) and secondary organic aerosol (SOA) make up a significant mass fraction of these particles. POA denotes aerosols that are directly emitted into the atmosphere. By contrast, SOA mostly forms from oxidation of precursor gases, followed by gas-particle conversion of the oxidation products with lower volatility. In order to describe SOA formation in atmospheric models, and predict their impact on air quality and climate, knowledge on the phase behaviour, i.e. the number and types of phases, in mixtures of POA and SOA is required. For instance, it is often assumed that SOA formation is enhanced in the presence of POA seed particles due to a lowering of the activities in the liquid organic aerosol phase in case of single-phase POA+SOA particles. The presence of POA will have a smaller effect on the formation of SOA mass in case of phase-separated particles.

Here, using optical and fluorescence microscopy, we observed the relative humidity dependent phase behaviour of individual particles containing mixtures of proxies of POA and SOA. Commercially available organic molecules were used as proxies for POA and SOA, covering a range of oxygen-to-carbon ratio between 0 and 1.0. For most of the mixtures investigated, phase-separated particles dominated, and the phase behaviour strongly depends on the oxygen-to-carbon ratio of the two mixed proxies. Results using more complex SOA material derived from environmental chamber studies confirm the dominance of phase separated POA+SOA particles. Our results have important implications for air pollution policies being considered to limit SOA formation in urban environments.

10CC.12

Atmospheric New Particle Formation from Gas Phase Reactions of Alkanolamines with Sulfuric Acid.

SANDRA FOMETE, Jack Johnson, Nanna Myllys, Coty Jen, *Carnegie Mellon University*

Chemical absorption using aqueous alkanolamine solutions such as monoethanolamine (MEA), diethanolamine (DEA), and triethanolamine (TEA) is widely used for CO_2 capture in several industrial processes. As such, these alkanolamines are likely to be released in large amounts into the atmosphere due to large-scale adoption of this process as countries work towards achieving net-zero carbon emission targets. In addition, these amines are also used in a wide variety of industrial and personal care products. Despite the extensive use of these chemicals, their fate in the atmosphere has not been extensively studied. One likely reaction pathway for these chemicals in the atmosphere is nucleation with sulfuric acid. Computational chemistry suggests that MEA plays a vital role in enhancing sulfuric acid nucleation. However, nucleation kinetics of MEA, as well as that of DEA and TEA with sulfuric, has not been experimentally measured. In this study, we examined nucleation reactions of MEA, DEA, and TEA with sulfuric acid in a flow reactor. 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 was analyzed using a custom-built high resolution, atmospheric pressure interface time of flight chemical ionization mass spectrometer (API-ToFCIMS). In addition, the Atmospheric Cluster Dynamics Code (ACDC) is also used to investigate how the formation rates of sulfuric acid-MEA/DEA/TEA compare with experimental measurements. Results indicate that MEA, DEA, and TEA at the parts per trillion (ppt) level can enhance sulfuric acid nucleation in the atmosphere. Though the enhancing potential of these alkanolamines is less than that of dimethylamine (DMA), one of the strongest enhancing agents, it will likely play a key role in new particle formation in the atmosphere as these compounds are increasingly used for the removal of CO_2 in the atmosphere. Results from this study improve the current understanding of how new particles form in the atmosphere and will help in evaluating the environmental impact of alkanolamines used for CO_2 capture.

10IM.1

Beyond Positive Matrix Factorization: The Strengths and Weaknesses of 3D Factor Analysis Methods.

MICHAEL WALKER, Brent Williams, *Washington University in St. Louis*

Advances in mass spectrometry have greatly expanded our understanding of aerosol chemistry and composition. With increasingly high time- and chemical-resolution measurements, a wealth of complex data necessitates more elegant analysis methods. Positive matrix factorization (PMF) has been widely applied within the aerosol science community to identify the key, physically-relevant features within datasets. When paired with mass spectrometry data, PMF generates factors of covarying mass-to-charge values and the corresponding time series that reconstruct the initial data. However, many of the newly developed and adopted analytical methods to probe aerosol composition feature an additional separation dimension that will not be considered in the two-dimensional PMF model. This separation dimension can be understood as retention time in chromatography measurements, temperature-based separation from thermograms, or size in particle-time-of-flight or mobility-based measurements. To enable a more detailed analysis of these types of datasets, the existing, Igor-based PMF Evaluation Tool that has utilized the PMF2 solver for PMF analysis has been enhanced to incorporate the Multilinear Engine 2 (ME-2) solver and three-dimensional factor analysis models. The PMF2 and ME-2 solvers offer various tradeoffs in terms of their computational efficiency, capabilities to handle large datasets, and ability to constrain solutions that should be considered when determining the proper data analysis approach. Furthermore, the specific model and solver choice needs to be directed by the scientific questions driving the study. Examples from a variety of laboratory and field measurements from different 3D mass spectrometry techniques will illustrate the importance of these decisions in the factor analysis process.

10IM.2

Airborne Flux Measurements of Ammonia over the Southern Great Plains.

SIEGFRIED SCHOBESBERGER, Emma D'Ambro, Ben H. Lee, Qiaoyun Peng, Mikhail Pekour, Jerome Fast, Joel A. Thornton, *University of Eastern Finland*

Ammonia (NH_3) plays an important role in atmospheric and environmental chemistry, from the formation of inorganic and organic aerosol, to soil acidification and nutrient cycles. Its dominant source are anthropogenic emissions, primarily from agricultural activities, and it thereby contributes substantially to fine-particle pollution in many regions. However, there are high uncertainties in attributing atmospheric NH_3 to specific sources, and current emission inventories substantially underestimate many major point sources. The quantification of NH_3 is challenging, due to the wide range of ambient mixing ratios and its infamous propensity to interact with surfaces, causing losses and slow response times.

In this study, we present a new technique for detecting NH_3 using a chemical ionization mass spectrometer (CIMS). The CIMS was deployed on a G-1 aircraft during the Holistic Interactions of Shallow Clouds, Aerosols, and Land Ecosystems (HI-SCALE) campaign over Oklahoma, specifically around the ARM Southern Great Plains field site, in 2016. The instrument was modified to enable quantifiable airborne measurements throughout tropospheric pressures, and to alternatingly use iodide anion and deuterated benzene cation ionization. In this mode, and aided by a high-flow core-sampling setup, we obtained a formidable device for measuring in-situ mixing ratios of NH_3. The high sensitivity and response time of ~1 s allowed us to calculate vertical NH_3 fluxes via eddy covariance. Besides measuring the free-troposphere and boundary-layer NH_3 levels, we detected sharp plumes of highly elevated (10’s of parts per billion) NH_3 downwind from a fertilizer plant. The fluxes let us also constrain the NH_3 emission rates for ubiquitous agricultural area sources. The HI-SCALE flight profiles focused on studying shallow convective clouds, and additional instrumentation provided aerosol chemical speciation and size distributions, which allows us to put our measurement results in perspective of aerosol properties and cloud processing.

10IM.3

Using Dynamic Principal Components to Analyze Mobile Particulate Matter Measurements. BLAKE ACTKINSON, Robert Griffin, Katherine Ensor, *Rice University*

Mobile monitoring is becoming an increasingly popular technique to measure particulate air pollution because of the high spatial resolution of its measurements. While the high spatial resolution of these measurements offers advances in understanding the distribution of particulate matter (PM), work is needed to characterize its sources. Past work has used Principal Component Analysis (PCA) to analyze source contributions to mobile PM measurements; however, it is problematic because these measurements are inherently non-stationary if collected over an extended period of time and space.

Here we discuss the use of Generalized Dynamic Principal Components (GDPC) to evaluate the sources of PM collected with a mobile platform in Houston, Texas. GDPCs are lagged principal component reconstructions of the data that are obtained through minimizing a mean-squared error loss function. GDPCs can be applied to non-stationary data to characterize the potential source contributions of that data. We also discuss differences between what this technique shows about source contributions compared to more traditional principal components. We believe that GDPC offer an improved way to identify source contributions of PM.

10IM.4

Introducing the Culebra Aerosol Research Lidar Project. JENS LAUTENBACH, Pedrina Terra, Josef Hoeffner, *Arecibo Observatory - UCF*

This poster presentation introduces and gives the status of the Culebra Aerosol Research Lidar (CARLA) project funded by the Puerto Rico Science, Technology & Research Trust.

CARLA's research instrument, an innovative high spectral resolution aerosol lidar is under development at the main site of the Arecibo Observatory, Puerto Rico. It will provide the scientific community with height resolved aerosol data at a Caribbean location. This includes dust coming across the Atlantic Ocean from the African continent that is named Saharan Air Layer (SAL). The SAL plays an important role in the lower atmosphere because it affects cloud and hurricane formation, weather, and the health of our population, among others. Based on SAL's track, CARLA will be deployed at the Remote Optica Facility of the Arecibo Observatory in Culebra Island. Culebra Island is located around 20 miles east of Puerto Rico mainland and a unique site to investigate the SAL before it reaches Puerto Rico mainland. The purpose of the CARLA project is twofold: (a) study and provide data to the scientific community of aerosol properties and SAL over the island of Culebra, and (b) increase opportunities for the educational system by outreach activities for Puerto Rico's K-12 schools as well as for university students to perform hands-on research experience.

10IM.5

Re-examination of the CAPS PMssa Monitor Scattering Channel Truncation. Brian Heffernan, Stephen Jones, Timothy Onasch, ANDREW FREEDMAN, *Aerodyne Research, Inc.*

We present measurements as well as detailed modeling of the truncation effect in the scattering channel of the PM_{SSA} monitor. Wavelength (450-780 nm) dependent measurements of relative scattering intensities as a function of optical extinction are determined using both polystyrene latex (PSL) and ammonium sulfate particles. These particles are size selected using either a differential mobility analyzer (DMA) or an aerodynamic aerosol analyzer (AAC). The effects of the degree of the non-monodisperse nature of the measured particles, determined using an optical particle counter (OPC), will be discussed. We will also present detailed Zemax-based ray tracing modeling of the optical system which includes the effects of multiple reflections caused by the presence of a glass tube in the integrating sphere. Finally, a comparison with recently published data by other researchers will be made.

10IM.6

Comparison of Particle Phase Data from FIGAERO CIMS and LTOF-AMS from Formation of Biogenic Particles in the CERN CLOUD Chamber. BRANDON LOPEZ, Mingyi Wang, The CLOUD collaboration, Neil Donahue, *Carnegie Mellon University*

The formation of particles by highly oxygenated molecules from the ozonolysis of biogenic precursors has been observed in the controlled environment of the CERN CLOUD chamber under conditions of the free troposphere. The composition and properties of particles in air masses depend on the formation conditions but can also be influenced by changing conditions as the particles are transported through the atmosphere. Here we present results from pure biogenic nucleation at constant temperatures from +5 to -50 ^{o}C at various values of relative humidity (RH). We explore the particle composition by comparing real-time data from two mass spectrometers using positive matrix factorization (PMF). The aerosol mass spectrometer (AMS) quantitatively measures the bulk composition of particles, while the Filter Inlet for Gases and AEROsols (FIGAERO) with an iodide chemical ionization mass spectrometer can provide aerosol molecular information. The bulk AMS data depend strongly on temperature but weakly on RH; however, PMF analysis of the FIGAERO data reveals that the particle composition is significantly different at different RH, despite the similar AMS spectra. The two data sets are thus complementary, suggesting that bulk aerosol properties may remain relatively unchanged even as the overall particle composition is influenced by the presence of water.

10IM.7

Sensor Environmental Test Chamber-2 (SEnTEc-2): Advancing Today's Sensor Testing to Meet Tomorrow's Sensor Needs.

DAVID HERMAN, Wilton Mui, Vasileios Papapostolou, Andrea Polidori, *South Coast Air Quality Management District*

The Air Quality Sensor Performance Evaluation Center (AQ-SPEC) program of the South Coast Air Quality Management District (AQMD) has evaluated the performance of over 100 low-cost sensors (LCS) measuring air pollutants both in the field and a controlled test chamber. The first AQ-SPEC Sensor Environmental Test Chamber (SEnTEc-1) capabilities included temperature, relative humidity, and pollutant control for gases and both liquid and solid dust particles. However, recent advances in LCS applications (i.e., sensor networks and mobile deployment) have necessitated more complex testing capabilities. Therefore, AQ-SPEC has developed a second larger Sensor Environmental Test Chamber (SEnTEc-2) capable of performing more comprehensive test procedures. The SEnTEc-2 system was designed using the knowledge and experience gained from SEnTEc-1 and expands the testing capabilities of AQ-SPEC. This updated chamber system can generate complex aerosol and gas mixtures using the following: an integrated zero-air generator, a dynamic dilution calibrator, two aerosol generators, an ozone generator, and certified gas cylinders; automation and feedback controls maintain the produced pollutants at chosen concentrations. A suite of Federal Reference Method and/or Federal Equivalent Method monitors measure both particulate matter and gaseous species, as well as particle size distributions. Preliminary test exercises demonstrate that the SEnTEc-2 system can generate a wide range of stable and reproducible aerosol and gas atmospheres. Specific/predetermined test sequences such as that in the EPA's Performance Testing Protocol for Fine Particulate Matter Air Sensors can also be reliably conducted. Furthermore, the development and execution of highly specialized testing scenarios by the SEnTEc-2 system (i.e., vibration, wind speed, and altitude tests) can provided additional validation into the use of low-cost sensors in environments with more turbulent weather conditions. When fully implemented, the SEnTEc-2 system will assist with sensor networks/sensor loan program calibration, performance target testing, and supplementary testing for low-cost sensors deployed on mobile platforms.

10IM.8

Assessment of Children's Personal and Land Use Regression Model-Estimated Exposure to NO2 in Springfield, Massachusetts.

DONG GAO, Sarah Esenther, Laura Minet, Alexander De Jesus, Tina Savvaides, Marianne Hatzopoulou, Krystal Godri Pollitt, *Yale University*

Ambient nitrogen dioxide (NO_2) is a widely available measure of traffic-related air pollution and has been found associated with a variety of health outcomes. The land use regression (LUR) models, which are frequently used to estimate air pollution exposures, is able to describe small-scale spatial variation in air pollution levels based on geographical predictor variables. In this study, an NO_2 monitoring network was established at 40 sites across the greater Springfield region in Massachusetts using cost-effective passive samplers and measured ambient NO_2 levels during a five-day period in winter 2018. The NO_2 measurements, along with the land use characteristics, were incorporated into a LUR model. A total of 25 children (age 12-13), meanwhile, were recruited from a local elementary school, and their personal NO_2 exposures were measured by novel wearable samplers. The personal NO_2 exposure was compared with LUR-derived NO_2 exposure estimates in different microenvironments including homes, school and commute paths. The results show that the variability in personal NO_2 exposure is greater than the typical individual outdoor exposures predicted by LUR, though the LUR model had a good prediction performance and could capture the NO_2 emission hotspots in outdoor settings. The findings suggest that human NO_2 exposure can be highly personalized based on different combustion sources and access to house ventilation, reaffirming the importance of measuring personal exposure.

10SW.1

Optical Properties of Absorbing Aerosol Emitted from Biomass Burning. YINGJIE SHEN, Rudra Pokhrel, Shane Murphy, Ezra Levin, Amy P. Sullivan, *University of Wyoming*

Black carbon (BC) and Brown carbon (BrC) emissions from wildfires absorb visible sunlight and have a significant impact on the global energy budget. Wildfires are one of the largest sources of both BC and BrC globally, but the optical properties and magnitude of these emissions remain uncertain. With the increasing number of wildfires in the United States and globally, the absorption, scattering and extinction caused by BC and BrC are of growing importance. In this presentation we will present results from ground campaigns in the Mountain West using a mobile lab and results from airborne measurements during the WE-CAN (Western Wildfire Experiment: Cloud Chemistry, Aerosol Absorption, and Nitrogen) field campaign. The impact of organic coatings of BC and brown carbon will be presented. We will also present results on the impact of photochemical aging, dilution, and physical aging on the contribution of both BC and BrC to total aerosol absorption. Finally, we will present summary results on the average overall optical properties of Western U.S. wildfires and discuss their relationship to global biomass burning emissions.

10SW.2

Investigating Carbonaceous Aerosol and its Absorption Properties from Fires in the Western US (WE-CAN) and Southern Africa (ORACLES and CLARIFY). THERESE CARTER, Colette L. Heald, Christopher Cappa, Jesse Kroll, Teresa Campos, Hugh Coe, Michael Cotterell, Nicholas Davies, Delphine K. Farmer, Cathryn Fox, Lauren A. Garofalo, Lu Hu, Justin Langridge, Ezra Levin, Shane Murphy, Rudra Pokhrel, Yingjie Shen, Kate Szpek, Jonathan Taylor, HuiHui Wu, *MIT*

Biomass burning (BB) produces large quantities of carbonaceous aerosol (black carbon and organic aerosol, BC and OA, respectively), which significantly degrade air quality and impact climate. Black carbon absorbs radiation, warming the atmosphere, while OA typically scatters radiation, leading to cooling. However, some OA, termed brown carbon (BrC), also absorbs visible and near UV radiation; although, its properties are not well constrained. We explore three aircraft campaigns from large BB regions with different dominant fuel and fire types (WE-CAN in the western US and ORACLES and CLARIFY off southern Africa) and compare them with simulations from the global chemical transport model, GEOS-Chem using GFED4s. The model generally captures the observed vertical profiles of carbonaceous BB aerosol concentrations; however, we find that BB BC emissions are underestimated in southern Africa. Our comparisons suggest that BC and/or BrC absorption is substantially higher off Africa than in the western US and that, while the Saleh et al. (2014) and FIREX parameterizations based on the BC:OA ratio improve model-observation agreement in some regions, they do not sufficiently differentiate absorption characteristics at short wavelengths. We find that photochemical whitening substantially decreases the burden and direct radiative effect of BrC (annual mean of +0.292 W m^{-2} without whitening and +0.083 W m^{-2} with). Our comparisons suggest that whitening is required to explain WE-CAN observations; however, the importance of whitening for African fires cannot be confirmed. Qualitative comparisons with the OMI UV aerosol index suggest that our standard BrC whitening scheme may be too fast over Africa.

10SW.3

Investigating the Southeast Asian Haze Impacts on Urban Organic Aerosol Composition Using a High-Mass Resolution Spectrometry and Factor Analysis. SRI HAPSARI BUDISULISTIORINI, Katie Balmer, Daniel Bryant, Liudongqing Yang, Jing Chen, Mikinori Kuwata, Jacqueline Hamilton, *University of York*

Organic aerosol (OA) is a major component of urban particulate matter. One of the contributing sources to urban OA is biomass burning emission. Recurring peatland fire has caused Southeast Asia countries, including Singapore, blanketed by haze for the last two decades. Studies found oxygenated organic aerosol (OOA) as the dominant OA component during the haze episode and linked it to biomass burning tracers. The limited samples and analysis capabilities hindered further assessing the peatland fires' impact on urban air quality. Hence, we aim to investigate the OA sources in Singapore using a high-mass resolution spectrometer. Intermittent daily samples of particulate matter with an aerodynamic diameter less than 2.5 µm ($PM_{2.5}$) were collected from 2018 to 2019, covering clean and haze episodes. The samples were analyzed using liquid chromatography with heated electrospray ionization coupled to a Q-Exactive Orbitrap mass spectrometer. We developed a novel targeted and non-targeted molecular identification to the high-resolution mass spectrometry (HRMS) data. We identified almost 2000 compounds. Moreover, we discovered enhancement of biomass burning markers, including 4-nitrocatechol, 4-hydroxy-3-nitrobenzoic acid, 4-nitro-1-napthol, vanillin, nitroguaiacols, nitrophenols, methyl-nitrophenols, and hydrocinnamic acids, during the haze period compared to the clean period. Interestingly, vanillic acid, methyl-dinitrophenols, and dinitrophenols, previously identified as biomass burning markers, did not display elevated levels during the haze event. Therefore, we applied, for the first time, a positive matrix factorization analysis technique to the identified HRMS compounds to further investigate the OA sources. The results indicate other major OA sources, including traffic and biogenic secondary organic aerosol sources. The hybrid non-targeted HRMS and factor analysis provide detailed OA sources characterization and powerful urban air quality observation tools.

10SW.5

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. If atmospheric aerosols are not internal mixtures, it could change how we understand their health and climate effects. When distinct aerosol populations come together, mixing should happen on a time scale of a few hours to support the internal mixing assumption. Gas-phase exchange between aerosol populations via evaporation and condensation of semi-volatile organics (“Marcolli mixing”) can be a major mechanism of mixing between accumulation-mode particles with slow coagulation. Viscous, semi-solid, or “glassy” particles may impede this by posing diffusion limitations to evaporation and/or condensation. Here we describe experiments on carefully prepared particle populations representing “glassy” aged organic particles (various non-volatile sugars as well as laboratory generated SOA with ammonium sulfate seeds) and fresh biomass burning particles (erythritol with black carbon seeds) to develop a model phase space for organic aerosol systems and better understand when particle “glassiness” impedes mixing. We quantify the mixing state of these particle populations 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 by “triggering” data acquisition when desired mass-to-charge ratios are detected and the SP mode enables refractory black carbon particles to be characterized. Our results suggest that the non-volatile sugar particles have no diffusive limitations to mixing at the conditions tested. Preliminary results suggest that laboratory generated SOA particles have diffusive limitations to mixing at certain conditions. Our hypothesis is that these limitations are alleviated at some relative humidity threshold, which increases with decreasing ambient temperatures.

10SW.7

Transported African Wildfire Smoke Acts as Cloud Condensation Nuclei in the Tropical Atlantic Marine Boundary Layer. HALEY ROYER, Mira L. Pöhlker, Ovid O. Krüger, Edmund Blades, Peter Sealy, Nurun Nahar Lata, Zezhen Cheng, Swarup China, Andrew Ault, Patricia Quinn, Hope Elliott, Patricia Blackwelder, Cassandra Gaston, *University of Miami*

The role of aerosols on cloud formation in the tropical Atlantic is important to understand as marine stratocumulus clouds reflect incoming solar radiation and obscure the low-albedo ocean surface. However, few studies have been conducted on aerosol-cloud interactions in this region. Ragged Point–a research station situated in Barbados–was established to study aerosol transport to the Caribbean including the summertime transport of African dust. The site is also uniquely situated to study cloud-aerosol interactions in the tropical Atlantic. In this study, we compared size-resolved chemical data from computer-controlled scanning electron microscopy coupled with energy dispersive x-ray spectroscopy (CCSEM/EDS) to size-resolved CCN measurements from a cloud condensation nuclei (CCN) counter (CCNC) coupled with a scanning mobility particle sizer (SMPS). Data were collected at the Ragged Point field station during the EUREC^{4}A and ATOMIC campaigns from January to February 2020. Results show unusual wintertime transport of African smoke and dust to the northwest tropical Atlantic. When long-range transported African aerosol arrived in Barbados, we observed a compositional change in the aerosol particle loading from marine sulfate to smoke particles as well as a decrease in aerosol hygroscopicity. Further, during these time periods, CCN number concentrations doubled, suggesting that transported smoke particles increase the CCN burden compared to marine background conditions. Previous research has shown the impact of African smoke on clouds over the tropical south Atlantic. However, our work shows that aerosol hygroscopicity and CCN number concentrations over the tropical North Atlantic are also affected by African smoke. These findings highlight the pervasive impact of African smoke in the Atlantic marine boundary layer and can be used to improve uncertainties in current climate models regarding the role of smoke particles on cloud formation and cloud properties in the tropical North Atlantic.

10SW.9

Aerosol Size Distribution Changes in Biomass Burning Plumes: The Competing Roles of Coagulation and OA Condensation/Evaporation. NICOLE JUNE, Anna Hodshire, Elizabeth Wiggins, Richard Moore, Edward Winstead, Claire Robinson, Kenneth Thornhill, Kevin Sanchez, Demetrios Pagonis, Hongyu Guo, Pedro Campuzano-Jost, Jose-Luis Jimenez, Matthew Coggon, Sonia Kreidenweis, Shantanu Jathar, Jeffrey R. Pierce, *Colorado State University*

The evolution of organic aerosols and aerosol size distributions within smoke plumes are uncertain due to the variability in rates of coagulation and OA condensation/evaporation across different smoke plumes and potentially in different locations of a single plume. We use aircraft data from the western US portion of FIREX-AQ campaign to evaluate differences in aerosol size distribution evolution (growing by 10s to over 100 nm in several hours) under different concentrations and amounts of dilution. We estimated the role of coagulation using model simulations and the role of OA condensation/evaporation using the observed time evolution of the observed total organic aerosol (OA) mass. We find that coagulation alone can explain a majority of the diameter growth in concentrated portions of the smoke plumes (i.e., when the initial ΔOA concentrations were >1000 µg m-3) and even overestimates the observed growth in some cases. In concentrated smoke plumes, there is observed OA evaporation, which helps reduce the over estimation of growth due to coagulation alone. In dilute portions of plumes (i.e., ΔOA < 100 µg m-3), coagulation alone tends to underestimate the observed aerosol growth. On the other hand, the ΔOA enhancement ratios tend to increase with age in the dilute portions of smoke plumes, implying that there is net condensational growth of these particles, and we infer that condensation plays a larger role than coagulation in particle growth in dilute smoke regions. In some smoke plumes, the combined growth from coagulation and OA changes still results in an overprediction in the concentrated portions yet an underestimation in dilute portions, may indicate that turbulent mixing between the percentile groups is important. Overall, we conclude that coagulation dominates growth in concentrated plumes, while OA condensation dominates in dilute plumes, and we discuss potential reasons for this.

10SW.10

High-intensity Forest Fires Emit High Concentrations of Diverse, Viable, and Ice-Nucleating Bioaerosols. LEDA KOBZIAR, David Vuono, Rachel Moore, Timothy Dean, Doris Betancourt, Adam Watts, Brent Christner, Johanna Aurell, Brian Gullett, Adam Kochanski, Ali Tohidi, *University of Idaho College of Natural Resources*

The atmosphere is known to harbor diverse and active microorganisms. However, the contribution of wildfire smoke as a vector for bioaerosol dispersal is unknown. To address this knowledge gap, we conducted the first molecular and cellular characterization of wildland fire smoke from high-intensity forest fires at the Fire and Smoke Model Evaluation Experiment (FASMEE) in Fishlake National Forest, Utah. Using unmanned aerial systems (UAS) to sample bioaerosols directly above the forest combustion zone, our results show that fire aerosolizes diverse and viable assemblages of microorganisms that are distinct from background aerosols, and that have ice nucleating potential three-fold above background levels. Nearly four times as many DNA-containing cells were found in smoke compared to ambient air, with 79% inferred to be viable. Both total and biological ice nucleation potential were higher in smoke at temperatures -8 to -15 °C. Molecular reconstruction of microbial assemblages from 16S and 18S rRNA genes as well as fungal ITS sequences show that effective diversity of bacterial taxa was twice as high in smoke than in ambient air. Ordination techniques show that ambient and smoke bacterial assemblages differed significantly. Our results indicate that living microbes constitute a non-trivial portion of the aerosols in smoke produced by high intensity wildland fires, and therefore may have impacts on weather, atmospheric chemistry, and the dispersal of human or plant pathogens. Such fires are capable of ejecting smoke plumes above the planetary boundary layer, challenging the concept of a wildfire’s perimeter of impact and introducing the possibility of smoke as a biological dispersal agent with global reach.

10SW.11

Impact of Wildfire Smoke and Biomass Burning on PAHs and Quinones. ELIZABETH NOTH, Frederick Lurmann, Charles Perrino, David Vaughn, S. Katharine Hammond, *Environmental Health Sciences, SPH, UC Berkeley*

As part of our ongoing research to understand the impact of polycyclic aromatic hydrocarbon(PAH) exposures on health in the San Joaquin Valley, we evaluated 20 years of airborne PAH data(2002-2021) in Fresno, California. We collected and analyzed 752 integrated 24-hour PM10 samples for PAHs collected on two 37mm pre-baked quartz fiber filters impregnated with ground XAD-4 resin. This method captures both vapor- and particle-phase compounds. These samples were analyzed for 17 PAHs and 19 quinones. We evaluated the impact of agricultural waste burning(AWB) and wildfire smoke(WFS) on these compounds and their relevant diagnostic ratios. We quantified agricultural burning in Fresno and Madera Counties from agricultural burn permit data with location and materials burned available from the local air district. To assign days of wildfire smoke impacts to Fresno, we used the NOAA Satellite Smoke Mapping product. The dataset had 67 days with both AWB and WFS, 24 days with just WFS, 502 days of AWB, and 159 days where neither type of impact was reported. We saw significant elevations in concentrations in many individual PAHs and quinones on days of WFS and AWB. The most dramatic differences were observed in 3- and 4-ring PAHs collected in July-October: compared to days with neither source, acenaphthylene was 13 times higher on WFS days, fluorene was 5 times higher and phenanthrene was 3 times higher. Retene concentrations during July-October that had AWB (and no WFS) were 37 times higher than days without. Samples during this same time period with both WFS and AWB showed the ratio of pyrene/benzo[a]pyrene was 12 times lower than days with neither source. Both pyrene and benzo[a]pyrene increased on WFS+AWB days, but benzo[a]pyrene increased more, relatively. PM2.5 and NO2 concentrations for these days do not exhibit similar dramatic differences in response to the change in source.

10SW.12

Photolytic Mass Loss of Secondary Organic Aerosol (SOA) Derived from Furan Species. NARA SHIN, Yuchen Wang, Taekyu Joo, Nga Lee Ng, Pengfei Liu, *Georgia Institute of Technology*

Biomass burning (BB) is one of the major global sources of primary organic aerosols and volatile organic compound (VOC)precursors which can produce secondary organic aerosols (SOA). These organic aerosol particles undergo further chemical processes in the atmosphere that result in changes in their mass concentration and physicochemical properties. One process involves photolysis in the particulate phase, which has been identified as a loss pathway of organic aerosols. However, this pathway can be confounded by other processes, such as photo-oxidation, in typical chamber experiments. In this study, we investigate the effect of photolysis on the mass of SOA formed by the oxidation of furan species. Furan compounds are known as a significant part of non-methane hydrocarbons and methylfuran is one of the major furans emitted from BB. The SOA produced by OH oxidation of furan species using an Oxidation Flow Reactor (OFR) and Georgia Tech Environmental Chamber are deposited onto a quartz crystal substrate and the mass-loss rates of SOA under specific UV wavelengths (300 and 340 nm) are measured using a Quartz Crystal Microbalance (QCM). During 48-h photolysis experiments on furan-derived SOA, we observed significant mass losses under two different wavelengths (300nm and 340nm), with a relatively higher mass-loss fraction at 300 nm wavelength than 340 nm. This study shows that particulate phase photolysis can be a potential fate and loss mechanism of BB-derived SOA in the ambient condition.

10UA.1

Simulation of SOA Formation from the Photooxidation of Long-chain Alkanes via Multiphase Reactions. AZAD MADHU, Myoseon Jang, David Deacon, *University of Florida*

Linear alkanes are hydrocarbon species that are emitted from gasoline and diesel automobile exhausts. It has been known that alkane SOA yield increases with increasing carbon number. The high molecular weight alkanes (larger than C9) are important SOA precursors from diesel combustion. In this study, the formation of alkane SOA is predicted by using the UNIfied Partitioning Aerosol Reaction (UNIPAR) SOA model via multiphase reactions of explicit products. In the model, oxidized gas products are predicted by using an explicit chemical mechanism (MCM V3.3.1) with the addition of auto-oxidation mechanisms that produce low volatility products. The SOA formation from photooxiation of n-nonane (C9), n-decane (C10), n-undecane (C11), and n-dodecane (C12) are first predicted and compared to observed SOA mass in the UF-APHOR chamber. The resulting SOA model is extended to the SOA formed from longer alkanes (C>12) by using the relationship between carbon length and distribution of products. The extended UNIPAR is also compared to chamber data (C13-C15). The sensitivity of alkane SOA yields to NOx levels, aerosol acidity, temperature, aerosol water content (humidity), and preexisting organic matter are analyzed through simulation with UNIPAR under varying conditions. Overall, alkane SOA yield is less sensitive to inorganic salted aqueous reactions of organic compounds because of the low solubility of its products, compared to other SOA precursors such as aromatics and biogenics.

10UA.2

Watching Paint Dry: Understanding I/VOC Emissions from Architectural Coatings and their Impact on SOA Formation. Rebecca Tanzer Gruener, Liam D. Dugan, Mark E. Bier, Allen Robinson, ALBERT A. PRESTO, *Carnegie Mellon University*

Volatile chemical products (VCPs) have become an increasingly important source of Volatile Organic Compounds (VOCs) and Intermediate-Volatile Organic Compounds (IVOCs) emitted into urban environments. These VOCs play a potentially important role in national Secondary Organic Aerosol (SOA) formation. In this study we conduct headspace and extended emissions tests of paints to quantify the emission factors of I/VOCs over paint's emission timescale. SOA yield predictions were also calculated. We found that paints are not expected to be a long term emission source of I/VOCs. The majority of all I/VOCs measured are indistinguishable from zero within two days post paint application. We found that on a national scale paints emit 0.51 kg/person per year of I/VOCs. This means that 291g of I/VOCs are emitted per kg of paint used in the U.S. each year. The SOA mass yield from these emissions were calculated to be 4.7% [+/-2%]. Even though the majority of the I/VOC emissions from the paints were VOCs (59%), the majority of the SOA formed from paint emissions (68%) were from the IVOC portion of the paint emissions. Interestingly the I/VOC paint emissions come predominately from Oil-based paints (making up 87% of the SOA formed from paints) and Semi-Gloss Exterior paints (making up the remaining 13% of SOA formed from paints). Both of these paints are primarily used outdoors where theoretically 100% of their I/VOC emissions enter the atmosphere and form SOA. This indicates that in order to best mitigate the SOA formed from paints, care should be taken to minimize the IVOC components of Oil and Semi-Gloss Exterior paints.

10UA.3

Key Role of NO3 Radicals in the Production of Isoprene Nitrates and Particulate Nitrooxyorganosulfates in Beijing. JACQUELINE HAMILTON, Daniel Bryant, Peter Edards, Archit Mehra, Thomas J. Bannan, Alfred Mayhew, James Hopkins, James Lee, Mike Newland, Bin Ouyang, Andrew Rickard, *University of York*

Poor air quality is the biggest environmental factor contributing to premature mortality globally. As the Earth's population has grown, the number of people living in urban areas has increased rapidly from 751 million in 1950 to 4.2 billion in 2018. By 2030, the UN estimates there will be 43 megacities (> 10 million inhabitants), with most of them located in developing countries in Africa, Asia and Latin America. Since many of these locations are situated in the tropics, high average temperatures can lead to significant emissions of biogenic volatile organic compounds (BVOC) to the urban atmosphere, in particular isoprene. Beijing, China, is a well-studied megacity, with significant air quality issues related to particle pollution and ozone (O3) production. Beijing experiences high average summertime temperatures (ca. 30 C) and has a high percentage of urban green space (> 41 % urban green space), which can lead to significant amounts of isoprene being emitted. Photochemical oxidation of isoprene in the presence of high levels of anthropogenic pollutants, in particular nitrogen oxides (NOx) and sulfur dioxide (SO2), can lead to enhanced secondary organic aerosol (SOA) production.

A key uncertainty in understanding SOA production from isoprene is the role of isoprene nitrates (IsN). IsN are formed in chain terminating reactions, during oxidation by hydroxyl radicals (OH) in the presence of NO, or by nitrate radicals (NO3). IsN can lead to significant secondary organic aerosol (SOA) production and they can act as reservoirs of atmospheric nitrogen oxides. Recent observations in a boreal forest by Liebmann et al. (2019) under low-NO conditions indicated that daytime alkyl nitrate production from NO3 chemistry can dominate over OH under certain conditions.

As part of UK-China Atmospheric Pollution and Human Health in a Chinese Megacity (APHH-China) program during the summer of 2017, we collected a comprehensive suite of gas- and particle-phase chemical observations. We estimated the rate of production of IsN from the reactions of isoprene with OH and NO3 radicals during the summertime in Beijing. Unusually low NO concentrations during the afternoon resulted in NO3 mixing ratios of ca. 2 pptv at approximately 15:00, which we estimate to account for around a third of the total IsN production in the gas phase (Hamilton et al., 2021). Heterogenous uptake of IsN produces nitrooxyorganosulfates (NOS). Offline filter samples were analysed using high resolution mass spectrometry coupled to chromatography to identify isoprene NOS for comparison to IsN levels in the gas phase. Two mono-nitrated NOS were correlated with particulate sulfate concentrations and appear to be formed from sequential NO3 and OH oxidation. Di-and tri-nitrated isoprene related NOS, formed from multiple NO3 oxidation steps, peaked during the night. This work highlights that NO3 chemistry can play a key role in driving biogenic-anthropogenic interactive chemistry in Beijing with respect to the formation of IsN during both the day and night. Further work will compare the production of NOS in other megacities and laboratory experiments to determine the role of NO3 in forming IsN in urban areas.

10UA.4

Air inequality: Global Divergence in Urban Fine Particulate Matter. JOSHUA S. APTE, Sarah Seraj, Sarah Chambliss, Melanie Hammer, Veronica Southerland, Susan Anenberg, Aaron van Donkelaar, Randall Martin, Michael Brauer, *University of California, Berkeley*

Fine particle air pollution ($PM_{2.5}$) is the largest global environmental risk factor for ill-health and is implicated in 7-12% of all human deaths. Improved air quality is a key policy goal for cities around the world, yet in-situ $PM_{2.5}$ measurements are missing for > 50% of the urban population. Here, we use satellite remote sensing of aerosol optical depth constrained by a geophysical model and in-situ observations to develop a 20-year time series of $PM_{2.5}$ for nearly all urban areas in the world with year-2010 population exceeding 100,000 people, encompassing 2.9 billion people in 4231 cities. Over this period, we find a growing divide in urban air quality between lower-income and higher-income world regions, with the $PM_{2.5}$ disparity increasing by > 50% between the highest- and lowest income quartiles of world cities. Within Asia, a sharp divergence is underway, with sustained increases in urban $PM_{2.5}$ in South Asia (+48%) contrasted against dramatic improvements in Chinese cities (-40% since 2011). While 85% of the world's urban population experiences $PM_{2.5}$ higher than World Health Organization guidelines, urban $PM_{2.5}$ concentrations are tightly linked to regional conditions, suggesting that city-level efforts alone may be insufficient to address this major health threat.

10UA.5

High-latitude Urban Air Quality: 20 Months of Aerosol Composition Data from Fairbanks, Alaska. ELLIS ROBINSON, Michael Battaglia, Meeta Cesler-Maloney, James Campbell, Athanasios Nenes, Jason St. Clair, Jingqiu Mao, Rodney J. Weber, William Simpson, Peter F. DeCarlo, *Johns Hopkins University*

We present continuous, sub-hourly measurements of aerosol composition from Fairbanks, Alaska, USA that span the past 20 months (January 2020 to August 2021) and include times before and after the social and economic disruption of the Covid-19 pandemic. Conditions of extreme cold, minimal sunlight, and Fairbanks' location within a river valley lead to wintertime aerosol concentrations that frequently exceed EPA 24-hour limits. We compare PM2.5 mass and composition measurements from winter 2020 (pre-Covid) with winter 2021 using an Aerodyne Aerosol Chemical Speciation Monitor (ACSM). The ACSM dataset identifies the relative contributions of different aerosol components to air quality in Fairbanks. Positive matrix factorization (PMF) of the mass spectral dataset is used to identify the major contributions to both organic and inorganic aerosol fractions, which include oxidized organic aerosol (OOA, 40-60% of OA mass), biomass burning OA (BBOA, 15-40%), and hydrocarbon-like OA (HOA, 15-25%). Wintertime sulfate concentrations display a diurnal pattern similar to HOA, implicating a primary vehicular source of sulfate in the region. Our analysis shows the relative contribution of the different major emissions sources to PM2.5 in Fairbanks, and how these sources change on diurnal and seasonal time scales and under the influence of different meteorological conditions.

10UA.6

Size-Segregated Ions and Carbonaceous Fractions of Ambient Aerosol in Bogota. LADY MATEUS, Nestor Rojas, Kelly Burbano, Rodrigo Jimenez, *Universidad Nacional de Colombia*

Size-segregated chemical characterization of ambient aerosol is useful to understand its sources and formation mechanisms, and complements information obtained from bulk aerosol composition. Elemental and Organic Carbon (EC/OC) make up a significant fraction of matter particulate emitted by combustion processes, and water-soluble ions provide an important information about the origin of ambient aerosols. Previous studies have determined the chemical composition and source contribution of PM_{10} and the temporal and spatial variability of polycyclic aromatic hydrocarbons (PAH) in Bogota, one of the main megacities of Latin America. However, the size-segregated chemical composition of ambient aerosol has not been studied. This work aims to better understand the size-segregated variability of the aerosol chemical composition in this city. A Tisch® 8-Stage Cascade Andersen Impactor was used to collect the samples of ambient aerosol in the southwest area of the city, which usually show the highest concentrations of $PM_{2.5}$. Eight sets of size-segregated ambient aerosol samples were collected over two periods in 2018 to quantify the concentration of OC/EC and water-soluble ions (ammonium, sodium, potassium, magnesium, calcium, chloride, nitrate, sulfate and oxalate). The average PM_1 concentration during the sampling campaign was 20.8 ±12.5 $\mu g/m^3$ (70.8 ± 10.7 % of $PM_{2.5}$). The mass size distribution was bimodal, with a coarse mode between 5.8 and 4.7 µm, and an accumulation mode between 0.43 and 0.65 µm. The carbonaceous fraction constituted over 75 % of PM_1 mass. The main component of the finest particles was EC, which can penetrate and deposit on alveolar sacs of people exposed to air pollution in this area of the city. The main inorganic ions were sulfate, nitrate, and ammonium, which had the maximum concentration in the range of 0.65 - 1.1 µm. The PM_1 concentration showed a moderate correlation with the concentrations of OC, EC, nitrate, calcium, and ammonium.

10UA.7

Aerosol Properties and Processing during Wintertime under Hazy Condition. SUSAN MATHAI, Zezhen Cheng, Rhenton Brimberry, Nurun Nahar Lata, Swarup China, *Pacific Northwest National Laboratory*

Atmospheric aerosols emitted into the atmosphere often as externally mixed compounds coagulate or condense on each other due to aging to exist in internally mixed state. Variability in mixing state of atmospheric aerosols play a major role in uncertainties associated with the estimated radiative forcing. Meteorological condition plays a major role in determining the mixing state of particles in the atmosphere. We collected samples during wintertime and under hazy condition from a polluted region which is impacted by biomass burning from household activities and agricultural burning. The collected samples were analyzed using multi-modal micro-spectroscopy and chemical imaging techniques such as computer controlled scanning electron microscopy, transmission electron microscopy and scanning transmission X-ray microscopy/near edge X-ray absorption fine structure spectroscopy to determine the size resolved morphology and chemical composition of individual particles. Due to extensive fire activities during winter the K-rich particles are dominant in the atmosphere. We also observed an abundance of sulfates in the sample which could be the result of aqueous phase reaction due to regional haze. Furthermore, we investigated phase state of individual particles with and without inorganic inclusions and our results suggest that particles with inclusions are in semi-solid state while particles without inclusions are in solid-state. The results from this study will help in understanding different mixing state of particles in an urban polluted region and the impact of mixing states on particle phase state.

10UA.8

Seasonal Influence on Urban Particulate and Black Carbon Pollution: Winter, Summer, and Wildfire.

REBECCA A. SUGRUE, Chelsea V. Preble, James D.A. Butler, Thomas W. Kirchstetter, *University of California, Berkeley*

Low-cost sensors can be deployed as dense monitoring networks to increase the spatial resolution of air pollution monitoring. This work collocated low-cost black carbon (BC) and fine particulate matter ($PM_{2.5}$) monitors in two California communities. In Richmond, a densely-populated urban community in the San Francisco Bay Area with a major refinery and surrounded by highways, 50 sensor pairs were installed. Eleven monitoring sites were distributed across Modesto, a sprawling Central Valley community impacted by agricultural and trucking activities. Month-long monitoring campaigns were conducted in summer (August) and winter (January) 2020–2021. Custom-built BC sensors (Aerosol Black Carbon Detectors, UC Berkeley) were collocated with Aeroqual AQY1 and PurpleAir PA-II $PM_{2.5}$ sensors in Richmond and Modesto, respectively, outside of homes and schools. This short-term monitoring captured seasonality in particulate pollution and spatiotemporal variability in $BC/PM_{2.5}$ ratios within and between these communities.

Despite differences in land-use and combustion sources, Richmond and Modesto had approximately the same average winter BC concentration, ~0.4 $\mu g\ m^{-1}$. During the summer campaign, both communities were heavily impacted by wildfire smoke, which resulted in more uniform $PM_{2.5}$ and BC. Compared to non-smoke affected summer periods, $PM_{2.5}$ and BC concentrations were 2–10× and 1.5–3.5× higher throughout the day, and the $BC/PM_{2.5}$ ratio was 50% lower when smoke impacted air quality in Richmond. Though historical records indicate a strong seasonal cycle with BC concentrations 2–4× higher in winter, the average winter BC concentration in Richmond during this study was only 50% higher compared to the non-wildfire summer period. Ongoing analysis is examining spatiotemporal differences of local air pollution between Richmond and Modesto, localized hotspots, and the influence of source-specific activity patterns. Additionally, we are examining data-driven approaches to distinguish between smoke and non-smoke impacted days and related wildfire smoke corrections for both low-cost BC and $PM_{2.5}$ sensor data.

10UA.9

Residential Wood Burning Aerosol Emissions and Secondary Aerosol Formation in the Wintertime Urban Atmosphere.

ANDREW HOLEN, Ryan Cook, Matthew Gunsch, Nathaniel May, Kathryn Kolesar, Kerri Pratt, *University of Michigan*

Wintertime air pollution is gaining attention due to air quality exceedances that impact human health. However, our current understanding is limited in terms of knowledge of primary emission source strengths and secondary aerosol formation. In particular, few studies have been done that examine the composition of individual atmospheric aerosols in urban environments during winter conditions. Therefore, a field campaign was conducted in Ann Arbor, Michigan from Feb. 4 – Mar. 8, 2016. An aerosol time-of-flight mass spectrometer (ATOFMS) was used to measure individual aerosol particle size, chemical composition, and mixing state. An ambient ion monitor – ion chromatography (AIM-IC) system provided online measurements of particulate inorganic ion concentrations. Simultaneous aerosol size distribution measurements were also conducted. Together these methods provided quantitative identification of individual sources, including residential wood burning, vehicle emissions, and road salt aerosol. In addition, we examined the formation of secondary aerosol, including ammonium nitrate. These results provide an improved understanding of wintertime aerosol chemistry in mid-latitude urban environments.

10UA.10

What is the Value of Information from Low Cost Sensor Networks? Balancing Sampling and Instrument Uncertainty. ROSE EILENBERG, R. Subramanian, Aliaksei Hauryliuk, Carl Malings, Albert Presto, Allen Robinson, *Carnegie Mellon University*

It is hypothesized that the increased spatial density enabled by networks of lower-cost sensors (LCS) can be used to better capture the spatiotemporal variability of urban air pollution. However, the measurement uncertainty of LCSs is larger than regulatory-grade instruments.

To test that hypothesis, we modeled their performance under different conditions. First, we characterized the measurement uncertainty for the O_3, $PM_{2.5}$, CO, and NO_2 sensors in the Real-time Affordable Multi-Pollutant monitor when collocated with regulatory-grade instruments. The overall uncertainties were concentration-dependent and ranged from 62%-133%; the slopes of concentration-dependent bias ranged from -0.22 to -0.66. Second, we performed Monte-Carlo simulations using highly spatially resolved data from a national land-use regression model as the ground truth to evaluate different hypothetical low-cost sensor networks. Using networks ranging from 1 to 100 nodes, we estimated population-weighted average concentrations, concentration disparities, and the influence of point sources.

Our analysis highlights that low-cost monitoring networks mainly provide advantages for pollutants with large spatial variability such as NO_2, for which the estimate uncertainty of a single-monitor network with no measurement error can be 70%. However, a large sensor network is unnecessary for a relatively spatially invariant pollutant like ozone, for which the sampling error of an error-free single monitor can be 2.5%. Concentration-dependent biases can cause substantial challenges; for example, when two areas have average concentrations that vary by 20%, on average 4 error-free monitors are needed in each area. With a concentration-dependent bias slope of -1/4, five monitors are required. With a concentration-dependent bias of -1/2, 18 monitors are required on average. We found similar results when identifying the influence of a point source; in most cases, no difference was detectable when the concentration-dependent bias slope exceeded -1/4. When measurement error models are unbiased, the performance of LCSs can be similar to regulatory monitors over long averaging times.

10UA.11

Aerosol Loadings across Africa - Results and Lessons from the AfriqAir Network. Michael R. Giordano, Julien Bahino, Matthias Beekmann, Thomas Bigala, Jimmy Gasore, Theobald Habineza, Aliaksei Hauryliuk, Carl Malings, Stuart Piketh, Albert A. Presto, Daniel Westervelt, Veronique Yoboue, Kofi Amegah, Emmanuel Appoh, Allison Hughes, Michael Gatari, Ezekiel Waiguru, James Nimo, Rebecca Garland, Pieter G. van Zyl, Miroslav Josipovic, R. SUBRAMANIAN, *OSU-EFLUVE, LISA/CNRS, UPEC, ENPC, UP*

AfriqAir is a global consortium that brings together air quality scientists and other researchers interested in using air quality data to tackle air pollution in African cities. A main activity of AfriqAir is to set up and operate hybrid networks of low-cost PM sensors centered around PM reference monitors. AfriqAir and our partners have deployed over 50 low-cost PM sensors as well as multiple reference-grade PM monitors in several cities across Africa, including Nairobi, Kenya, Accra, Ghana, Zamdela, South Africa, Kigali, Rwanda, and many more.This presentation will focus on the results from these sensor networks deployed over the past 2 years. Specifically, the results of a secondary COVID lockdown in Nairobi, Kenya compared to other cities in E., W., and South Africa which did not experience lockdowns in 2021 along with the temporal trends of dry (biomass burning) seasons in a pre- and post-COVID Africa will be presented. Results suggest that subsequent lockdowns after the first in Nairobi have had some effect on aerosol loadings but not as significantly as the first. An updated analysis of the mobility of low-cost sensor models in Africa will also be discussed.

10UA.12

Characterization and Variability of Urban Cooking Emissions Sources.

SUNHYE KIM, Jo Machesky, Drew Gentner, Albert A. Presto, *Carnegie Mellon University*

Primary aerosols, including cooking organic aerosol (COA) constitute a minority of total $PM_{2.5}$ mass on average, however, their fresh emissions dominate intra-city spatial variations in $PM_{2.5}$ concentrations and exposure. This study focuses on characterizing the variability of COA composition using a mobile laboratory to measure fresh cooking emissions from 9 restaurants in two cities. We quantified particle size distributions and number concentrations with a fast mobility particle sizer (FMPS) and condensation particle counter (CPC) and COA mass and composition with an aerosol mass spectrometer (AMS). Particle number concentrations and size distributions emitted from the restaurants studied were highly variable. These concentrations varied maximally by 100-fold over 50 minutes from some restaurants, likely due to on-demand cooking activities as food orders were placed. The mode diameter of particles was ~10.08 nm, suggesting that restaurant cooking is a major source of ultrafine particles in urban areas.

The overall AMS mass spectra of our samples strongly correlated with typical cooking emissions measured in the laboratory and to ambient COA factors derived via factor analysis ($R>0.8$ and $\theta<20°$). However, emissions from a commercial bakery demonstrated exceptional chemical features that were unreported in prior literature with lower correlations ($\theta=45°-83°$, $R=0.03-0.67$). The AMS analysis suggests that bakery samples had distinctive N-containing fragmentation ions (*m/z* 58 $C_3H_8N^+$, *m/z* 86 $C_5H_{12}N^+$, and *m/z* 100 $C_6H_{14}N^+$).

These reduced-nitrogen containing peaks were also detected at other cooking sites which likely include bread as part of their menu. To examine potential sources of the nitrogen features in the laboratory, we measured emissions with and without the dough stabilizer azodicarbonamide ($C_2H_4N_4O_2$) as a possible source of N-containing peaks. However, the reduced nitrogen peaks were not detected, suggesting that another by-product of bread production is the source of these nitrogen-containing species.

11BA.1

No SARS-CoV-2 Detected in Environmental Samples Collected at a Fitness Center That Reopened Following CDC Guidelines.

HONGWAN LI, Sripriya Nannu Shankar, Chiran Witanachchi, John Lednicky, Julia Loeb, Md. Mahbubul Alam, Z. Hugh Fan, Karim Mohamed, Arantzazu Eiguren-Fernandez, Chang-Yu Wu, *University of Florida*

Fitness centers are considered high risk for SARS-CoV-2 transmission due to their high human occupancy and the type of human activity that takes place in them, especially when individuals pre-symptomatic and asymptomatic for COVID-19 exercise in them. In this study, air (N=21) and surface (N=8) samples were collected five times from August to November 2020 at a fitness center. The total attendance throughout samplings was ~2500 of patrons. Air samples were collected using BioSpot-VIVAS, VIVAS, PTFE filters in-line holders, and NIOSH bioaerosol samplers. Moistened flocked nylon swabs were used to collect samples from high-touch surfaces. We did not detect SARS-CoV-2 by rRT-PCR analyses in any air or surface sample. A simplified infection risk model based on the Wells-Riley equation predicts that the probability of infection in this fitness center is 1.77% following its ventilation system upgrades based on CDC guidelines, and that risk was further reduced to 0.89% when patrons used face masks. The combination of high ventilation, minimal air recirculation, air filtration, and UV sterilization of recirculated air reduced the infection risk up to 94% compared to poorly ventilated facilities. Amongst these measures, high ventilation with outdoor air is most critical in reducing the airborne transmission of SARS-CoV-2. For buildings that cannot avoid air recirculation due to energy costs, the use of high filtration and air disinfection devices are mandatory to reduce the probability of acquiring SARS-CoV-2 through inhalation exposure. The infection risk in fitness centers that follow CDC reopening guidance including implementation of engineering and administrative controls, and use of personal protective equipment, can be low, and these facilities can offer a relatively safe venue for patrons to exercise.

11BA.3

Measuring Short Time Course Reduction of SARS-CoV-2 Infectivity in Aerosol.

HENRY OSWIN, Allen E. Haddrell, Mara Otero, Jamie Mann, Tristan Cogan, Andrew Davidson, Jonathan P. Reid, *University of Bristol*

The COVID-19 pandemic has been a major source of mortality and morbidity across the globe, as well as imparting a significant economic burden. Yet a year into this pandemic there remain many questions surrounding the transmission dynamics of SARS-CoV-2. New research tools are needed to provide a more detailed picture of the factors influencing the airborne and droplet borne transmission of disease.

A novel method was developed at the University of Bristol for the airborne study of bacteria (Fernandez, 2019) and has been adapted for the study of viruses in a BSL-3 laboratory. Using electrodynamic levitation, virus containing droplets of controllable size and composition can be suspended within a humidity (RH 5-95%) and temperature (0 C – 50 C) controlled chamber. The droplets can be suspended from 5 seconds to days or even weeks and are then extracted from the chamber allowing the virus within to be quantified by cytopathic effect.

Using this technique, it was determined that the airborne stability of SARS-CoV-2 in culture media droplets was linked to the physical state of the droplet. If the relative humidity was below 50% the droplet effloresced, forming a dry crystalline particle, which caused the infectivity of the virus to almost immediately drop by up to 60%. At high enough RH's to keep the droplet remaining liquid, the virus underwent a more gradual drop in infectivity. For example, at 90% RH SARS-CoV-2 took over 5 minutes to reach a 60% drop in infectious virus. But the rate of viral decay in the liquid droplet does not slow down as much as the dry particle meaning that after 10 minutes the infectivity of the virus was similar at both high and low RH.

These measurements are significantly more refined than previously reported data from rotating drum measurements (Van Doremalen 2020) and cover a much wider range of environmental conditions. The data provides an insight into potential seasonal and geographical impacts on COVID-19 transmission dynamics, as well as information that may aid the development of new infection control procedures.

11BA.6

Size Distribution of Chemical and Biological Particles during the Saharan Dust Episodes over Europe in February 2021.

KALLIOPI VIOLAKI, Andrea Mario Arangio, Athanasios Nenes, *EPFL, Switzerland*

Dust plays a major role in Earth's climate, by absorbing and scattering radiation, and modifying clouds that alter the planetary radiation balance and hydrological cycle. Dust also affects ecosystems through its nutrient content. Aeolian dust is a significant carrier of iron and phosphorus which are limiting nutrients in many regions of the global ocean. This deposition of dust is thought to significantly increase ocean primary productivity, hence its carbon uptake through photosynthesis. Annually, Europe receives millions of tons of dust affecting public health and ecosystems – and with climate change, the frequency and severity of dust episodes are expected to change as well.

During this study, aerosol particles were collected with a size-segregated hi-volume sampler (Tisch 230-High Volume Cascade Impactor). The impactor separated the particles in five different stages; from larger than 7.2µm to less than 0.49µm. Those samples were used to characterize the properties of dust particles during the severe dust episodes in Spring, 2021 in a forest site near Lausanne, Switzerland. We analyzed trace metals and nutrients (Fe, Cu, P, N), inorganic ions, sugars, phospholipids, and biological particle content (fungi, bacteria, and pollen). The deposition flux of nutrients is also quantified and related to their acidity state. We found that one dust episode alone can be responsible for a large fraction of the deposition of soluble metals and P – and that biological P may constitute a significant fraction of the total deposition of the nutrient. These results are related to work we have carried out in the E. Mediterranean (Violaki et al., 2021) and provide an overall synthesis of the importance of dust events for nutrient deposition.

11BA.7

Environmental Surveillance for SARS-CoV-2 from September 2020-February 2021 on a University Campus that Followed CDC Reopening Guidance.

HONGWAN LI, Sripriya Nannu Shankar, Chiran Witanachchi, John Lednicky, Julia Loeb, Md. Mahbubul Alam, Z. Hugh Fan, Michael Lauzardo, Karim Mohamed, Arantzazu Eiguren-Fernandez, Chang-Yu Wu, *University of Florida*

College and university campuses are densely populated areas with communal residential arrangements, shared dining spaces, and a population of adolescents interested in socialization; this means respiratory viruses can be efficiently transmitted on campuses. We conducted one of the first environmental surveillances for SARS-CoV-2 on a university campus in the U.S. that complement epidemiological studies. This study aimed to provide environmental surveillance data for evaluating the transmission risk of spreading SARS-CoV-2 around foot traffic areas on a university campus that followed CDC reopening guidance. Environmental samples were collected at the university which had the second highest COVID-19 cases amongst higher education institutions in the U.S. in Fall 2020. Air samples near foot traffic areas and swabs from high touch surfaces were collected at six campus locations: three residence halls, one dining hall, one student union, and one basketball arena. After 16 sampling events throughout Fall 2020 and Spring 2021 and nearly 8400 visits of students during the measurements, a total of 60 air (N=41) and surface (N=19) samples were collected. We did not detect SARS-CoV-2 in any air or surface samples by rRT-PCR. The sampled university followed CDC guidance for campus reopening, including COVID-19 testing, case investigations, and contact tracing. At the six facilities, control measures were implemented such as reduced capacity, cleaning and disinfection, and one-way traffic management. Students, faculty, and staff were asked to maintain physical distancing, wear face masks, and hand washing, to further reduce the transmission. Although the COVID-19 cases were relatively high at the sampled university, the transmission of SARS-CoV-2 at foot traffic areas in the sampled facilities was minimal due to the adopted CDC reopening measures. Identification of low risk areas allows resources to be focused on higher risk areas on campus for more effective risk minimization.

11BA.8

Direct-Read Fluorescence Based Measurements of Bioaerosols Produced during Activities of Daily Living.

VISHAL D. NATHU, Jurate Virkutyte, M.B. Rao, Marina Nieto-Caballero, Mark T. Hernandez, Tiina Reponen, *University of Cincinnati*

Biological indoor air pollutants or bioaerosols such as bacteria, fungi, and pollen, may adversely affect human health. More specifically, workers employed in home healthcare (HHCWs) occupations are at risk of bioaerosol exposures in their workplaces. Furthermore, there are significant data gaps concerning how everyday activities influence the distribution and accumulation of different types of bioaerosols indoors. Due to HHCWs job responsibilities and activities in patients' homes, elevated bioaerosol exposures are expected while on the job. We collected residential indoor bioaerosol data using a novel direct-reading fluorescence instrument (InstaScope, DetectionTek, Boulder, CO). The experiments consisted of measuring residential bioaerosols at background and performing seven daily living activities, including cooking, dusting, showering, vacuuming, walking, bedsheet changing, and sleeping. Each activity was repeated 4-7 times. Averages of the concentrations from the repeated experiments were taken. Compared to the background of 71,489 particles/m3, pollen concentrations were 973 and 443 percent higher during showering and cooking, respectively. Fungal particles during showering and cooking were 2,301 and 489 percent higher than the background (2,371 particles/m3), respectively. The highest increases in bacterial particles were observed during sleeping and cooking activities. Respective bacterial concentrations were 170 and 195 percent higher compared to background concentrations measured at 135 particles/m3. These results show that showering, cooking, and even sleeping may produce larger amounts of bioaerosols compared to other studied activities. Pollen concentrations were affected by the activities more than fungal and bacterial concentrations. Further analyses are required to understand bioaerosol distribution in residential environments.

11BA.9

Surface Virus Inactivation Using Compact Non-Thermal Plasma Reactors.

ANTHONY TANG, Igor Novosselov, Scott Meschke, Angelo Ong, Ivy Terry, *University of Washington*

Viable SARS-CoV-2 virus and viral RNA has been found on surfaces up to several days, depending on the type of surface and ambient environments, such as temperature and humidity. Thus, COVID19 transmission may occur through touching objects or surfaces with virus from an infected person followed by touching the mouth, nose, or eyes. Surface virus inactivation by exposure to non-thermal plasma (NTP) is investigated utilizing an axisymmetric electrohydrodynamic (EHD) reactor and the MS2 bacteriophage virus. The NPT is generated by a compact 0.75 in. diameter concentric dielectric barrier discharge (DBD) reactor that produces high concentrations of reactive species, which are expelled from the reactor by an air jet. In our experiment the jet impinges on a coupon inoculated with MS2. The effect of exposure time and reactor residence time are studied by varying NTP reactor flow rate. The virus inactivation is measured using a double agar layer plaque assay. At a jet velocity of ~ 5 m/s and exposure time of one minute, the NPT surface treatment offers greater than 2log10 of viral inactivation. The non-chemical and non-contact surface treatment ultimately offers an attractive alternative to traditional surface treatments.

11BA.10

Study of Airborne Microbial Diversity in a University Campus Using a Portable Electrostatic Bioaerosol Sampler. KAVINDRA KUMARAGAMA, Shane Rogers, Shantanu Sur, Suresh Dhaniyala, *Clarkson University*

Environmental bioaerosol monitoring using portable devices has recently gained interest to assess the risk for airborne transmission of diseases such as COVID-19. To address such a need, a portable, low-power, and low-cost device was recently developed in collaboration with TelosAir, a local startup. Our device, called Trace Aerosol sensor and Collector for Bio-particles (TracB), is capable of real-time air quality monitoring and capturing airborne particles for offline analysis. The device utilizes the principle of electrostatic precipitation to efficiently capture bioaerosol on a collection plate. The collection efficiency of the device is tested using bacteria, fungi, and virus model organisms. Here we present a detailed characterization of the biosampler component of the device, including the impact of an ionizer, precipitation voltage, and collection plate substrate on collection efficiency and viability of captured microorganisms. We have deployed multiple TracB units for one year in various indoor and outdoor locations of Clarkson University campus. Culture-based and sequencing-based analysis of the collected samples were conducted to determine the diversity, abundance, and seasonal variation of airborne microbial populations in these locations. Our preliminary results show that Actinobacteria and Proteobacteria are the most abundant bacterial phyla, and Ascomycota and Basidiomycota are the most abundant fungal phyla among all four seasons. Furthermore, our data suggests the high microbial abundance in spring and summer for indoor and outdoor sampling locations, respectively.

Keywords: Bioaerosol, low-cost sensor, electrostatic precipitator

11BA.11

Effect of Sampling Duration on Bioaerosol Culturability When Using Passive Sampling Devices. SYDONIA MANIBUSAN, Gediminas Mainelis, *Rutgers, The State University of New Jersey*

Bioaerosols are aerosolized biological particles with the potential to cause negative health effects such as disease transmission or exacerbation of respiratory diseases. 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 extended sampling times. Culture-based techniques remain widely used to determine bioaerosol presence, including in countries with a regulatory framework for bioaerosols. However, few studies have documented the impact of sampling duration on bioaerosol culturability over extended periods. The Rutgers Electrostatic Passive Sampler (REPS) is a passive bioaerosol area sampler that has demonstrated the ability to capture bioaerosol particles over long time frames. However, the impact of sampling duration on REPS culturable samples has not been determined. Therefore, the objective of this study was to identify the optimal duration for the REPS sampler based on sample culturability over extended sampling campaigns (24 hours to 21 days).

REPS samples were collected at different time periods over 21 days. Sample collection was repeated twice in both an outdoor and indoor location. The SAS Super 180, an active culture-based sampler, was used to collect collocated grab samples twice daily over two to three-minute durations to determine average daily bioaerosol concentrations. All REPS samples were plated on tryptic soy agar (TSA) and malt extract agar (MEA) plates for bacteria and fungi, respectively. REPS samples were also analyzed for ATP activity and total bacteria. In addition to colony counts, REPS performance to determine culturable bioaerosols was also evaluated based on its equivalent sampling flow rates normalized to the SAS sampler. Initial results showed REPS’ equivalent sampling rates of 0.981 ± 0.801 L/min (5 days) to 2.83 ± 1.43 L/min (3 days) for culturable bacteria outdoors. The 21-day samples had similar rates of 1.18 ± 0.606 L/min. We conclude that passive samplers such as REPS offer affordable and unobtrusive sampling over time periods ranging from days to weeks.

11CC.1

Water Uptake of Atmospheric Organosulfates at Sub and Supersaturated Conditions. Chao Peng, Patricia Razafindrambinina, KOTIBA A. MALEK, Lanxiadi Chen, Weigang Wang, Rujin Huang, Yuqing Zhang, Xiang Ding, Maofa Ge, Xinming Wang, Akua Asa-Awuku, Mingjin Tang, *University of Maryland*

Organosulfates (OS) are ubiquitous in the atmosphere, but their role in atmospheric chemistry and physics is poorly understood. Hence, exploring the water uptake extent of OSs can improve our understanding of their, dry and wet deposition, and impact on cloud formation. In this study, the subsaturated and supersaturated droplet growth of four atmospherically relevant OSs: sodium methyl sulfate (methyl-OS), sodium ethyl sulfate (ethyl-OS), and sodium octyl sulfate (octyl-OS) were investigated. The droplet activation is measured with a cloud condensation nuclei counter (CCNC) at supersaturated conditions (SS; 0.4, 0.6, 0.8, and 1.0%). The hygroscopic growth, under subsaturated conditions, of these aerosolized chemicals were studied using a vapor sorption analyzer and a humidity tandem differential mobility analyzer (H-TDMA). Results show that supersaturated hygroscopicity derived from κ -Köhler theory analysis can be larger than sub-saturated hygroscopicity. κ-values range from 0.2 to 0.5 and vary with supersaturation. The organosulfate solubility limit and droplet surface tension depression play an important role in determining droplet activation at supersaturated regimes.

11CC.2

Viscosity of Secondary Organic Aerosol: Effects of Composition and Oxidation Method. GIUSEPPE CRESCENZO, Vahe Baboomian, Natalie R. Smith, Sergey Nizkorodov, Allan Bertram, *University of British Columbia*

Forests emit large quantities of volatile organic compounds (VOC) into the troposphere. Upon oxidation, lower volatility products condense and form secondary organic aerosol (SOA). SOA constitutes a large mass fraction of submicron atmospheric aerosols. SOA is important for air quality and influences climate. Information on the viscosity of SOA is needed to predict their role in air quality and climate. For example, the viscosity of SOA can impact the growth and evaporation rate of SOA, their ability to act as ice nucleating particles, and their ability to transport pollutants over long distances. Nevertheless, the viscosity of SOA remains uncertain. Here we report viscosities as a function of relative humidity for SOA derived from terpene and sesquiterpene photooxidation and dark ozonolysis. From the measured viscosities and the Stokes-Einstein equation, we determined diffusion coefficients and mixing times of organic molecules within the SOA. We show that particle viscosity and mixing times within the SOA depends strongly on the oxidation method and the type of VOC used to generate the SOA. Photooxidation lead to higher viscosities compared to dark ozonolysis, and a complex mixture of VOCs resulted in a higher SOA viscosity compared to SOA generated from α-pinene alone.

11CC.3

Is Black Carbon the 2nd Largest Contributor to Climate Change? GEORGIOS A. KELESIDIS, David Neubauer, Liang-Shih Fan, Ulrike Lohmann, Sotiris Pratsinis, *ETH Zurich, Switzerland*

The climate models of the Intergovernmental Panel on Climate Change list CO_2, CH_4 and black carbon (BC) as the most potent contributors to global warming based on their radiative forcing, *RF* [1]. Among them, the BC contribution comes with the highest uncertainty. Examining closely these models, it becomes apparent that they might underpredict significantly the direct *RF* for BC, largely due to their assumed spherical BC morphology [1].

Here, the Rayleigh-Debye-Gans (RDG) theory is interfaced with discrete dipole approximation simulations to estimate the light absorption [2] and scattering [3] of BC accounting for its composition, morphology and coating by weakly or non-absorbing compounds. The RDG-derived mass absorption cross-section of bare and coated BC is coupled with ECHAM-HAM simulations [4] to estimate the regional and global direct *RF* from BC. Accounting for the fractal-like morphology of BC increases its direct *RF*, explaining satellite observations of the aerosol absorption optical depth [5] and revealing that BC is the 2nd largest contributor to global warming. So, reducing BC emissions can have an immediate impact on global warming and delay climate effects induced by CO_2.

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11CC.4

Annual Variability of Particle Size, Cloud Condensation Nuclei and Particle Hygroscopicity in the Central Arctic. XIANDA GONG, Jiaoshi Zhang, Heike Wex, Chongai Kuang, Janek Uin, Matthew Shupe, Jian Wang, *Washington University in St. Louis*

Temperatures in the Arctic are rising at more than twice the global average rate. The climate-relevant properties of Arctic aerosols and the processes that drive these properties remain poorly understood, especially in the central Arctic where observations are scarce. Here we present the seasonal variations of central Arctic aerosol properties, including particle number size distribution (PNSD), CCN number concentration (NCCN), and particle hygroscopicity based on the measurements onboard the R/V Polarstern during the recent Multidisciplinary Drifting Observatory for the Study of Arctic Climate (MOSAiC) campaign, which took place from October 2019 to September 2020.

The seasonal variation of PNSD in the central Arctic is similar to those observed at other Arctic sites, including Mt. Zeppelin and Svalbard. The PNSD exhibited a high accumulation mode number concentration during springtime due to Arctic haze and high Aitken mode number concentration during summertime as a result of more frequent new particle formation events. NCCN during the springtime was often the highest (~110 cm-3 at a supersaturation of 0.30%), whereas, during summertime, NCCN is usually low (~ 20 cm-3) except when newly formed particles grow and reach a sufficiently large size to act as CCN. Particle hygroscopicity (expressed as a single parameter, κ) was low (~0.2 to 0.3) during summertime due to strong contributions of organics to particle composition. During springtime, κ ranged from ~0.5 to 0.8, consistent with mixtures of long-range transported continental aerosols and sea-salt particles. During the polar night, high NCCN (~200 cm-3) and elevated κ (~1.0) were observed under strong winds, suggesting a substantial contribution from blowing snow or highly hygroscopic particles transported from lower latitudes during storms. The processes that drive the seasonal variations of the aerosol properties in the central Arctic will be discussed.

11CC.6

Mixing State and Properties of Aged Aerosols in the North Atlantic Free Troposphere. MEGAN MORGENSTERN, Rhenton Brimberry, Nurun Nahar Lata, Swarup China, Lynn Mazzoleni, Paulo Fiahlo, Diamantino Henriques, Andrea Baccarini, Silvia Henning, Birgit Wehner, Bo Zhang, Simeon Schum, Claudio Mazzoleni, *Michigan Technological University*

Aerosols influence several physical and chemical processes in our atmosphere, with interactions depending on their properties. As aerosols travel, they age, and these properties transform. While important, characterization of ‘well-aged’ particles in remote regions is scarce, often due to logistical challenges. To fill this gap, we collected and analyzed well-aged particles from Pico Mountain Observatory in the Azores in the North Atlantic.

Analysis included computer controlled scanning electron microscopy with energy dispersive X-ray spectroscopy, and scanning transmission X-ray microscopy with near-edge X-ray absorption fine structure spectroscopy on samples from June and July of 2015 and 2017. The micro-spectroscopic analyses were used to determine the mixing state parameter (χ) of each sample. The mixing state parameter is a numerical representation of how similar (internally mixed) or different (externally mixed) the particles’ elemental composition in the sample is. The elemental composition was also used to determine the particles’ hygroscopicity. Data from a collocated nephelometer and aethalometer were used to determine the scattering and absorption Angström exponents and the single scattering albedo. The Angström exponents provide information about the aerosol size and chemical composition, while the single scattering albedo determines their radiative forcing. For 2017, we also measured cloud condensation nuclei concentrations (CCNc). The aerosol transport and potential sources were investigated using the FLEXible PARTicle dispersion model (FLEXPART).

Aerosol composition varied, with groupings such as carbonaceous, sea salt, and dust. The FLEXPART analysis also suggested different potential sources and source regions, such as dust from North Africa, and biomass burning aerosols from North America. We will present the analyses of - and links between - the aerosol mixing state, composition, optical properties, hygroscopicity, and CCNc. These analyses can help understand how aerosol aging affects their interactions with radiation and clouds.

11CC.7

Compositional Analysis of Cloud Droplet Residuals by High Resolution Time-of-Flight Aerosol Mass Spectrometry: A CAMP2Ex Case Study. CLAIRE ROBINSON, Rachel O'Brien, Matthew Brown, Ewan Crosbie, Francesca Gallo, Carolyn Jordan, Richard Moore, Kevin Sanchez, Taylor Shingler, Michael Shook, Kenneth Thornhill, Elizabeth Wiggins, Edward Winstead, Bruce Anderson, Luke Ziemba, *NASA, SSAI*

The complexity of cloud-aerosol interactions remains a significant research front in atmospheric chemistry. Variations in the chemical composition of cloud condensation nuclei play a role in cloud formation and reactions that occur in the cloud droplets. Determining the chemical composition and carbon oxidation state of sub-cloud aerosols and their corresponding cloud droplet residuals helps us further understand the overall formation of clouds and the effect on the radiative budget. The Cloud, Aerosol and Monsoon Processes-Philippines Experiment (CAMP^{2}Ex) is a collaborative field campaign between NASA and the Philippines research community that flew during the 2019 southwest monsoon season. One of its focuses was to characterize aerosol and cloud microphysics in the region utilizing a complex suite of instrumentation on the NASA P-3B aircraft.

Here, we present a case study examining on-line High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS) data from CAMP^{2}Ex. This specific flight was conducted on 16 September 2019 over the Sulu Sea targeting biomass burning aerosol originating from the Borneo region. The HR-ToF-AMS sampled from a forward-facing isokinetic inlet for the majority of the flight, but was switched to sample from a Counter-Flow Virtual Impactor inlet when passing through clouds to characterize cloud droplet residual composition. Clouds sampled during the flight were a mixture of shallow marine cumulus (i.e., with cloud tops reaching approximately 1 km) and a more-developed convective cell reaching 4-5 km altitude. Organic aerosol elemental ratios and mass spectra for this flight give insight into the chemical composition of the sampled aerosol and cloud droplet residuals. This unique set-up allows us to observe the effects of cloud processing on the chemical composition of the sampled biomass burning aerosol and determine relevant scales of altitude or spatial variability during the flight.

11CC.8

An Overview of Aerosol Measurements and Process Studies During the TRacking Aerosol Convection interactions ExpeRiment (TRACER) and Partner Field Campaigns.

MICHEL JENSEN, James Flynn, Laura Judd, Pavlos Kollias, Chongai Kuang, Greg McFarquhar, Raj Nadkarni, Heath Powers, John Sullivan, Allison Aiken, Brian Argrow, Sarah Brooks, Christopher Cappa, Rajan K. Chakrabarty, Philip Chilson, Don Collins, Gijs de Boer, Darielle Dexheimer, Manvendra Dubey, Jiwen Fan, Robert Griffin, Petra Klein, Alex Kotsakis, Markus Petters, et al., *Brookhaven National Laboratory*

Beginning in August 2021 for 14 months, a multi-agency succession of field campaigns will take place in the coastal, urban regime of Houston, TX to study the interactions among clouds, aerosols, pollutants and the environment. A major component of these campaigns is the measurement of aerosol properties to better understand their lifecycle and influences on clouds and air quality.

The DOE TRacking Aerosol Convection interactions ExpeRiment (TRACER; October 2021 - September 2022) includes the deployment of the ARM Mobile Facility (AMF1) near the polluted Houston ship channel. The AMF1 includes the Aerosol Observing System providing continuous, surface-based measurements of aerosol and trace gases. During summer 2022, additional aerosol measurements will be made in a cleaner region southwest of Houston, and mobile and tethered balloon system platforms will capture aerosol regional variability.

TRACER-Air Quality (NASA and TCEQ; September 2021), brings a network of ground-based remote-sensing observations of ozone and other pollutants, balloon-borne measurements and remote-sensing aircraft measurements. The measurements will be used to address questions related to pollution, influences of photochemistry and local meteorology, the evaluation of air quality models and satellite products, and the intersection of air quality and socioeconomic factors.

The NSF Experiment of Sea Breeze Convection, Aerosols, Precipitation and Environment (ESCAPE) campaign will take place from mid-June through mid-July 2022 and brings an array of aircraft, and surface-based fixed and mobile measurements. Specific to aerosol studies, the ESCAPE aircraft will measure aerosol and ice nucleating particle concentrations.

These campaigns bring together a diverse cross-section of scientists, employing an array of surface-, aircraft- and satellite-based measurements, combined with state-of-the-art Earth system modeling to answer fundamental questions important for our understanding of weather, climate and air quality that would not be possible without these cooperative efforts.

11CC.9

Black Carbon Aerosol-Cloud Effects over the Eastern North Pacific Ocean.

Nilima Sarwar, Dongli Wang, Walt Williams, 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 the marine environment is affected both directly and indirectly by BC aerosol.

In this talk, the influence of BC aerosol on the formation and properties of the marine boundary layer are assessed. The mass concentration, size distribution, and mixing state of BC aerosol particles are used to evaluate the different sources of BC aerosol and their influences on the marine stratocumulus layer. During the sampling campaign, we observed both clean and BC-perturbed clouds off the California coast. Major findings from this study include - observing an increase in average BC mass and number concentrations from the marine boundary layer to an above-cloud BC layer, pollution of clouds by entrainment of BC aerosols, and evidence of wet scavenging of BC by cloud droplets. Overall, the marine environment in this region is characterized by a complex mixture of marine engine exhaust, transported wildfire plumes, and long-range transported aerosol.

11CC.10

On the Effects of Wet vs. Dry and Seeded vs. Unseeded Conditions on SOA Hygroscopicity. Patricia Razafindrambinina, Kotiba A. Malek, Joseph Dawson, Miriam Freedman, Akua Asa-Awuku, Tim Raymond, DABRINA DUTCHER, *Bucknell University*

Volatile organic matter that are suspended in the atmosphere such as α-Pinene and trans-caryophyllene undergo the aging process, chemical, and photooxidation reactions to create secondary organic aerosols (SOA) that are thought to be viscous and inhibit water uptake. Currently, the influence of the indirect effect of SOA on the radiative budget is yet to be fully understood, and little is known of the impact of water vapor and ammonium sulfate (ubiquitous species in the atmosphere) presence on the hygroscopicity and CCN activity of SOA. In this research, three water-uptake measurement methods: cavity ring-down spectroscopy (CRDS), hygroscopic tandem differential mobility analysis (H-TDMA), and cloud condensation nuclei counting (CCNC) are employed to study the hygroscopicity of α-Pinene and trans-caryophyllene SOA formed under dark ozonolysis, and observe the changes in water uptake of SOA in the presence of water vapor at 76 % RH and ammonium sulfate seeds. Hygroscopicity was parameterized by the single hygroscopicity parameter (κ) and showed that water vapor and ammonium sulfate modify the water uptake behavior of α-Pinene SOA, but not trans-caryophyllene. It is proposed that a difference in the viscosity and hydrophobicity of the SOA may be the primary factor that leads to changes in hygroscopicity.

11CC.11

Water Uptake of Alginic Acid Sodium Salt as a Proxy for Marine Hydrogels and Its Mixtures with Different Inorganic Salts. BEHNAZ ASADZADEH, Hichem Bouzidi, Jakub Ondráček, Jaroslav Schwarz, Vladimír Ždímal, *ICPF of CAS, Prague, Czech Republic*

Sea spray aerosol (SSA) represents the largest source of natural primary aerosol with climate relevance in cloud formation. Marine hydrogel has been postulated to represent large fraction of sea spray aerosols due to their unique physicochemical and hydrological properties. Alginate is the most abundant marine biopolymer and, next to cellulose, the most abundant biopolymer in the world. Alginates (ALG) are a group of naturally occurring anionic polysaccharides derived from brown algae cell walls, and several bacteria strains. In this study we used alginic acid sodium salt (HAG) as a proxy for marine hydrogels. Hygroscopic measurements were performed for pure (HAG) aerosol particles and their mixtures with sodium chloride NaCl, ammonium sulfate $(NH_4)_2SO_4$, and sodium sulfate Na_2SO_4 at different dry mass ratios with a hygroscopicity tandem differential mobility analyzer (H-TDMA). The Zdanovskii–Stokes–Robinson (ZSR) mixing rule is used to estimate the hygroscopic growth of internally mixtures. Pure (HAG) aerosol particles and their mixtures with $(NH_4)_2SO_4$ and Na_2SO_4 show the obvious diameter reduction at medium RH. For all mixtures, the ZSR-calculated *GF*s are in relatively good agreement with the measured hygroscopic growth at high RH. Furthermore, the aerosol hygroscopicity parameter κ_{HTDMA} is derived from hygroscopic growth factor measurements at water activity (a_w) = 0.9. The obtained κ_{HTDMA} of different mixtures indicates that the mixed HAG/NaCl particles have high κ_{HTDMA} at high NaCl mass fractions and can be considered as highly CCN-active compounds.

11CC.12

Secondary Organic Aerosol and Brown Carbon Formation from Furanoid Oxidation via OH Radicals: Important Precursors from Biomass Burning. TAEKYU JOO, Linghan Zeng, Yuchen Wang, Tori Hass-Mitchell, Rodney J. Weber, Drew Gentner, Benjamin Brown-Steiner, Matthew Alvarado, Nga Lee Ng, *Georgia Institute of Technology*

Biomass burning is an important source of both primary and secondary organic aerosol (SOA), and recent studies demonstrate the importance of nontraditional organic vapors, such as furanoids, as precursors of SOA formation. Furfural and 2- and 3-methylfuran are the major furanoid species emitted from biomass burning. Here, we investigate SOA and secondary brown carbon (BrC) formation from photooxidation of these compounds in the Georgia Tech Environmental Chamber. Experiments were performed under dry (RH<5%) and humid (RH 50-60%) conditions with ammonium sulfate seeds in the presence of NO_x. Light absorption spectra of soluble SOA extracted from filter samples were measured with a Liquid Waveguide Capillary Cell (LWCC) and higher absorption was observed for furfural SOA compared to 2- and 3-methylfuran SOA. SOA bulk composition and functional group distributions were measured using a high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) and an offline electrospray ionization and high-resolution quadrupole time-of-flight tandem mass spectrometry (LC-ESI-Q-TOF), respectively. The results showed that the fraction of nitrogen-containing aerosol to total organics was 4 times higher in furfural SOA compared to methylfuran SOA. For furfural oxidation under humid conditions, the time evolution and thermogram of particle-phase nitrogen-containing compounds measured using a Filter Inlet for Gases and AEROsols coupled with time-of-flight chemical ionization mass spectrometer (FIGAERO-HR-ToF-CIMS) confirmed the occurrence of rapid uptake of first-generation products followed by oligomerization in the particle phase. Unlike 2- and 3-methylfuran, furfural contains a carbonyl that leads to the production of multi-functionality compounds. This facilitates hydration and higher yields of carbonyl-containing products via fragmentation during photochemical aging, which can then undergo heterogeneous browning reactions with ammonium salts. Consequently, enhanced brown carbon species formation can be expected. Results from this study contribute to our understanding of SOA and BrC formation of furan-containing compounds in biomass burning plumes as well as its impact on the climate.

11SA.2

Characterization of Vehicular Emissions of Ammonia and Other Nitrogen-Containing Volatile Organic Compounds under Real-World Driving Conditions. JUN ZHENG, Dongsen Yang, Yan Ma, *Nanjing University of Information Science and Technology*

Ammonia (NH3) and amines are believed to play a pivotal role during nucleation processes in the atmosphere. Globally, agriculture-related activities may dominate NH3 and amines emissions. However, the most populated urban centers that are often suffered from severe haze events, are less likely impacted by agriculture emissions. In this work, we found that vehicular emissions may be the dominant source of NH3 and other nitrogen-containing volatile organic compounds (NVOCs, including amines and amides) in metropolitan areas. A set of curbside experiments were conducted to characterize NH3 and NVOCs emissions from motor vehicles (including gasoline-, diesel- and natural gas-powered automobiles) under real-world driving conditions. The emission character of each subject vehicle with respect to NH3 and NVOCs emitted per kilogram fuel consumed was inferred from synchronized CO2 measurements. Although NH3 emitted from any individual subject vehicle predominated that of NVOCs by orders of magnitude, vehicular emissions of amines still can be overwhelming comparing to their typical ambient background levels and can significantly impact nucleation processes based on recent field observations. The typical emission profiles (mass spectra) of each type of vehicle were also determined from this study, which could be a set of valuable information for the purpose of NH3 and NVOCs source apportionments and hence to formulate effective air pollution abatement strategies.

11SA.4

Organic Aerosol Components across Europe Using 22 ACSM/AMS Year-long Datasets and a Harmonized Source Apportionment Protocol. GANG CHEN, MariCruz Minguillon, André S. H. Prévôt, Team COLOSSAL, *Paul Scherrer Institute*

Atmospheric aerosol can indirectly and directly affect climate, reduce visibility, and cause adverse public health issues. Organic aerosol (OA) is a significant air pollutant, representing 20-90% of the total submicron aerosol mass. However, the spatial and temporal variabilities of OA sources remain poorly characterized in Europe. In this study, we collected year-long data using 21 Aerosol Chemical Speciation Monitors (ACSM) and one Aerosol Mass Spectrometer (AMS) (Aerodyne Research Inc., MA, USA) between 2014 and 2019 in Europe. We performed OA source apportionment (SA) applying Positive Matrix Factorization (PMF) analysis using novel techniques within SoFi Pro (Datalystica Ltd., Villigen, Switzerland), including rolling mechanism, a-value approach, bootstrap re-sampling, criteria-based selection, and uncertainty assessments.

Overall, we found that oxygenated OA (OOA) factors dominated at all sites, and their contribution was more significant at non-urban sites than urban environments. On the contrary, hydrocarbon-like OA (surrogate of road traffic emission, HOA) showed higher contributions in urban locations, although identified at most non-urban sites. Biomass burning OA (BBOA) was present at most stations with the larger temporal variation throughout the year. Cooking-like OA (COA) only exited in cities (mostly in southern Europe). The median of normalized diurnals of HOA showed clear patterns with morning and evening rush-hour peaks in urban sites, while it did not show prominent morning peak in non-urban environments. However, both urban and non-urban sites showed similar patterns for BBOA, coal combustion OA (CCOA), and OOA factors.

These high-time resolution SA results from 22 ACSM/AMS long-term European datasets offer a more comprehensive picture of OA sources' spatial and temporal variabilities. Air quality and climate modellers and policymakers can benefit from our results, as they provide essential knowledge to understand and eventually mitigate OA from different sources.

11SA.6

A Coupled Volatility and Molecular Composition Based Source Apportionment of Atmospheric Organic Aerosol. PHILIP RUND, Ben H. Lee, Claudia Mohr, Daniel Jaffe, Noah Bernays, Qi Zhang, Ryan Farley, Tuukka Petäjä, Joel A. Thornton, *University of Washington*

Improvements in organic aerosol (OA) source apportionment are needed to improve our understanding of the processes and precursors that control its atmospheric abundance. We apply Non-Negative Matrix Factorisation (NNMF) to molecular-level particle composition and volatility measurements obtained using a Time-of-Flight Chemical Ionization Mass Spectrometer (ToF-CIMS) coupled to a custom Filter Inlet for Gases and AEROsols (FIGAERO) at a mixed temperature forest site during summer, a boreal forest site during spring, and a remote mountain top observatory during late summer. We conduct NNMF of resolved thermogram timeseries containing >350 molecular components, utilizing volatility and abundance information. We also conduct NNMF using only the molecular-level abundance information. Typically, 5 to 10 factors explain a significant fraction of the spectral variance at each site. Factors derived from the resolved thermograms show distinct volatility, molecular composition, and temporal variations that illustrate different biogenic and anthropogenic OA precursors and aging timescales. The median mass contributions of NNMF factors produced for the temperate forest site, without a priori information imposed, align well with categories determined by an independent study of the same data using a spectral basis set produced from multiple laboratory chamber experiments. A weakness of the NNMF approach is the lower dynamic range of separation, as particulate organic nitrates, which were observed to have distinct patterns of variability but low overall abundance at some sites, were not separable. The routine is shown to be more robust using resolved thermograms as input rather than concentration timeseries, likely due to the additional component variability in volatility space. The added layer of volatility information and molecular-level identification of OA composition provided by the FIGAERO-CIMS shows potential with the NNMF algorithm to reproduce atmospherically relevant sources from observations as well as providing a framework to further identify chemical processes that lead to volatility lowering.

11SA.7

Source Apportionment and Real-Time Measurement of pm10 Trace Metals Released from Car Brakes, Tire Wear and Construction Dust.

ZAINAB BIBI, James Allan, Hugh Coe, Nicholas Marsden, Michael Flynn, *University of Manchester, UK*

With a population of about 66.04 million (2017) and an area of 242,495 km², United Kingdom (UK) is one of the most densely populated regions worldwide. There are 28 million cars currently on UK roads, which are accounting for 79% of the road traffic. Traffic-related particles can be distinguished into exhaust emissions (EE), which are emitted because of incomplete fuel combustion and lubricant volatilisation during the combustion procedure, and non-exhaust emissions (NEE), which is either generated from non-exhaust sources such as brake, tire, clutch and road surface wear or already exist in the environment as-deposited material and become resuspended due to traffic-induced turbulence (Amato et al., 2011). In the current study, we are introducing the most recent instrument for the detection of NEE, i.e., Cooper Xact 625i ambient metal analyser (Cooper Environmental Services, Beaverton, Oregon, USA). PM10 samples were collected from 1st July 2019 to 17th Sept 2020 at the new Air Quality Site in Manchester, UK. The site is well documented with respect to the good urban background site that should offer a contrast to the more central Piccadilly site and the Whitworth observatory in the main campus of the University. Later, PMF analysis was performed to do the source apportionment of metals (Paatero and Tapper, 1994). The results showed that the first factor is brake lining and mineral dust, dominating by Fe and Cu metals. The second marker has the highest m/z of K, Zn, S and Pb. Zn is the marker for tire wear while Pb is a marker for road paint and S & K was used as the marker of biomass burning. The third factor is sea salt/sea spray particles mainly dominated by Cl. The fourth factor is secondary sulfates dominated by S and the fifth factor is construction dust representing the signals at m/z 26.9 (Al), 28 (Si), 40 (Ca) and 55.8 (Fe). The significant loads of the traffic-related and road dust factors with strong diurnal variations highlight the continuing importance of vehicle-related air pollutants at this site. The results emphasize the large influence of non-exhaust emissions sources on the composition of PM10. Other factors such as road dust and domestic burning contribute to the influence of local activities such as construction site near the AQ site and domestic burning from waste burning. This study will provide a piece of important additional information about sources of NEE in the urban background site along with construction dust and domestic burning sources and will be helpful for policymaking in the future.

11SA.9

Spatiotemporal Analysis of PM2.5 in Chicago Using Data from EPA and Low-Cost Sensor Network.

VIJAY KUMAR, Dinushani Senarathna, Suresh Dhaniyala, Shantanu Sur, Supraja Gurajala, Sumona Mondal, *Department of Mathematics, Clarkson University, Potsdam-NY*

PM2.5 has been linked to numerous pollution-mediated adverse health effects and their monitoring is key for taking preventative and mitigative measures. Accurate measurements of PM2.5 concentrations are available from EPA sites, but such data lacks spatial resolution due to a limited number of monitoring locations. In recent years the deployment of low-cost sensor networks has opened up the possibility of acquiring air quality data at a high spatiotemporal resolution. In this study, we aimed to build a model to estimate the PM2.5 concentrations at high resolution in the Chicago area, using PM2.5 measurements from EPA and low-cost PurpleAir (PA) sensors network. Time series clustering analysis was first performed to identify spatial patterns in daily and weekly PM2.5 data collected from 4 EPA and 10 PA sampling sites between January to December 2020. The predictor variables in our model included: land-used variables such as road length, annual average traffic, land type, and chemicals releasing industries around the sampling locations, and also included meteorological variables such as temperature, humidity, wind speed, and wind direction. Multivariate linear regression models for daily and weekly PM2.5 concentrations were developed after checking multicollinearity among the predictor variables. By selective incorporation of variables, a reasonable prediction of PM2.5 was obtained with coefficient of determination (R2) of 0.6-0.8. Our findings show promise of using low-cost sensor network data to complement EPA data to build models with higher spatiotemporal accuracy.

11SA.11

Impacts of Residential Wood Burning Curtailment Program on Wintertime PM Pollution in the San Joaquin Valley of California. JUSTIN TROUSDELL, Caroline Parworth, Ryan Farley, Deepchandra Srivastava, Qi Zhang, *University of California, Davis*

Over the past three decades extensive efforts have been made to decrease particulate matter (PM) related to residential wood burning (RWB) in the San Joaquin Valley (SJV) of California. This effort goes hand in hand with decreasing violations of the National Ambient Air Quality Standards (NAAQS) for PM and reducing the health risks of wood smoke. The control district and the counties place restrictions on RWB based on forecasted meteorology and PM emissions under rule 4901. Here we investigate the compliance rate of curtailment restrictions and the effects of rule 4901 on PM2.5 pollution in SJV. A key tracer species for biomass burning in this region is biomass burning organic aerosol (BBOA) resolved via source apportionment of organic aerosol spectra acquired with aerosol mass spectrometers. To see if RWB species mass concentrations were reduced in accordance with curtailment restrictions, hourly percent changes in BBOA concentrations were calculated by comparing average diurnal concentrations of RWB species during curtailment to those during burning-allowed periods for the 2018-2019 and 2012-2013 winter seasons. The comparison was then performed after normalizing the diurnal concentrations with background corrected CO or NOx, which are expected to have relatively low contributions from RWB, to correct for well-known systematic meteorological differences. The percent differences between 6 pm to midnight, when RWB emissions primarily occur, are small for the 2018-2019 winter. This suggests that compliance with restrictions was low for this winter. However, significant reduction of RWB emissions was observed in the 2012-2013 winter season when BBOA concentration was 2 times higher than the 2018-2019 season. Although compliance is low decreasing trends in PM2.5 and BBOA suggest that the total number of people burning is less than in previous years.

11SA.12

One-year ACSM Source Apportionment Analysis at the Central European Research Station Melpitz. SAMIRA ATABAKHSH, Laurent Poulain, Gang Chen, André S. H. Prévôt, Alfred Wiedensohler, Hartmut Herrmann, *Leibniz Institute for Tropospheric Research*

Atmospheric aerosol negatively affects human health and also has important climate impacts. Since organic aerosol (OA) represents the largest fraction of the aerosol and comprise huge variety of compounds, the molecular identification of OA constituents, their impact on physico-chemical properties as well as the corresponding source identifications remain challenging. Although source apportionment as a common approach for the OA source identification was is much applied in field campaigns using Aerosol Mass Spectrometer (AMS), a strong need for source apportionment analysis covering longer time series data, as well as several seasons or years exists.

In this study, a one-year time series data set (Sep 2016-Aug 2017) of an Aerosol Chemical Speciation Monitor (ACSM) operated at the TROPOS research station Melpitz (51.54° N, 12.93° E, 86 m a.s.l., Germany) was analysed using the SoFi Pro software (Datalystica Ltd., Villigen, Switzerland). The recently developed ‘rolling windows mechanism’ was applied to properly capture the temporal variability of the source finger-print (here their mass spectra). The results show that OA dominates the total mass concentration with a clear seasonal variability (39% in winter to 59% in summer). Five factors were identified as having a distinct temporal variability and mass spectral signature. Three of them were associated with primary organic sources: hydrocarbon-like OA (HOA), biomass burning OA (BBOA) and coal combustion OA (CCOA), and two oxygenated OA (more-oxidized OOA (MO-OOA) and less-oxidized OOA (LO-OOA)).

The present work aims to investigate the seasonal variability of the identified organic factors, the time series, and the diurnal cycle of mass concentrations for each factor over all time periods. Moreover, factors influencing the mass concentration of the different OA sources will also be discussed.

11SW.1

Intercomparison of Spectroscopic Measurements of Biomass Burning Aerosol Optical Properties during a Wildfire in Southern California. ESTHER MORALES, Danielle Rocco, Jaebin Ju, Jorge Gonzales, Anissa Barrera, Stephanie Salas, Daniel B. Curtis, *California State University, Fullerton*

The optical properties of atmospheric aerosols remain one of the largest uncertainties in our understanding of Earth's radiative balance. Wildfire events are expected to increase in size and frequency in certain areas, such as the Western United States, due to climate change and other anthropogenic activities. Therefore, it is crucial to better understand the optical properties of biomass burning aerosol.

In this study a suite of instruments was deployed indoors and outdoors at California State University, Fullerton to measure ambient aerosol particles during a nearby wildfire event in Southern California during October 26, 2020 through November 2, 2020. The instruments used were an Integrating Nephelometer (Ambilabs 2-WIN) to measure scattering coefficient at wavelengths of 450 nm and 525 nm, a Cavity Attenuated Phase Shift Spectrometer (CAPS, PMex Aerodyne, Inc.) to measure extinction coefficient at a wavelength of 450 nm, and two co-located Purple Air Sensors (one indoors and one outdoors). Absorption coefficients were calculated using an extinction minus scattering coefficient comparison. Particle aerodynamic size distributions were measured using a Scanning Mobility Particle Sizer (SMPS, TSI, Inc.) and were used to perform a Mie retrieval of the effective refractive index of the particles over time. Measurements were intercompared and compared with mass measurements from a reference monitoring station (South Coast Air Quality Management District, Anaheim-Loara) located approximately 10 km away.

All instruments were located indoors at California State University, Fullerton (CSUF) with the exception of one PurpleAir sensor that was placed outdoors at CSUF and the AQMD reference monitor. The indoor and outdoor PurpleAir sensors were compared to better understand penetration of particles into the indoor environment and potential exposure of residents to particles during a wildfire. Results of these comparisons will be discussed as well as how each instrument performed against the others.

11SW.2

Plume Heights Affect the Evolution of Organic Aerosol Optical Properties: Insights from FIREX-AQ Field Measurements. CHENCHONG ZHANG, Benjamin Sumlin, Nishit Shetty, Pai Liu, Rajan K. Chakrabarty, *Washington University in St. Louis*

Light-absorbing organic carbon (LAOC) is one of the major components of smoke plumes from biomass burning (BB) events. The atmospheric processing of emitted LAOC in atmospheric transport could have a significant influence on regional radiative forcing and air quality. The spatiotemporal evolution of LAOC optical properties from BB events and their radiative implications are poorly understood, which limits this process-based parameterization in radiative transfer (RT) and chemical transport models (CTMs). Here we synergistically integrate the insights gained from satellite measurements, CTM, and field measurements to investigate the impacts of atmospheric processing on LAOC emitted during the field study portion of the 2019 Fire Influence on Regional to Global Environments and Air Quality (FIREX-AQ) campaign. We incorporate an experimentally constrained radical volatility basis set (VBS) into the WRF-Chem (Weather Research and Forecasting model coupled with Chemistry) CTM to account for the chemical composition of the spatially evolving plume particles. The optical properties of LAOC as a function of photochemical aging are correlated with their fractional compositions in this model. Our simulation results from the CTM are further compared with satellite observations and ground-based measurements to validate the reliable representation of the atmospheric processing for LAOC. Our constrained modeling results show that atmospheric processing of LAOC significantly depends on the smoke plume heights, resulting in stratified vertical profiles of absorption optical depths as a function of photochemical aging. We anticipate our findings to provide better insights for improving LAOC representation in current RTs and CTMs.

11SW.3

Ground-based in Situ Hyperspectral Optical Measurements of Smoke Aerosols during FIREX-AQ, Relating Spectral Characteristics to Aerosol Composition, Fuels, and Fire State.

CAROLYN JORDAN, Bruce Anderson, John Barrick, Kathleen Brunke, Jiajue Chai, Gao Chen, Ewan Crosbie, Jack Dibb, Ann Dillner, Emily Gargulinski, Jackson Kaspari, Robert Martin, Richard Moore, Rachel O'Brien, Claire Robinson, Gregory Schuster, Taylor Shingler, Michael Shook, Amber Soja, Kenneth Thornhill, Andrew Weakley, Elizabeth Wiggins, Edward Winstead, Luke Ziemba, et al., *NASA*

A recent study from the Korea – United States Ocean Color (KORUS-OC) field campaign explored using two-dimensional mapping of in situ aerosol hyperspectral (300-700 nm) characteristics to provide additional discrimination between differing ambient aerosol populations than can be provided by the use of Ångström exponents alone. Here, we apply that methodology to smoke aerosol samples collected from the NASA Langley Research Center's (LaRC) Mobile Aerosol Characterization (MACH-2) laboratory during the western portion of the Fire Influence on Regional to Global Environments and Air Quality (FIREX-AQ) field campaign in July and August of 2019. MACH-2 traveled over 7000 miles sampling 8 fires in 6 states. Here, we report hyperspectral absorption coefficients measured in a liquid waveguide capillary cell from deionized water and methanol extracts of aerosols collected on Teflon filters from 5 of those fires: Williams Flats in Washington state, Nethker in Idaho, Little Bear in Utah, Castle in Arizona, and 204 Cow in Oregon. We also report commensurate mean in situ hyperspectral extinction coefficients for those filter samples obtained from our custom spectral extinction instrument (SpEx). Second order polynomials were used to fit each of the logarithmically transformed spectra, along with the traditional linear fits known as Ångström exponents. Samples from each fire mapped into distinct regions in the two-parameter (a_1,a_2) fit space of the second order polynomial fit coefficients. Variations in aerosol composition deriving from differing biomass fuels, fire state, and atmospheric processing are explored to interpret the separation found in (a_1,a_2) space. In addition, residuals (the difference between the fit and measured spectrum) from the second order polynomials more clearly reveal individual spectral features than are evident from residuals from the linear fits. These features provide specific wavelength targets for further exploration of relationships to physicochemical aerosol properties.

11SW.4

Characterizing the Physical and Chemical Evolution of Organic Aerosol in Biomass Burning Smoke using Gas- and Particle-phase Molecular Tracers from Laboratory and FIREX-AQ Observations.

MELINDA SCHUENEMAN, Douglas Day, Demetrios Pagonis, Seonsik Yun, Olivia Jenks, Pedro Campuzano-Jost, Hongyu Guo, Benjamin A. Nault, Wyatt Brown, Julia Lee-Taylor, Joost de Gouw, Jose-Luis Jimenez, *CIRES, University of Colorado, Boulder*

Fire plumes introduce large amounts of diverse gas- and particle-phase species into the atmosphere, which have been shown to negatively impact human health and the environment. This diversity makes characterizing fire impacts challenging. The abundant emissions of volatile organic compounds (VOCs), particles, and NOx suggest that substantial organic aerosol (OA) formation should occur downwind of fires. However, typically no enhancement of total OA is observed in most cases. One explanation that we are exploring is that primary OA (POA) evaporation is balanced by the condensation of less-volatile oxidized VOCs from VOC precursors onto existing aerosols (forming SOA). During the NASA/NOAA FIREX-AQ mission, for the first time, an Extractive Electrospray Soft Ionization Time-of-Flight Mass Spectrometer (EESI) was used to perform an extensive study of the OA composition in fire plumes. While the identity of some key molecules is clear based on previous literature and other evidence, most of the hundreds of OA species detected in the fire plume are not yet identified. These species hold essential information needed to understand the overall chemical evolution of OA. A suite of laboratory chamber experiments using the EESI and Vocus-PTR-ToF were conducted, targeting known and suspected biomass burning SOA precursors (e.g., phenol, catechol, and styrene). Catechol, nitrophenol, nitrocatechol, 5-nitro-1,2,3-benzenetriol, dinitrocatechol, and two ring-opened products were identified in the particle phase. Many of those species were also identified in the gas phase with the Vocus PTR-ToF-MS. A box model was constructed to represent these experiments, along with selected wildfire plumes from FIREX-AQ, to aid us in interpreting and chemically quantifying the evolution of aerosols in biomass burning plumes. Both the chamber and field models match measured nitrocatechol well. Chemical budgets were created using the direct measurements from the field and chamber studies.

11SW.5

Physicochemical and Toxicological Profiles of Particles from the Combustion of Individual California Biomass Species.

AMBER KRAMER, Tiancong Ma, Tian Xia, Yifang Zhu, *University of California, Los Angeles*

Wildfires driven by global climate change are rapidly becoming more common in daily life in California. The incomplete combustion of biomass, as seen in wildfires, produces plumes of emissions filled with toxic gasses and particulate matter (PM) that lead to increased morbidities and mortalities. To protect populations from harmful wildfire PM emissions, a better understanding of the specific risks associated with biomass combustion in different environmental biomes is needed. Here, we developed a unique contained chamber method which allows us to combust several individual species found throughout California under controlled temperature and relative humidity conditions as well as simultaneously characterize physicochemical and toxicological profiles of emitted PM. We characterize differences in PM emissions between the different species and under different combustion conditions. Particle size distribution was measured using SMPS (10 – 500 nm) and APS (0.5 µm – 20 µm in diameter). The PM-bound organic chemical properties and toxicological outcomes were assessed by collecting PM samples on glass fiber filters and in impingers. We perform oxidative stress, cellular viability, and cytokine assays, and pair these toxicological results with the organic chemical speciation from each biomass species, to provide novel data about specific risks of PM exposure to California residents based on specific biota found throughout the state. To better understand how PM may change between the combustion zone and community exposure zone downwind from wildfires, we assessed the organic chemical concentrations, toxicological properties, and particle size distribution changes after PM aging in the chamber. Our developed chamber method not only allows for measurements during combustion, but also allows us to monitor PM over an aging period. Results from this study could provide practical knowledge for comprehensive risk assessment related to wildfire emissions.

11SW.6

Quantifying Emission Factors from Mixed Conifer Forest Controlled Burns Aimed to Reduce Wildfire Risk at Blodgett Forest Research Station California.

DEEP SENGUPTA, Nathan Kreisberg, Coty Jen, Yutong Liang, James D.A. Butler, Rebecca A. Sugrue, Robert Weber, Paul Van Rooy, Afsara Tasnia, Emre Ozen, Edward Gonzalez, Jason Kriesel, Kevin K. Schwarm, Mitchell R. Spearrin, Thomas W. Kirchstetter, Robert York, Daniel Foster, John Battles, Scott Stephens, Kelley Barsanti, Allen Goldstein, *University of California, Berkeley*

Climate change and prolonged fire suppression strategies in California have led to an increase in the frequency and severity of large wildfire events in recent years. The particulate matter (PM) concentrations across the western United States have increased broadly following these events, impacting air quality and human health over large areas. In order to reduce wildfire risks, California is increasing application of controlled or prescribed burning to reduce accumulated fuels that could otherwise be conducive to wildfires. Extensive field and laboratory studies have been conducted to develop emission profiles from wildfires, but emission factors from prescribed burns under realistic conditions have been less widely studied.

We present emissions profiles from prescribed burns of managed and unmanaged land located in a mixed conifer forest of California conducted in 2017 and 2021. In Fall 2017, we measured emissions factors/profiles of gaseous species (carbon dioxide (CO_2), carbon monoxide (CO), nitrogen oxides (NO_x)) and PM characteristics from filter-based measurements mounted on an All-Terrain Vehicle platform. PM samples were analyzed for total elemental (EC) and organic carbon (OC) using thermal-optical method and organic compounds (using two-dimensional gas chromatography mass spectrometry method). We were able to distinguish the emissions between active and smoldering phase of burning and between managed and unmanaged forest plots. In order to capture the variability of emissions in smoke plume we developed a drone-based sensor platform that includes real-time sampling of CO, CO_2, NO_x, black carbon and collection of sorbent tubes for volatile organic compounds and filter samples for $PM_{2.5}$ to be analyzed for organic compounds, OC, and EC. The drone was deployed for a set of four burns in spring 2021. We observed the evolution of smoke plumes during flaming and smoldering combustion phases and associate them with temperature profiles from thermal imageries, and computed modified combustion efficiencies using the drone sensor package. The resulting data will provide emission profiles and emission factors for prescribed burns to improve the FOFEM model of emissions used by the California Air Resources Board for air quality modeling.

11SW.7

Chemical Transformations of Biomass Burning Organic Aerosol within Wildfire Plumes - From Near-source to the Regional Scale. RYAN FARLEY, Timothy Onasch, John Shilling, Shan Zhou, Sonya Collier, Lawrence Kleinman, Arthur J. Sedlacek, Qi Zhang, *University of California, Davis*

The atmospheric processing of biomass burning organic aerosol (BBOA), and the resulting implications on tropospheric aerosol composition and physicochemical properties, is still uncertain. This study investigates the transformation of BBOA within wildfire plumes during the DOE sponsored Biomass Burning Observation Project (BBOP) in the U.S. Pacific Northwest. Measurements of submicron particulate matter (PM_1) concentration and composition between <1 and ~10 hours of photochemical processing were performed using a high-resolution aerosol mass spectrometer (HR-AMS) aboard the DOE G-1 aircraft. A second HR-AMS at the Mt. Bachelor Observatory (MBO) ground site provided complementary measurements of BBOA having undergone > 6 hours of processing during the campaign. In addition, highly aged plumes with more than 10 days of transport were sampled at MBO in summer 2019. Here we present the analyses of these strategically combined airborne and mountaintop measurements to investigate the near-field (< 1 hr) and regional evolution of BBOA properties in wildfire emissions located in the western U.S. We examine the evolution of the chemical properties of BBOA as a function of photochemical age, estimated by the ratio of NO_x/NO_y or NO_x/CO. The freshest plume had extremely high OA loadings of up to 2000 $\mu g\ m^{-3}$ and an average O/C of less than 0.25. After 6-8 hours of atmospheric transport, the BB plumes sampled at MBO had an increased O/C of 0.70 ± 0.04. The increase of O/C in aged wildfire plumes was associated with a decrease in the organic fraction at m/z 60 (f_{60}), a HR-MS tracer ion for primary BBOA. Additionally, we also explore the formation of secondary organic aerosol (SOA) within the wildfire plumes by comparing the enhancement of OA relative to CO. Finally, positive matrix factorization analysis will be used to disentangle the contribution of primary BBOA from SOA formed through atmospheric reactions of volatile organic compounds. These results can be used to better understand and model the evolution of aerosols and the formation of SOA within these systems.

11SW.8

Reconciling Assumptions in Bottom Up and Top Down Approaches for Estimating Aerosol Emissions from Wildland Fires in the Western US Using Observations from FIREX-AQ. ELIZABETH WIGGINS, Bruce Anderson, Matthew Brown, Gao Chen, Ewan Crosbie, Josh DiGangi, Glenn Diskin, Marta Fenn, Michael Shook, Amber Soja, Francesca Gallo, Emily Gargulinski, Hongyu Guo, Johnathan Hair, Demetrios Pagonis, Anne Perring, Claire Robinson, Kevin Sanchez, Melinda Schueneman, Chelsea Stockwell, Kenneth Thornhill, Carsten Warneke, Joshua P. Schwarz, Taylor Shingler, et al., *NASA*

Wildland fires in the Western United States emit a substantial quantity of trace gas and particulate matter that can severely degrade local to regional air quality and ultimately influence climate. However, it is difficult to accurately quantify biomass burning emissions due to the highly variable composition of the fuels they consume and their dynamic behavior. There are two traditional methods to calculate fire emissions, the “bottom up” approach and the “top down” approach. The bottom up approach aims to calculate the mass of fuel consumed by the fire on the ground to quantify emissions, while the top down approach uses fire radiative power (FRP) observed from remote sensing as a proxy for the mass of fuel consumed. The fraction of the total mass emitted in the form of particulate matter (PM) can then be determined via the use of an emission factor for the bottom up approach or through aerosol optical depth observations for the top down approach. The two approaches often disagree by an order of magnitude or more on the mass of PM emitted by fires, but validation is challenging, and it remains difficult to determine which approach is correct.

In situ and remote sensing airborne measurements from the recent NASA/NOAA campaign Fire Influence on Regional to Global Environments and Air Quality (FIREX-AQ) provide the opportunity to evaluate the two traditional approaches to calculate emissions. In this study, we calculate fire PM emission rates from Western US wildland fires sampled during FIREX-AQ using an independent approach that relies on the integration of smoke plume observations and information gleaned from airborne LIDAR measurements from HSRL. We also calculate fire PM emission rates using the traditional bottom up and top down style approaches. We compare our PM emission rate estimates from the in situ based approach with the traditional approaches to investigate potential bias. We find the bottom up approach has the best agreement with the in situ approach, but with a high level of noise. The top down approach systematically overpredicts fire emissions on the lower end of the range compared to the in situ approach, but the data is much more tightly clustered. The results of our analysis improve our understanding of how to correctly quantify fire aerosol emissions, and have larger implications for using aerosol optical depth remote sensing observations to estimate the mass of PM emitted by fires.

12BA.1

Determining the Composition of Ice Nucleating Particles from Marine Phytoplankton.

ALYSSA ALSANTE, Daniel Thornton, Sarah Brooks, *Texas A&M University*

Sea spray aerosol (SSA) plays a significant role in climate, both directly by scattering solar radiation and indirectly by affecting cloud properties. In the marine environment, aerosol contains a significant amount of organic matter derived from phytoplankton productivity. A subset of aerosol facilitates the freezing of atmospheric ice crystals by acting as ice nucleating particles (INP) at temperatures above the homogeneous nucleation threshold (-38°C). Our previous laboratory experiments demonstrated that high growth rates result in increased production of INP. Therefore, we focus on biologically relevant individual amino acids, proteins, and nucleic acid that are involved in rapid phytoplankton growth as possible candidates for effective INP. Our results indicate amino acids and DNA are effective INP nucleating ice at -19.2°C to -24°C ± 3.4°C and -18.3°C ± 1.8°C, respectively. In contrast, RuBisCo, an important enzyme in carbon fixation, has the highest average freezing temperature (-7.8°C ± 0.6°C). These results demonstrate that phytoplankton production is an important source of INP from the ocean and that resource allocation by phytoplankton potentially affects the properties of marine INP.

12BA.2

Species-Specific Chemical Analysis of Pollen for Source Identification of Atmospheric Aerosol.

KEVIN AXELROD, Vera Samburova, Andrey Khlystov, *Desert Research Institute*

Biological aerosols, or bioaerosols (aerosols that are biological in origin) are a subject of increasingly intense study in recent years due to their potential impact on atmospheric chemistry. However, information related to chemical composition of bioaerosols is still largely unknown. In our study, we characterized the chemical composition of fresh pollen, one of the most common bioaerosols in the atmosphere that has a significant impact on human health and could also influence climate by providing cloud nuclei. Different pollen species (aspen, corn, pecan, ragweed, eastern cottonwood, paper mulberry, rabbitbrush, bitterbrush, lodgepole pine, and Jeffrey pine) were purchased or collected around the area of Reno, Nevada, USA. Water extracts of these pollens were chemically analyzed, including analysis of saccharide content via GC-MS and free amino acid content via UPLC-MS analysis techniques. The saccharides ß-D-fructose, α-glucose, and β-glucose were found across all ten pollen samples analyzed. In addition, sucrose was found in five samples, while galactose was found in pine species. Analyzed saccharides constituted 3.97-28.54% of total dry weight among samples, while total free amino acids constituted 0.29% to 15.05%. The free amino acid proline was ubiquitous among all analyzed pollen samples. In addition, chemical profiles of surface-deposited aerosol in the pine-dominated Lake Tahoe area correlated most closely with pine pollen than any of the other analyzed pollen species. Our results demonstrate that saccharide and free amino acid profiles of pollen can be used to infer sources of aerosol in the environment.

12BA.3

Pollen as a Source of Atmospheric Particles and Ice Nucleating Particles.

BRIANNA HENDRICKSON, Alyssa Alsante, Sarah Brooks, *Texas A&M University*

Annual emissions of primary biological aerosol particles (PBAPs) contribute 10-1,000 Tg to the aerosol population. With pollen acting as a substantial fraction of annual PBAP emissions (47-84 Tg), it is important to accurately quantify pollen emissions. Whole pollen grains are released from plants and rupture during pollen season, releasing pollen grain fragments referred to as subpollen particles (SPPs). Whole pollen grains and SPPs can act as ice nucleating particles (INP) influencing cloud formation and precipitation. Accurate characterization of meteorological conditions required for pollen emissions to occur is needed to quantify the contribution of pollen to the aerosol population. This study is an evaluation of various mechanisms (conventional relative humidity and wind versus wind only) to determine the threshold parameters needed for live oak pollen grain rupture in a laboratory chamber. To represent the conventional mechanism, branches were exposed to high relative humidity >95%, followed by reduced relative humidity (<80%) and winds (up to 4mph). In contrast, wind-only experiments were conducted by cycling fans on and off at constant relative humidity. While both conventional relative humidity cycling and lightning have been proposed as SPP production mechanisms, neither are essential elements of the production of the high concentrations of SPP as evidenced by concentrations as high as 2.4E+02 ± 1.3E+02 SPPs per cm^3 observed in wind-only experiments here. In fact, the mean SPP emissions during relative humidity cycling was lower than that during wind-only with concentrations as high as 7.3E+01 ± 3.4E+01 SPPs per cm^3. The concentration of SPPs generated from whole pollen grains was characterized and used to calculate SPP emission factors. Live oak SPP emission factors were determined to be between 1.4E+04 and 7.7E+04 SPPs per pollen grain, representing a significant source of cloud-forming aerosol. Concentrations and ice-nucleating behavior of pollen and SPP will be reported, and atmospheric implications discussed.

12BA.4

Miniature High-Flowrate Biosampler for Distributed Deployment.

DAVID ALBURTY, Andrew Page, Ann Packingham, David Goad, *InnovaPrep LLC*

A 200 LPM dry-electret sampler weighing less than a kilogram with 4-hr rechargeable battery was developed for fieldable use and tested in April, 2020 for collection of killed SARS-CoV-2 using portable qPCR. The sampler features an omnidirectional inlet and simple faceplate button operation. The sample filter is contained in an interface ring to avoid cross-contamination and provide ease of sample handling. Filter elution is performed with a wet foam which collapses to a small volume for analysis, providing a higher concentration ratio than is possible with vortexing. Selection of the filter material in combination with the sample inlet was done to maximize the collection of particles across the size range from 10 nanometers to 11 microns. The sampler is constructed of materials compatible with bleach and other disinfectants and cleaners. It has built-in feet allowing exhaust flow away from the inlet and can be tripod-mounted or hung in location. This sampler combines rapid, effective, bioaerosol sampling with a 30-second sample elution process that is compatible with fieldable qPCR to provide a simple solution for public health monitoring of airborne pathogens.

12BA.5

Airborne Dust and Bioaerosol Concentrations in Canadian Laying Hen Facilities Using Battery Cages, Enriched Cages and Aviaries. MAGALI-WEN ST-GERMAIN, Valérie Létourneau, Araceli Dalila Larios Martínez, Stéphane Godbout, Caroline Duchaine, *Laval University, Quebec Heart and Lung Institute*

Since 2017, the Canadian egg industry has begun a transition from conventional cages to alternative housing systems for laying hens. While enriched cages and aviaries provide improved animal welfare conditions, the greater freedom of movement provided by alternative systems and the presence of litter in aviaries may affect air quality and consequently have adverse effects on worker's respiratory health. This project aims to evaluate airborne dust (PM2.5, PM10, and total dust) and bioaerosols concentrations in conventional and alternative laying hen facilities. Twelve farms within 200 km of Quebec City (Canada) were visited during winter and fall 2020 and winter 2021. Facilities housed at least 20 000 hens and were visited after 55 to 65 weeks of production. Airborne dust, molds, and bacteria were sampled using the DustTrakTM DRX Aerosol Monitor (Model 8534, TSI) and the high-volume samplers Coriolisµ (Bertin Technologies) and SASS3100® Dry Air Sampler (Research International). Triplicates were taken in each facility. Median total dust concentrations were 1.161 (IQR: 0.188) mg*m^{-3} in conventional facilities, 1.608 (IQR: 0.831) mg*m^{-3} in enriched cage facilities and 32.581 (IQR: 7.528) mg*m^{-3} in aviaries. Median culturable bacteria concentrations were respectively (7.7, IQR: 4.1)*10^{4} CFU*m^{-3}, (2.2, IQR:1.7)*10^{5} CFU*m^{-3} and (5.1 , IQR: 5.0)*10^{6} CFU*m^{-3}, while median culturable mold concentrations were (1.0, IQR: 1.0)*10^{2} CFU*m^{-3} , (2.6, IQR: 8.5)*10^{2} CFU*m^{-3} , (1.7, IQR: 1.5)*10^{2} CFU*m^{-3}. qPCR analyses revealed median 10^{7} 16s rRNA copies*m^{-3} in conventional and enriched cage facilities and 10^{8} 16s rRNA copies*m^{-3} in aviaries. Dust and culturable bacteria concentrations were higher in aviaries while other bioaerosol concentrations seem to be similar across facility types. Concentrations of endotoxins and pathogenic agents will be evaluated in upcoming analyses.

12BA.6

Development and Characterization of an Environmental Rotating Aerosol Chamber for Long-term Bioaerosol Suspension. Esther Monroe, Nishit Shetty, Benjamin Sumlin, Joshin Kumar, GANESH CHELLUBOYINA, Rajan K. Chakrabarty, *Washington University in St. Louis*

In traditional chamber studies, aerosols are subject to gravitational settling and other wall losses which must be considered when studying the temporal evolution of the size distribution. To mitigate such losses, an Environmental Rotating Aerosol Chamber (ERAC) was conceived for bioaerosol applications where it is necessary to prolong the suspension of particles, especially in the sub-micron size range. Our ERAC is comprised of a 37.9-L cylindrical vessel which rotates about its axis, and the resulting centrifugal force counteracts the rate of gravitational settling. The ERAC is also equipped to control environmental factors such as temperature and relative humidity and is capable of disinfection by an internal 254 nm UV-C lamp. These parameters are monitored by integrated sensors, and the data acquisition is done via a microcontroller which interfaces to an external computer.

The suspension efficiency of the ERAC was evaluated using aerosolized 600 nm and 1 µm polystyrene latex beads. Measurements using an Aerodynamic Aerosol Classifier (Cambustion Inc.) coupled with a TSI condensation particle counter showed that at size-dependent optimal rotation rates, the ERAC can suspend sub-micron particles for over 24 hours, and that the steady-state rate of aerosol loss approaches the theoretical prediction values of the Gruel model. Following the chamber characterization, ERAC was used to investigate the effects of environmental conditions on inactivated virus particles over a 7-day period. In this talk, we will present experimental characterizations of the decay constants of the aerosol number concentration as a function of relative humidity, temperature, and particle aerodynamic diameter.

12BA.7

Application of Long-read Nanopore Sequencing for the Analysis of Airborne Microbes. AUSTIN MARSHALL, Daniel Fuller, Kavindra Kumaragama, Suresh Dhaniyala, Shantanu Sur, *Clarkson University - Potsdam, NY*

The ongoing COVID-19 pandemic has raised global awareness of airborne diseases, generating a larger interest in the microbial population in the air. Next-generation sequencing (NGS) offers a robust approach to analyze the microbiome, however, one major challenge to analyze airborne microbes arises from their extremely low concentration in air compared with other environments such as soil, water, and gut. This, thus, necessitates the use of high-pressure drop, high flow-rate sampling devices or long collection time periods to capture sufficient amount of bioaerosol samples for analysis, a severe restriction for several applications. In this work, we explored how long-read nanopore sequencing technology could be utilized to establish an analytical workflow to obtain sequencing data from a small quantity of genomic material without compromising the quality and resolution of measurements. Bacterial abundance and diversity in bioaerosol samples were estimated by 16S rRNA amplicon analysis using a MinIon flow-cell device, which enables a full-length read of the 16S rRNA gene, thus increasing the sequencing read depth. We found that by modifying and optimizing the sample preparation procedure, we could extract reliable and accurate results from less than 0.5 ng of genomic DNA, which is over an order of magnitude lower than the amount needed for conventional NGS platforms such as Illumina. Additionally, the ability to perform the sequencing locally in the laboratory without the need for expensive instrumentation and the capability of multiplexing samples on a single run enable a fast, cost-effective means to get sequencing results following sample collection. Using this workflow, we have successfully analyzed bioaerosol samples collected by a low pressure-drop, low power, portable bioaerosol sampler deployed at various outdoor and indoor locations.

12BA.8

Measuring the Viability of Airborne Virus under Different Environmental Conditions and Fomites. ROBERT ALEXANDER, Mara Otero-Fernandez, Henry Oswin, Allen E. Haddrell, Jamie Mann, Adam Finn, Tristan Cogan, Andrew Davidson, Richard J. Thomas, Jonathan P. Reid, *University of Bristol*

The increasing number of airborne outbreaks worldwide, such as the current severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) pandemic, have raised the need to understand parameters affecting the airborne survival of pathogens in order to develop measures for effective infection control. The dynamics involved in the airborne transmission of disease relies on the ability of pathogens to survive aerosol transport and, subsequently, cause infection when interacting with a host. The length of time airborne microorganisms remain infectious in the aerosol phase is a function of a wide range of variables (e.g. atmospheric, microbiological, etc.) that affect their viability and, therefore, have the potential to impact the dissemination of the disease outbreak. Representing the dynamics of airborne disease transmission under laboratory conditions is challenging due to systematic limitations that can impact the accurate representation of the processes that these particles would experience in the natural environment.[1]

To be presented is the adaption of the CELEBS (Controlled Electrodynamic Levitation and Extraction of Bioaerosols onto a Substrate) technique which has been previously used to study the airborne survival of bacteria.[2] The present methodology also enables the robust study of airborne survival of viruses as a function of relevant environmental conditions within a high containment laboratory, using Mouse Hepatitis Virus (MHV) as a surrogate for more pathogenic viruses. The instrument uses piezoelectric dispensers to generate droplets of highly reproducible size and composition, which are then suspended using electrodynamic levitation within a path of temperature and RH controlled air. This technique also presents the ability to subject viruses to airborne transport prior to deposition on surfaces, to better simulate fomite transmission.

Results outlined in this presentation will contribute to understand the impact of several variables such as: (a) relative humidity, (b) temperature and (c) absolute humidity, while featuring some of the benefits of this novel technique including (1) the characterization of the rapid initial decay in viability occurring within the first couple of minutes after aerosolization, representing the importance of close range transmission and (2) the study of airborne pathogens stability on surfaces to accurately simulate the deposition of small particles which have deposited onto a surface after spending time airborne.

[1] Douwes, J., Thorne, P., Pearce, N. & Heederik, D. Bioaerosol health effects and exposure assessment: Progress and prospects. Ann. Occup. Hyg. 47, 187–200 (2003).
[2] Otero-Fernandez, M. et al. Assessing the airborne survival of bacteria in populations of aerosol droplets with a novel technology. J. R. Soc. Interface 16, 20180779 (2019).

12BA.9

Characterization of Sub-Pollen Particles in Atmospheric Aerosol During Summer Rain Events. CHAMARI MAMPAGE, Dagen Hughes, Lillian Jones, Nervana Metwali, Peter Thorne, Elizabeth Stone, *University of Iowa*

Osmotic rupturing of pollen grains (10-100 µm) can release sub-pollen particles (SPP; <2.5 µm). Due to their smaller size, SPP have longer atmospheric lifetimes, and are capable of long-range transport, affecting the Earth's climate, and penetrating deeper into the lung. The current study examines SPP in size-resolved atmospheric particulate matter (PM) in August – September 2019, during ragweed season in the Midwestern United States. On rainy days, $PM_{2.5}$ concentrations of fructose and sucrose, which are chemical tracers of pollen, increased suggesting possible pollen rupturing events that released SPP to the atmosphere. Co-located single-particle measurements showed an influx of submicron fluorescent particles during rain, especially convective thunderstorms. The concentrations of submicron SPP remained elevated after rain events, continuing to the next day, consistent with elevated chemical tracer concentrations. The size-resolved PM collected using a 5-stage impactor indicated that SPP ranged <0.25-2.5 µm in diameter. Field observations of SPP were complemented by laboratory studies of giant ragweed pollen rupturing, which released an estimated 1400 SPP per pollen grain ranging 0.02 - 6.5 µm in diameter, and suggested ragweed can be a contributing factor to submicron SPP during summertime. Mannitol, a fungal spore tracer and bacterial endotoxins were also analyzed, and their size-resolved concentrations showed minimal contribution to submicron particles during summer rain events. Collectively, the results show that the highest increase of pollen tracers in submicron particles compared to fungal spores and bacteria, indicating that SPP were likely responsible for the submicron fluorescent particles observed during summer rain events.

12BA.10

Carbonyls in Cloud Water: Their Biodegradation by Bacteria. 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 bacterial biotransformation in more polluted environments such as urban fogs is limited. Also, few observations exist on the biotransformation of carbonyl compounds in the interaction with other chemical components in cloud water. In this study, we aim to investigate the biodegradation rate of common aldehydes found in atmospheric water by bacterial strains isolated from samples collected in Bakersfield (California, USA). The initial results showed that the biodegradation of formaldehyde, acetaldehyde, glyoxal, and methylglyoxal occurred at 17°C and ranged from 10^{-21} to 10^{-20} mol $cell^{-1}$ s^{-1}. These observations suggest an important role of metabolic pathways in the chemical properties of atmospheric water. Moreover, we found that the biodegradation of formaldehyde by bacteria in an artificial cloud medium is inhibited in the presence of sulfur (IV), when hydroxymethanesulfonate (HMSA) has been formed.

12CA.1

Physical and Optical Properties of Aerodynamically Classified BC and BrC. JAMES ALLAN, Dawei Hu, Rami Alfarra, Kate Szpek, Justin Langridge, Michael Cotterell, Claire Belcher, Ian Rule, Zixia Liu, Chenjie Yu, Yunqi Shao, Aristeidis Voliotis, Mao Du, Brett Smith, Gregory Smallwood, Prem Lobo, Dantong Liu, Jim Haywood, Hugh Coe, *University of Manchester and NCAS*

Accurately characterising the optical properties of carbonaceous particulate matter is hampered by our ability to be able to study the compositional components in isolation and in particles of a single size. The Soot Aerodynamic Size Selection for Optical properties (SASSO) project aims to address this by using an Aerodynamic Aerosol Classifier (AAC), which eliminates the multiple charging problems associated with electrostatic classification. A variety of soot sources were studied, including wood burning (using a controlled combustion technique to separate elemental and organic carbon combustion phases), an automotive diesel engine and an inverted propane flame. In addition, SOA was generated in a chamber to provide both non-absorbing and 'brown' coatings. The particles were analysed using various online chemical, physical and optical instruments to evaluate composition, morphology and refractive index. The science themes addressed include the applicability of the standard SP2 Aquadag calibration, effect of wood type and moisture content, effect of humidification-induced restruturing and accuracy of mixing assumptions used in optical models. The outcomes of this research will be used to improve the HadGEM climate model in the UK.

12CA.2

A Novel Approach for Carbon Constant Calibration and Validation of the Magee Scientific Total Carbon Analyzer TCA08. Gašper Lavrič, KLEMEN KUNSTELJ, Martin Rigler, *Aerosol d.o.o.*

Introduction

Carbonaceous aerosols are usually the most significant contributor to fine particulate matter (PM2.5). They are frequently separated into organic carbon (OC) and elemental carbon (EC) based on their volatility using thermal-optical methods.

The Magee Scientific Total Carbon Analyzer, Model TCA08, is a newly developed scientific instrument that measures the Total Carbon Content ("TC") of suspended aerosol particles in near real-time using a simplified thermal method (Rigler et al., 2020). The combination of Total Carbon Analyzer TCA08 and the Magee Scientific Aethalometer® model AE33 provides a novel approach for measuring TC, eBC, OC, EC content of suspended aerosol particles near-real-time with high-time resolution.

The TC-BC method determines OC fraction of carbonaceous aerosols defined as

OC=TC-b·eBC

The determined proportionality parameter b is region/site-specific and depends mainly on the thermal protocol used to determine the EC fraction with a conventional OC-EC method.

Carbon constant Calibration/validation procedure

Carbon Constant calibration of the Total Carbon Analyzer TCA08 is a key operation to ensure the carbon detector's proper operation during measurement campaigns. The procedure is performed using punches of dry ambient filters that were previously measured with calibrated laboratory OC/EC instrument to determine their TC concentration.

Keywords: ambient filters, total carbon, calibration

References

Rigler, M., et al.: The new instrument using a TC–BC (total carbon–black carbon) method for the online measurement of carbonaceous aerosols, 13, 4333–4351, https://doi.org/10.5194/amt-13-4333-2020, 2020.

12CA.3

High-time Resolution Apportionment of Primary and Secondary Carbonaceous Aerosols Using Advanced TC-BC Method.

MARTIN RIGLER, Matic Ivančič, Jerzy Debosz, Uwayemi Sofowote, Jonathan Wang, Robert Healy, *Aerosol d.o.o.*

High-time resolution apportionment of carbonaceous aerosol is essential to identify the main pollution sources and separate species that have the highest impact on public health and planetary radiation balance. Carbonaceous aerosols were measured by the CASS system (Carbonaceous Aerosol Speciation System, Rigler et al., 2020), which combines the Total Carbon Analyzer TCA08 and the Aethalometer AE33, providing high time-resolved data on carbonaceous aerosol composition and optical properties in real-time.

Apportionment of the carbonaceous matter is based on the simplified TCA08 method, where the organic carbon (OC) content is calculated as the difference between total carbon (TC) and black carbon (BC). The BC tracer method is used to separate organic carbon into the primary and secondary OC (Wu and Yu, 2016). Furthermore, multiple-wavelength analysis of the AE33 absorption data provides optical apportionment to BC and brown carbon (BrC).

The intensive measurement campaign was conducted between 30 April and 14 May 2019 at a roadside monitoring station located adjacent to Highway 401 in Toronto, Canada. This is the busiest section of highway in North America, with average traffic volumes of over 400,000 vehicles per day. Measurement results were evaluated with complementary measurements of OC/EC, PM2.5, organics measured by an aerosol chemical speciation monitor (ACSM), and various trace gases. During workdays, the diurnal variations of BC, BrC, primary and secondary OC were strongly influenced by the temporal patterns of emissions from traffic. On the weekend evenings, a small contribution from biomass burning was also observed. Primary carbonaceous emissions (BC+POC) contributed 60% to TC during workdays, while secondary OC prevailed during weekends with a share of almost 70%.

[1] Rigler, M., et al.: Atmos. Meas. Tech., 13, 4333–4351, 2020.
[2] Wu, C. and Yu, J. Z., Atmos. Chem. Phys., 16, 5453–5465, 2016.

12CA.4

Connecting Composition to Reactivity for Fragrances and Their Emissions.

JAMES HURLEY, Jessica Gilman, Brian McDonald, Matthew Coggon, Gabriel Isaacman-VanWertz, *Virginia Tech*

Atmospheric oxidation of volatile chemical products (VCPs), which include consumer items such as personal care products, air fresheners, cleaning agents, etc., has been recently shown to account for a substantial fraction of organic aerosol in urban environments. Many of these products include fragrances, which are often comprised of volatile and reactive components, though their composition is frequently proprietary and/or unpublished. In this study, 11 commercially available fragrances were analyzed for their composition, and their evaporation and impacts on air chemistry were modeled. The liquid fragrance components were identified by Gas chromatography-Mass spectrometry (GC-MS) and quantified through GC-FID (Flame Ionization Detection). 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%). Fragrance compounds were generally less than half the mass of liquid fragrances, with the balance comprised of solvents and plasticizers and unresolved mass thought to be dominated by solvents and plasticizers. 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. Terpenes and terpenoids account for nearly all the emitted mass and reactivity while only comprising ~10% w/w on average of the liquid fragrances, and evolve on timescales of only a few hours. Due to varying fragrance composition, particularly the quantities of terpenes, there are orders of magnitude differences in the amounts of carbon and oxidant reactivity emitted by the different fragrances. 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.

12CA.5

Molecular Characterization of Aerosolized Bio-Oil.

EMILY HALPERN, Christopher West, Anusha P.S. Hettiyadura, Alexander Laskin, *Purdue University*

The chemical characterization of various volatility-separated fractions of bio-oils is very challenging due to the complexity of the mixture and the range of physicochemical properties of the components. It is essential to classify bio-oil components with respect to their major chemical types and functional groups to inform the deoxygenation processing of crude bio-oil surrogates and their viability as an energy source. Due to the range of volatilities of the molecular components, fractionation of the bulk bio-oil can be used to modify the composition so that it contains only components of interest. Here, we investigate aerosolized bio-oil fractions when deposited onto the different stages of a Microorifice Uniform Deposit Impactor (MOUDI), where fractionation was achieved by aerosol size-segregation and consequently reduced pressures on each of the stages. The molecular characterization of the bio-oil fractions was achieved using ultrahigh performance liquid chromatography equipped with a photodiode array detector and high-resolution mass spectrometry (UHPLC-PDA-HRMS) with both electrospray ionization (ESI) and dopant-assisted atmospheric pressure photoionization (APPI). Molecular characterization allowed description of the individual species present in the bio-oil sample based on estimated values of volatility, glass transition temperature, aromaticity, and elemental ratios. By comparing the mass absorption coefficients of bio-oil fractions with different volatilities, we were able to show that the less volatile fractions absorb more than the bulk sample due to the evaporation of volatile compounds at lower pressures in the MOUDI. This work provides insight on the molecular components of representative bio-oils and provides an opportunity to improve design and engineering of novel bio-oil fuels.

12CA.6

Secondary Organic Aerosol Formation from the Oxidation of Volatile Organic Compound Mixtures.

YUMENG CUI, Kunpeng Chen, Ying-Hsuan Lin, Roya Bahreini, *University of California, Riverside*

Smog chamber experiments have been widely used to simulate the ambient aerosol formation, and to understand the gas-phase and particle-phase chemistry. The chemical and microphysical properties of resultant aerosols formed from chamber experiments are generally applied to atmospheric models to estimate the aerosol formation and its radiative effects. However, most of the chamber studies focus on secondary organic aerosols (SOA) formation from a single volatile organic compound (VOC), while in the ambient atmosphere, VOCs from different sources usually mix after emissions. In this study, we explored the SOA formation and the chemical and optical properties of resulting particles from pure or the mixture of longifolene with 1-methylnaphthalene and phenol using continuous-flow chamber experiments under high-NO_x conditions, and single scattering albedo (SSA) and mass absorption coefficient (MAC) of SOA at 375nm were calculated (1-methylnaphthalene SOA: $SSA_{375}\approx0.85$, $MAC_{375}\approx0.6m^2/g$; phenol SOA: $SSA_{375}\approx0.75$, $MAC_{375}\approx3.1m^2/g$; longifolene SOA: $SSA_{375}\approx0.99$, $MAC_{375}<0.1m^2/g$). Our preliminary results show that the addition of longifolene weakened the absorption of aromatic SOA. In 1-methylnaphthalene and longifolene mixture experiments, the SSA_{375} increased from 0.85 in the pure system to 0.96, and MAC_{375} decreased from $0.6m^2/g$ to $0.3m^2/g$; in phenol and longifolene mixture experiments, the SSA_{375} increased from 0.75 in the pure system to 0.88, and MAC_{375} decreased from $3.1m^2/g$ to $1.1m^2/g$. The aerosol mass spectrometer (AMS) data showed the formation of organonitrate and/or nitroorganic compounds ($NO_x{}^+{}_{org}$) in SOA, and the ratio of $NO_x{}^+{}_{org}$ concentration to measured organics (R_{ON}) varied under different VOC schemes. Time-integrated aerosol samples collected at the end of the experiments will be analyzed with offline instruments (UV-Vis spectrophotometer and liquid chromatography coupled with a diode array detector and a high-resolution time-of-flight mass spectrometer equipped with an electrospray ionization source) for molecular characterization. More details about the aerosol optical properties and chemical composition will be presented to discuss the effects of mixing VOC precursors.

12CA.7

Fine Particulate Matter and Black Carbon Emissions from Non-Cooking Residential Sector Activities over Rural India.

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The residential sector including cooking, water heating (WH), space heating (SH), and kerosene lighting (KL) significantly injects pollutants into the atmosphere. Non-cooking residential (NCR) activities are understudied due to the lack of availability of data in rural India. Past studies used experience-based assumptions to estimate such emissions, however, without region-specific information on variables including device type and temporal usage. Here, we report spatial (5km resolution) and seasonal variation of $PM_{2.5}$ and BC emitted from NCR activities in rural parts of India. The month-device specific fuel consumption for each of the three NCR activities is prepared using primary data from ~5200 new residential surveys conducted across 41 districts of India under the National COALESCE project (Venkataraman et al., 2020, Bull. Am. Met. Soc., 101(7):E1052-68). This is combined with secondary demographic and housing data as predictors in multivariate regression models. Satellite-derived night-time light data are used to identify urban and non-urban areas. We estimate 1223 and 210 Gg/year of $PM_{2.5}$ and BC are released to the atmosphere from NCR activities, where SH, WH and KL contribute 58%, 41% and 1% of $PM_{2.5}$, respectively. The corresponding share of BC emissions is 65%, 28%, and 7%, respectively. Emissions are dominant in rural areas (86-88%), where, firewood (FW), and coal combustion contribute 35% and 39%, respectively to the total BC emissions. Similarly, FW (35%) and dung-cake (32%) dominate the $PM_{2.5}$ emissions. Devices such as traditional stoves (27%) and wick lamps (6%) used for WH and KL, respectively dominate BC emissions. Emissions found higher during winter (Nov-Feb) (52-56%), whereas, BC emission due to KL is higher (3%) during summer/monsoon (May-Aug). The regression model estimates a majority of BC emission from KL over the states of Uttar Pradesh, Bihar, and Assam, consistent with independent Census 2011 data. Further analysis examining the spatial variability of pollutants from a different device and fuel use for the three NCR activities is currently underway.

12CA.8

Molecular-Specific Photolysis of Atmospheric Brown Carbon.

DIEGO CALDERON-ARRIETA, Ana Morales, Anusha P.S. Hettiyadura, Chunlin Li, Yinon Rudich, Alexander Laskin, *Purdue University*

Light-absorbing organic aerosol (aka Brown Carbon, BrC) produced by biomass burning (BB) has a significant impact on global and regional air quality, public health, and climate. In this work we investigate molecular composition of BrC and its atmospheric transformations in laboratory experiments simulating their photolytically-induced transformations. We probe composition and optical properties of individual BrC species using high performance liquid chromatography (HPLC) equipped with a photodiode array (PDA) detector for UV-visible analysis of separated chromophores along with high resolution mass spectrometry (HRMS) for compositional analysis. Results of the HPLC-PDA-HRMS analysis reveal composition-specific atmospheric lifetimes of BrC species, indicating highly complex physicochemical properties of atmospheric BrC. This study provides insight to the atmospheric ageing of BrC in BB emission plumes.

12CA.9

Elemental Versus Black Carbon: Are They Interchangeable? Insights from Extensive Measurement Campaigns in Southern California. FARAZ AHANGAR, Payam Pakbin, Sina Hasheminassab, Mohammad Sowlat, Avi Lavi, Christopher Lim, *South Coast Air Quality Management District*

Elemental Carbon (EC) is one of the key components of ambient particulate matter with many adverse climate and health impacts. Traditionally, EC has been quantified by time-integrated filter-based EC measurements with subsequent laboratory analysis across the United States. In the past decade, continuous black carbon (BC) measurements are being more commonly used due to their higher time resolution and lower detection limit. While EC and BC are operationally defined, previous studies found good correlations among these two parameters. However, the relationships between EC and BC are not similar across the studies. Also, the spatial and temporal changes of EC-BC relationships are rarely explored.

In this work, we explore if the relationship between BC and EC is dependent on the characteristics of the location or whether it changes over time. We used the results from two air monitoring campaigns conducted in Southern California in 2012-2013 and 2018-2019. The data included EC measurements acquired through the IMPROVE thermal/optical reflectance method and BC measurements by seven-wavelength aethalometers at ten distinct locations in the South Coast Air Basin. The preliminary results showed that while highly correlated, BC concentrations were consistently higher than EC, especially at lower concentration levels. This is probably due to the different measurement techniques as well as the better detection limit of the aethalometers. Also, no significant trend between EC-BC relationship and the measurement season or location was observed during the study period. However, this relationship changed between the two campaigns which might be caused by the lower BC and EC levels during the second campaign, elevating the effects of higher BC-EC ratios at lower concentration levels.

12CA.10

Humidity-Dependent Brown Carbon Light Absorption and Photobleaching: Laboratory and Model Synthesis of Organic Dyes. KYLE GORKOWSKI, Katherine Benedict, James E. Lee, Allison Aiken, Christian Carrico, Tyler Capek, Manvendra Dubey, *Los Alamos National Laboratory*

Non-refractory light-absorbing molecules can photochemically oxidize to become more hygroscopic and less absorbing on a per molecule basis. This dynamic process occurs during aerosol transport in the atmosphere and is particularly important during the aging of biomass-burning plumes. We will discuss both laboratory measurements and modeling comparisons for this process using brown carbon mimics (photobleaching, hygroscopicity, and light scattering).

We performed aging experiments on mono-disperse surrogate brown carbon aerosol using an Aerodyne oxidation flow reactor. The humidity-dependent optical absorption was measured at 450 nm using a newly developed humidity-controlled single scattering albedometer. We observed a decrease in absorption and increased single scatter albedo as the days of equivalent OH exposure increased (1 to 10 days). We interpret our observations using an integrated modeling framework that combines thermodynamics and optical modeling. Specifically, we used a binary activity thermodynamics model to simulate water uptake. We predicted the complex-refractive index from the molecular structures using a newly developed molecular-optical model. We then combined these two steps in a hygroscopic-Mie model to compare our simulation to the observed humidity-dependent optical absorption.

Our synthesis combines the multiple processes by which brown carbon undergoes photo-bleaching in the atmosphere that we will develop into a simplified parameterization for use in climate models.

12CA.11

The Determination of Source-separated Black Carbon Emission Rates Using Radon as a Tracer of Atmospheric Dynamics.

ASTA GREGORIč, Luka Drinovec, Janja Vaupotič, Irena Jezek, Matic Ivančič, Janja Tursic, Griša Močnik, *Aerosol d.o.o.*

Black carbon (BC) is known as a good indicator of primary emissions. However, atmospheric conditions play an important role in the magnitude and time evolution of ambient BC concentrations, which makes it difficult to reliably quantify the intensity of sources.

We present a new method for the determination of the source-specific black carbon emission rates. The methodology was applied in two different environments: an urban location in Ljubljana and a rural one in the Vipava valley (Slovenia, Europe). The atmospheric dynamics was quantified using the atmospheric radon (^{222}Rn) concentration to determine the mixing layer height (MLH) for periods of thermally driven planetary boundary layer evolution. The BC emission rate was determined using an improved box model taking into account MLH and a horizontal advection term, describing the temporal and spatial exponential decay of BC concentration. The rural Vipava valley is impacted by a significantly higher contribution to black carbon concentration from biomass burning during winter (60 %) in comparison to Ljubljana (27 %). Daily averaged black carbon emission rates in Ljubljana were 210 ± 110 and 260 ± 110 $\mu gm^{-2}h^{-1}$ in spring and winter 2016/17, respectively. Overall BC emission rates in Vipava valley were only slightly lower compared to Ljubljana: 150 ± 60 and 250 ± 160 $\mu gm^{-2}h^{-1}$ in spring and winter, respectively. The yearly trend of BC emission rates, including the CoViD-19 lockdown period, for Ljubljana location will be presented.

Coupling the high-time-resolution measurements of BC concentration with atmospheric radon concentration measurements can provide a useful tool for direct, highly time-resolved measurements of the intensity of emission sources. Source-specific emission rates can be used to assess the efficiency of pollution mitigation measures over longer time periods, thereby avoiding the influence of variable meteorology.

12CA.12

Evaluation of Regional Model Predictions of Secondary Organic Aerosol from Aromatic Compounds and Monoterpenes with Precursor-Specific Tracers.

JIE ZHANG, Xiao He, Yaqin Gao, Shuhui Zhu, Shenggao Jing, Hongli Wang, Jian Zhen Yu, Qi Ying, *Texas A&M University*

The Community Multiscale Air Quality (CMAQ), with modifications to track precursor-specific SOA, was applied to model SOA formation from aromatic compounds and monoterpenes in Shanghai in November 2018. The modeled aromatic SOA showed a moderate correlation with measured 2,3-dihydroxy-4-oxopentanoic acid (DHOPA) concentrations in the ambient aerosols (R~0.4 for hourly data and R~0.5 for daily average data). The ratios of DHOPA and modeled aromatic SOA using robust regression are approximately 1-3×10^{-3} when SOA from aromatic glyoxal (GLY) and methylglyoxal (MGLY) is excluded, which is comparable to the average tracer-to-aromatics SOA ratio of 2.3±1.2×10^{-3} determined in the chamber studies. This indicates that the model can reasonably predict aromatic SOA. The ratio is around 0.5-1×10^{-3} with GLY and MGLY SOA included, suggesting that tracer-based aromatics SOA estimations need to be adjusted to account for the SOA from the secondary GLY and MGLY. The predicted monoterpene SOA shows a stronger correlation with the sum of two α-pinene tracers (α-pinT), pinic acid and 3-MBTCA, with R=0.5 and 0.6 for hourly and daily data, respectively. The α-pinT to modeled monoterpene SOA ratios are 0.11-0.16, which generally match the ratio of 0.168±0.081 reported in chamber studies. However, since the current model does not treat α-pinene and its SOA explicitly, future modeling studies should include a more detailed treatment of monoterpene emis-sions and reactions so that the predicted SOA from these important precursors can be directly compared with the ambient precursor-specific SOA-tracers.

12CC.1

Organosulfates in Primary and Secondary Sea Spray Aerosols.

DILINI KIRINDIGODA GAMAGE, Elias Hasenecz, Glorianne Dorcé, Kathryn Mayer, Jon Sauer, Chris Lee, Timothy Bertram, Christopher Cappa, Kimberly Prather, Elizabeth Stone, *University of Iowa*

Organosulfates are components of sea spray aerosols (SSA) that include anthropogenic surfactants and secondary organic aerosol. The composition and abundance of organosulfates in $PM_{2.5}$ nascent and aged sea spray aerosols were determined using liquid chromatography coupled to high resolution and tandem mass spectrometry with negative mode electrospray ionization (MS/MS). Ethylhexyl sulfate ($C_8H_{17}SO_4^-$; 209.0853), dodecyl sulfate ($C_{12}H_{25}SO_4^-$; 265.1479), and tridecyl sulfate ($C_{13}H_{27}SO_4^-$; 279.1636), which are anthropogenic anionic surfactants had the strongest signals among identified organosulfates and had the highest contributions to the bisulfate (*m/z* 97) product ion as determined by precursor-ion MS/MS. Among the 24 quantified organosulfates, dodecyl sulfate was the most abundant organosulfate in both nascent and aged SSA. A homologous series of fatty acid-derived organosulfates, which can be formed through heterogeneous reactions and specific for the marine environment was observed in aged SSA. Isoprene-derived, monoterpene-derived organosulfates, and other organosulfate species derived from unknown sources were also identified in both nascent and aged. The presence of monoterpene-derived organosulfates with a nitroxy functional group ($C_{10}H_{16}NSO_7^-$; 294.0653) in both nascent and aged indicates the role of nitrogen oxides in the marine environment. MS/MS signal abundance of isoprene derived organosulfates (e.g., 2-methyltetrol sulfate, $C_5H_{11}SO_7^-$; *m/z* 215) was greater than monoterpene-derived organosulfates in both nascent and aged SSA. Findings from this study provide insight into the molecular composition of sea spray aerosol and reveal insight to the likely primary and secondary sources of organosulfates in the marine environment.

12CC.2

Synergistic Particle Formation in the Upper Troposphere by Nitric Acid, Sulfuric Acid, and Ammonia.

MINGYI WANG, The CLOUD collaboration, Neil Donahue, *Carnegie Mellon University*

New particle formation in the free troposphere is a major global source of cloud condensation nuclei (CCN). But it remains ambiguous what precursor vapors drive the process in the relatively cold upper troposphere, especially over the tropical convective regions where abundant newly-formed particles have been consistently observed. With experiments performed in the CLOUD chamber at CERN with nitric acid, sulfuric acid, and ammonia levels as well as temperatures characteristic of the upper troposphere, we show that this multicomponent system forms particles synergistically, with formation rates orders of magnitude higher than those from any two of the three components. Particle formation may be ammonia limited in much of the upper troposphere. While the conventional expectation holds that ammonia is efficiently scavenged by cloud and rain droplets during convection, strongly enhanced levels of ammonia and ammonium nitrate are observed in the Asian monsoon upper troposphere. By co-condensing with abundant nitric acid, ammonia can drive the growth of newly-formed ammonium sulfate/nitrate particles to well above CCN size. Our simultaneous ice nucleation ability measurements confirm that these particles are almost all efficient ice nucleus (IN). Further, we present complementary global model and cloud trajectories simulations that corroborate these implications. We show that ammonia can be transported by the convective systems, and subsequently drive intense HNO_3–H_2SO_4–NH_3 nucleation in the Asian monsoon upper troposphere, producing particles that can travel across the mid-latitude Northern Hemisphere.

12CC.3

Measuring Brown Carbon Aerosol Deliquescence: Effect of Reaction Time and Composition. RACHEL M. HESGARD, Ariana Cruz Cruz, Paula K. Hudson, *California State University, Fullerton*

Atmospheric brown carbon (BrC) is a class of light absorbing secondary organic aerosol (SOA), which range in color from light yellow to dark brown. Measuring the hygroscopic properties of atmospheric BrC, and the role of cloud cycling on aerosol hygroscopicity, are essential to understanding the overall effect that BrC aerosol have on climate. To better understand and predict cloud formation properties of BrC, aerosol are generated from aqueous phase laboratory reactions of glyoxal (GX) and glycine (Gly). The composition of the BrC varied in initial reactant composition, using 2:1, 1:1 and 1:2 mole ratios of GX:Gly, and reaction time, after 3, 51, and 165 days of reaction. The water uptake and deliquescence of BrC aerosol was measured using a quartz crystal microbalance (QCM). BrC particles deposited on the quartz crystal are first dried then exposed to increasing relative humidity resulting initially in decreases in crystal oscillation frequency (water adsorption) then increases in oscillation frequency (deliquescence). The effect of cloud cycling on BrC deliquescence was also examined by repeatedly measuring the deliquescence relative humidity (DRH) of an individual BrC sample after drying each time. Although reaction time has a large effect on the light absorption of the BrC aerosol, there is no effect on the measured DRH supporting previous reports of a single BrC product formed from glycine / glyoxal reactions. As expected, DRH increases from 74% to 89% with increasing glycine concentration given the much higher DRH of glycine relative to glyoxal. Similarly, DRH increases from 74% to 85% over five “wet-dry” cycles, suggesting BrC composition becomes more glycine-like due to glyoxal evaporation from aqueous droplets. Results suggest that while reaction time or cloud cycling enhances the warming direct effect of BrC, these processes have no effect, or a negative effect, on cloud formation.

12CC.6

Evaluating Machine Learning Models for Estimating Submicron Aerosol Mixing State at the Global Scale. REETAHAN MUKHOPADHYAY, Zhonghua Zheng, Matthew West, Robert Healy, Laurent Poulain, Valerie Gros, Nicole Riemer, *University of Illinois at Urbana-Champaign*

Aerosol mixing state refers to how different aerosol species are distributed throughout a particle population. It impacts aerosol optical properties and concentrations of both cloud condensation nuclei and ice nuclei and is therefore important for determining the aerosol impact on climate. We can quantify mixing state through a metric known as X (chi), which is based on the mass fractions of aerosol species present in the particles of the population. Mixing state is difficult to represent in current aerosol models, especially on larger scales, due to the high computational cost. Recently, we developed machine-learned emulators for aerosol mixing state that were trained on data from the high-detail particle-resolved model PartMC-MOSAIC, a benchmark for simulating mixing state. While these emulators allow for the efficient prediction of the spatial and temporal distribution of X around the globe, they remain to be validated with observations. In this study, we validated these emulators against observational data from the MEGAPOLI field campaign, which provided single-particle measurements from a site in Paris, France, from mid-January to mid-February 2010. From this observational data, X was directly calculated. We then trained a machine learning model to predict X using extreme gradient boosting (XGBoost) on training data generated with PartMC-MOSAIC. As features, we used quantities that were measured during MEGAPOLI, including the mass concentrations of sulfate, nitrate, ammonium, organic aerosol, and black carbon, concentrations of various VOCs, O3, CO, NO and NOx, as well as temperature and relative humidity. In this poster, we present the validation results and discuss their implications for the use of emulators for predicting global aerosol mixing state based on both experimental observations and Earth system model output.

12CC.7

Sensitivity of the Hydrological Cycle to Aerosol Type and Amount Using High Resolution Weather Research and Forecasting Model over India. SAUVIK SANTRA, Shubha Verma, Roxy Mathew Koll, Olivier Boucher, *Indian Institute of Technology Kharagpur*

An inconsistent prediction of aerosol species distribution over the Indian subcontinent has so far limited the understanding of their potential linkage to the observed regional signals of changing spatial patterns of Indian summer monsoon (ISM) rainfall over the recent years, comprising of both enhancing and weakening effects. The present study is aimed to provide a quantitative prediction of the comparative impact of aerosol types on the changing pattern of ISM rainfall over recent years. Here we show a spatial concordance between the regional signals of ISM rainfall as visualized in the temporal trend (2000-2019) of the Indian Meteorological Department (IMD) ISM observations, the Multi-angle Imaging Spectroradiometer (MISR) aerosol optical depth (AOD), and the adequately simulated aerosol species distribution. The spatial distribution of aerosol species were estimated using constrained aerosol estimation which could well represent the measured values across the Indian subcontinent. We executed high resolution WRF aerosol radiative feedback simulation to examine the governing mechanism to the sensitivity of ISM rainfall regional signals to aerosol species types. A significant increase in rainfall with respect to no aerosol scenario was identified along the western coast of India due to combined aerosols (both anthropogenic and dust), which is notably in line with the current observations of high rainfall incidents over the region. Overall an increase and decrease in the ISM rainfall was observed over the northwestern India region (NWI) and Indo-Gangetic plain (IGP) region respectively, being spatially concordant to respectively abundant dust aerosols and anthropogenic aerosols (mostly sulfate aerosols). The potential governing mechanism to contrasting features of changing ISM rainfall distribution was attributed to the enhanced regional evaporation rate due to dust induced weakening of the surface cooling over the NWI region compared to that due to aerosols induced potential suppression of the effective evaporation over the IGP region.

12CC.8

A Review of Satellite Cloud Condensation Nuclei Retrieval Methods for Evaluation with In-situ Measurements from Aircraft-Based Observations in the Marine Boundary Layer. KEVIN SANCHEZ, David Painemal, Matthew Brown, Ewan Crosbie, Francesca Gallo, Carolyn Jordan, Claire Robinson, Taylor Shingler, Michael Shook, Kenneth Thornhill, Elizabeth Wiggins, Edward Winstead, Luke Ziemba, Bruce Anderson, Richard Moore, *NASA*

Aerosol-cloud interactions are the most uncertain component of the Earth system, due to their major influence on cloud properties, and as a result, Earth's energy budget. We need to better characterize these interactions, which requires constraining the cloud condensation nuclei (CCN) budget and disentangling the influences of aerosol microphysics from meteorology. Observational data are essential for evaluating and improving climate models, but airborne field campaigns have, until recently, been limited to a few (mostly continental) regions worldwide. CCN measurements over the remote ocean are scarce and only occur during extensive field missions involving airborne or ship-based measurements of limited spatial and temporal extent. Polar-orbiting satellite observations hold great promise for expanding the spatial coverage of observations to remote regions, however, it is currently not well understood to what extent these active and passive remote sensing observations can be considered adequate proxies for CCN. Recent literature make use of column integrated retrievals, such as aerosol optical depth or aerosol index, to characterize aerosol concentration and CCN, and the utility of vertically resolved optical properties from active sensors is only now becoming more fully understood. The NASA ACTIVATE, NAAMES, CAMP2EX and ORACLES field campaigns are particularly well suited for evaluating the skill of advanced satellite aerosol and cloud microphysical retrievals, given the comprehensive suite of airborne aerosol, cloud, and trace gas measurements, combined with airborne High Spectral Resolution Lidar (HSRL) and polarimetric imaging instruments that will be the basis for the next generation of space-based remote sensors. Here, we characterize the properties of aerosol and CCN from these NASA field campaigns and critically assess methods for deriving CCN and CCN proxies using visible and infrared satellite remote sensing retrievals.

12CC.9

Physicochemical Properties of Vertically Resolved Aerosols Collected over the Arctic via Tethered Balloon System. NURUN NAHAR LATA, Darielle Dexheimer, Fan Mei, Zezhen Cheng, Rhenton Brimberry, Swarup China, *Michigan Technological University*

The Physicochemical properties of aerosols play a vital role in affecting the Arctic climate via both aerosol-radiation and aerosol-cloud interactions. Though several ground-based observations demonstrate the seasonal variation of Arctic aerosol climatic impacts, the current understanding of the aerosol-cloud interaction in vertically stratified Arctic atmosphere is still limited. Thus, we aim to understand the physicochemical properties, sources, and atmospheric processing of aerosol at different altitudes by investigating ground-based in-situ and remote sensing data, backward trajectory analysis, and off-line size-resolved chemical composition analysis. The vertical profile of the aerosols was studied with the tethered balloon system (TBS), which was deployed at the U.S. Department of Energy Atmospheric Radiation Measurement Program's mobile facility (AMF3) at Oliktok Point, Alaska, on the Arctic Ocean coast. The aerosol sampling was performed at different altitudes, ranging up to 1100 m employing a cascade impactor during August 2019. We perform single-particle analysis using chemical imaging and multi-modal micro-spectroscopy techniques such as computer-controlled scanning electron microscopy with energy-dispersive X-ray spectroscopy (CCSEM/EDX), transmission electron microscopy (TEM) and scanning transmission X-ray microscopy with near-edge X-ray absorption fine structure spectroscopy (STXM/NEXAFS). Aerosol chemical compositions observed by TBS showed a clear temporal and spatial variation. Wider size distribution of the particles at high-altitude was observed compared with that of low-altitude particles on the same sampling day. A relatively higher percent of sulfate and sulfate coated dust aerosols were observed at higher altitudes, suggesting the possibility of cloud processing of aerosols. Altogether, the findings from this study will improve the understanding of the implication of Arctic aerosol on Arctic cloud formation and radiative properties.

12CC.10

New Particle Formation during the CAMP2Ex Campaign: Statistics and Impact of Emission Sources. QIAN XIAO, Jiaoshi Zhang, Yang Wang, Luke Ziemba, Ewan Crosbie, Edward Winstead, Claire Robinson, Jeffrey Reid, Josh DiGangi, Glenn Diskin, Sebastian Schmidt, Armin Sorooshian, Miguel Hilario, Sara Woods, Paul Lawson, Ryan Bennett, Jian Wang, *Washington University in St. Louis*

Nucleation and subsequent growth of new particles occur frequently within the upper troposphere over tropical oceans, and this new particle formation (NPF) presents a globally important source of cloud condensation nuclei (CCN). However, there have been few studies of NPF at lower altitudes over the tropical oceans. In addition, the impact of anthropogenic emissions and biomass burning on the NPF remains unclear. In this study, we examine NPF in lower and mid troposphere in Southeast Asia using airborne measurements during the recent the Cloud, Aerosol and Monsoon Processes Philippines Experiment (CAMP^{2}Ex). CAMP2Ex took place from 25 August through 5 October 2019, including both late southwest and early northeast monsoon phases. Recent NPF events, as evidenced by elevated concentrations of newly formed particles (i.e., particles with diameter between 3 and 10 nm), were observed during 4% of the total flight time (5 out of 128 hours). The frequency of NPF increases with altitude, reaching 49% above altitude of 8000 m. All NPF was observed at altitude above 3000 m and coincided with elevated RH, suggesting that new particles were formed in the outflow of convective clouds, where both the temperature and existing particle surface area are low. Based on trace gas measurements, airmasses are categorized as background, biomass burning, and pollution. Under the background condition, the highest concentrations of newly formed particles were mostly observed above 8 km. Weaker NPF was observed at lower altitudes under the background condition. Below 8 km, NPF mostly occurred in airmasses influenced by biomass burning or pollution and was facilitated by enhanced radiation contributed by clouds. NPF was more frequent during the more convectively active southwest monsoon period than more quiescent northeast monsoon, again indicating the impact of airmass origin and convective activities on the NPF in the lower to mid troposphere in the region.

12CC.11

Entrainment of Long-Range Transported Aerosols in the Marine Boundary Layer in the Azores. SHREYA JOSHI, Paulo Fialho, Diamantino Henriques, Renato Pinto Reveggino, Andrea Baccarini, Silvia Henning, Birgit Wehner, Lynn Mazzoleni, Simeon Schum, Bo Zhang, Raymond Shaw, Jian Wang, Claudio Mazzoleni, *Michigan Technological University*

Atmospheric aerosols have significant impacts on Earth’s radiation budget by interacting with solar radiation and by affecting the properties of clouds. Aerosols can be transported over long distances in the free troposphere to remote regions such as the Azores, in the mid-North Atlantic ocean. Free-tropospheric long-range transported aerosols like Saharan desert dust or North-American biomass burning carbonaceous particles can contribute to the aerosol loading and properties in this region. We analyzed data from two sites in the Azores: (a) Pico mountain observatory at 2225 m a.s.l., and (b) Eastern North Atlantic (ENA) DOE-ARM facility, near sea level. The two sites are within a horizontal distance of 70 km from each other. Pico generally lies in the lower free troposphere, while ENA lies in the lower marine boundary layer. These sites provide a unique opportunity for the analysis of aerosols at two different elevations. Aerosol properties from these facilities are used to understand the statistical and mechanistic connections between the aerosol properties in the free troposphere and those in the boundary layer and their potential effects on clouds and radiation. We used continuous aerosol data (e.g., light scattering, and absorption) at the two sites to detect possible events of entrainment of free tropospheric aerosols into the boundary layer. Candidate events were studied in more detail including determining their frequency, and duration. We will discuss these analyses and links between these events and the cloud condensation nuclei concentrations at the two sites, as well as, the properties of the stratocumulus clouds in the region.

12SA.3

Comprehensive Analysis of Marine Particulate Matter Impacts to Atmospheric Pollution in Coastal Communities. RYAN DROVER, David R. Cocker III, J. Wayne Miller, *University of California, Riverside*

Marine shipping is the most efficient mode of transporting goods, with 90% of global merchandise transported by sea. However, ocean-going vessels (OGVs) used for transportation are significant emitters of criteria pollutants. Port and coastal communities bear the impacts of these emissions, in addition to inland environments such as the Southern California Air Basin (SCAB), as OGVs navigate near coastlines as they follow major shipping lanes. 70% of ship-related emissions occurring within 216 nautical miles of the coastline; pollutant contributions include that marine vessel traffic produces nearly 75% of NOx emissions in Santa Barbara County, California. Additionally, estimates of particulate matter (PM) and NOx presence using emission factors on OGVs underpredict emissions as compared to on-ship measurements. Evolution of engine technology, marine oil and fuel composition changes, control methods including vessel speed reduction, and the use of emissions control technology further motivate the need to continue to update accounting of OGV emissions. As trade volume continues to increase, contributing to as well as interacting with a changing urban aerosol environment, marine emissions continue to be a segment of importance.

PM emissions, in addition to gaseous and pollutant speciation, were measured from 60 in-use marine engines on a wide range of vessels over numerous sampling campaigns. The measurements have been used in this exploration of the evolution of emissions from the shipping industry and its relationship to coastal urban air quality. This work aimed to characterize and quantify anthropogenic marine source contributions to PM in coastal urban air and identified trends and impact through the proportional contribution of marine emissions, including addressing mitigation strategies. Near-shore shipping emissions have an effect on the volume and composition of regional PM and gaseous components, and may also enhance new particle formation in coastal and inland urban areas.

12SA.5

Quantifying Linear and Non-Linear Influences of Aerosol Precursor Emissions on Pollutant Concentrations Using CMAQ-hyd.

JIACHEN LIU, Eric Chen, Ryan Russell, Shannon Capps, *Drexel University*

Chemical transport models (CTMs) are essential assets to understand complex physico-chemical reactions in the atmosphere. They provide estimates of concentrations of air pollutants based on emissions and meteorological parameters. Sensitivity analysis in CTMs has helped researchers determine the uncertainty in the CTMs and make policy recommendations. The simplest method to compute sensitivity coefficients is the finite difference method (FDM). The sensitivity coefficients are calculated by running the model multiple times with incremental values for the input variable of interest. However, this method suffers from truncation (i.e., ignoring higher-order terms) and cancellation errors (i.e., numerical issues caused by subtracting two very close numbers). The truncation error can be minimized by taking smaller perturbation step, thus eliminating the impact of higher-order sensitivity terms on the first-order result. However, the cancellation error will dominate if the perturbation step is too small. Other methods, including the direct decoupled method (DDM) and the adjoint method, involve formulating new forward sensitivity or adjoint equations to the CTM. When the CTM is updated, new equations must be modified manually, thus reducing their applicability in various complex CTMs. Here, we propose an alternate approach for sensitivity coefficient calculations in CTMs: the hyperdual number approach (Fike et al., 2011). Instead of a real number perturbation in the FDM, we applied a hyperdual perturbation to the emission variable of interest. The method is more accurate and does not depend on the perturbation step size. The method is also easier to implement compared to the DDM and the adjoint method. We applied this method in the Community Multiscale Air Quality (CMAQ) model v.5.3 to formulate the CMAQ-hyd model. We have calculated the exact first- and second-order sensitivities of aerosol and gas concentrations to select aerosol precursor emissions based on this new method.

12SA.6

Real-time Source Apportionment of Organic Aerosols in Three European Cities.

GANG CHEN, Francesco Canonaco, Jay G. Slowik, Kaspar R. Daellenbach, Iasonas Stavroulas, Nikolaos Mihalopoulos, Evangelos Gerasopoulos, Jean-Eudes Petit, Olivier Favez, Urs Baltensperger, André S. H. Prévôt, *Paul Scherrer Institute*

Currently, European countries are still suffering from poor air quality: 70% of air quality monitoring stations within Europe exceed the annual $PM_{2.5}$ value of the WHO guidelines (10 $\mu g/m^3$). Considering organic aerosol (OA) is one of the major air pollutants, the knowledge of OA sources is crucial for policymakers to design effective mitigation strategies.

Positive matrix factorization (PMF) on Aerosol Mass Spectrometer (AMS) data is still the most common technique to conduct source apportionment (SA) analyses. However, conventional PMF suffers mostly from rotational ambiguity and a high degree of subjectiveness from the analyst, which prevents from providing high-quality information in near real-time. To overcome these disadvantages, we propose a novel and innovative real-time SA methodology. In addition to running PMF (rolling PMF) for a short time window in the order of 1-2 weeks with a small step (one day or few hours), we assess source loading in real-time for the latest scan by performing chemical mass balance (CMB).

To test this concept of real-time SA technique, we will conduct rolling PMF analyses by following a standardized protocol on three ACSM datasets collected in Athens, Paris, and Zurich. Then, we will compare CMB results and rolling results in many aspects (time series, relative contributions, and factor profiles) to investigate the performance of the real-time approach. So far, we found that it showed a good agreement (R2 >0.94) between the time series of resolved factors from CMB and rolling results using Athens ACSM data.

This project's success will minimize user interactions and subjective judgments and provide up-to-date, trustable information for policymakers and air quality modellers. Finally, reliable SA results in real-time pave the way for air quality forecast, especially relevant for safeguarding public health in megacities.

12SA.8

Using Constrained Source Apportionment to Characterize Water Soluble Brown Carbon in Los Angeles Summertime Organic Aerosol.

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Water soluble brown carbon (WS-BrC) and non-refractory aerosol chemical composition were quantified across two summers in Claremont, CA using collocated instruments. Claremont is located approximately 30 miles east of downtown Los Angeles in the foothills of the San Gabriel mountains. A Brechtel Particle-Into-Liquid Sampler (PILS) in series with a UV/visible wave-guide spectrometer (LWCC) and GE Analytical Total Organic Carbon Analyzer (TOC) provides continuous measurements of WS-BrC in PM1 at one minute resolution while an Aerodyne quadrupole Aerosol Chemical Speciation Monitor provides non-refractory PM1 organic and inorganic aerosol composition and loading every 10-15 minutes. Organic aerosol concentration obtained from the ACSM is well correlated to water-soluble OC and source apportionment of the OM show that a large fraction is secondary (OOA type I or II). WS-BrC was characterized by wavelength-dependent absorbance measurements from 300-700 nm, allowing more detailed analysis than a single-wavelength approach. Aerosol absorptivity at 365 nm is greatest in the morning, like HOA, with afternoon SOA formation appearing to dilute the absorptivity by the addition of non-absorbing OOA. However, absorptivity is only mildly correlated to HOA fraction of OM, indicating that a more complex set of processes governs its formation during these periods in Los Angeles. To deconvolute the observed absorbance, ACSM-derived organic aerosol spectra were first processed using the multi-linear engine (ME-2) in SoFi (Datalystica). We explored a range of model solutions from 3-6 factors. These model solutions were then used as constraints on a second factor analysis, targeting the wavelength-dependent absorbance time series. With some variation, most solutions indicate that we observed factors characterized by strong UV and weak visible absorbance (“non-absorbing”), strong UV absorbance with a tail of absorbance extending into the visible region (“typical BrC”), and a wavelength-independent BrC factor, with modest, constant absorbance extending beyond 400nm. Preliminary analysis suggests that although most WS-BrC is connected to rapidly forming chromophores associated with HOA type aerosol, other sources of WS-BrC contribute to the total observed signal in the Los Angeles basin.

12SA.9

Impacts of Stay-at-home Orders on Ozone in California Using an Ozone Source Apportionment Technique.

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The outbreak of the 2019 coronavirus disease (COVID-19) has posed great challenge on public safety and economics globally. However, it also brought an opportunity for researchers to study the outcome of reduced human activities.

California issued a COVID-19 shelter-in-place order asking people to stay at home between March 19 – May 8, 2020. Personal mobility decreased significantly during this period leading to generally improved air quality across the state. Several studies have found that monthly-average concentration of nitrogen dioxide (NO_2) and airborne particulate matter (PM) decreased relative to levels in the previous years, but the effects on ozone (O_3) are mixed. In the Los Angeles area, the 8-hr daily maximum O_3 concentration increased rather than decreased.

Multiple factors could have contributed to the increased O_3 concentrations during spring 2020, including NOx disbenefit and unfavorable meteorological conditions. Previous model simulations have great uncertainty when predicting the root cause because they lack direct measurements to confirm O_3 response to NOx and VOC perturbations. Here we address this shortcoming by performing the first direct comparison between predicted and measured O_3 response to NOx and VOC perturbations. Chemical transport model (CTM) predictions for O_3 sensitivity will be compared to direct chamber measurements carried out for multiple months at Sacramento, California, during the year 2020. CTM predictions will also be compared to TROPOMI satellite measurements of $HCHO/NO_2$ as an indirect measure of O_3 sensitivity to NOx and VOC perturbations across the entire state of California. Changes to the 2020 emission inventory due to COVID-19 impacts are estimated by adjusting emissions in several sectors: on-road vehicles, air traffic, restaurants, rail and freight transport to estimate the emissions affected by the pandemic. Source apportionment algorithms built into the CTM will quantify NOx and VOC sources that contribute to O_3 formation in the presence of these changes. The combined CTM predictions and direct measurements will identify the source contributions to O_3 formation from different emission sectors under the altered COVID-19 conditions. The results will provide new strong guidance for future emissions control strategies to reduce O_3 in California.

12SA.10

Quantitative Source Apportionment of Organic Aerosol by Combined Factor Analysis: Extractive Electrospray Ionization and Aerosol Time-of-Flight Mass Spectrometry (EESI-TOF/AMS). Yandong Tong, Lu Qi, Giulia Stefenelli, Dongyu S. Wang, Francesco Canonaco, Urs Baltensperger, André S. H. Prévôt, JAY G. SLOWIK, *Paul Scherrer Institute*

Primary and secondary organic aerosol (POA and SOA) are significant components of aerosol pollution and are linked to adverse health effects. Efficient mitigation strategies require quantitative characterization of POA and SOA sources. Although the aerosol mass spectrometer (AMS) has proven to be a reliable method for quantitative source apportionment of POA, it usually lacks the chemical resolution to distinguish different SOA sources due to its extensive thermal decomposition and ionization-induced fragmentation. In contrast, softer ionization techniques such as extractive electrospray ionization time-of-flight mass spectrometry (EESI-TOF) or chemical ionization mass spectrometry (e.g., FIGAERO-CIMS) have the chemical resolution to resolve SOA sources, but are unable to provide quantitative results due to uncertainties in molecule-dependent sensitivities.

Here we introduce a method for quantitative source apportionment of the total organic aerosol, including both POA and SOA sources, by conducting positive matrix factorization (PMF) on a single dataset including both AMS and EESI-TOF mass spectra. Because each factor profile includes both AMS and EESI-TOF components, quantitative mass concentrations and EESI-TOF factor sensitivities are direct outputs of the mode. In this way, the model optimally combines the strengths of the AMS (quantification) and EESI-TOF (chemical resolution). We demonstrate the model's ability to incorporate factors detectable by only a single instrument vs. both instruments, incorporate profile constraints for selected factors, and provide uncertainty analysis.

The combined PMF method is applied to summer and winter datasets from Zurich, Switzerland. Resolved sources include traffic, cooking, biomass burning, and cigarette smoke POA, as well as SOA from daytime and nighttime oxidation of biogenic emissions and biomass burning. The retrieved EESI-TOF sensitivities agree well with measurements of chemical standards, laboratory-generated SOA from known precursors, and parameterizations based on the chemical formulae of molecular ions. Comparison of these results to standalone EESI-TOF PMF highlights the importance of accounting for factor-dependent sensitivities.

12SA.11

Chemical Characterization of Organic Nitrogen Aerosol Particles from Prescribed Burns of U.S. Wildland Forests. FARRAH HAERI, Daniel Foster, Deep Sengupta, Afsara Tasnia, Paul Van Rooy, Nathan Kreisberg, Scott Stephens, John Battles, Robert York, Kelley Barsanti, Allen Goldstein, Coty Jen, *Carnegie Mellon University*

A significant source of organic nitrogen (ON) compounds in the atmosphere are emitted from biomass burning (BB) events, including wildfires. ON compounds can absorb light, contributing to a warming climate, or deposit onto land and oceans resulting in disruptions of the nitrogen cycle. As wildfire frequency increases in the western U.S., prescribed burning is being implemented U.S. wildlands to reduce fuel loading and thus the probability of high-intensity wildfires. However, the implications of these prescribed burning emissions on air quality or environment are not well characterized, especially in regard to the ON contribution from prescribed burning emissions. Thus, to understand the impact large-scale prescribe burning has regional air quality, the chemical composition of ON compounds from prescribed burning emissions needs to be examined.

For this study, we chemically characterize and quantify emission factors (EF) of ON compounds from freshly emitted smoke $PM_{2.5}$ particles, collected via Sequential Spot Sampler, during prescribed burns (in collaboration with University of California, Berkley (UCB) and Riverside (UCR) at Blodgett Forest Research Station (Georgetown, CA)) using a high-performance liquid chromatographers (HPLC) coupled to an orbitrap mass spectrometer. We find that speciated ON compounds' (amino acids, nitro vanillin, and nitrocatechols) EF is correlated with the modified combustion efficiency and reflects the prevalence of ON compounds in less efficient burning conditions in the field. In addition, smoke particles were collected downstream of the burn at nighttime compared to near the burn during the day. Certain compounds, such as amino acids, were observed to have higher EFs during nighttime smoldering compared to daytime active burning, suggesting a difference between day and nighttime smoke emissions for ON compounds. Results from this study can be applied toward linking the effects ON compounds from prescribed burning have on the atmosphere and climate.

12SW.1

Lessons Learned from Deployment of a Novel Multiwavelength Photoacoustic Spectrometer to FIREX-AQ.

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The Multiwavelength Integrated Photoacoustic-Nephelometer (MIPN) is a field-portable, in situ, real-time, contact-free instrument designed for laboratory and field measurements of brown carbon (BrC) aerosol by targeting relevant wavelengths where BrC is known to absorb. A prototype MIPN (MIPN v1) was deployed to the FIREX-AQ field campaign where it measured light absorption by wildfire aerosols in the western United States in August 2019. As with many prototype instruments, the MIPN v1 had successes and failures during its first deployment which informed the next iteration of refinements, culminating in a modified MIPN v2.

During FIREX-AQ, The MIPN v1 measured light absorption by wildfire aerosols in parallel with a variety of instrumentation aboard the Aerodyne Mobile Laboratory. The month-long field campaign in this dynamic environment revealed several opportunities for improvement. Among the refinements are a modernized absorption sensor design, real-time self-diagnostics and internal monitoring, and a robust demodulation algorithm for recovering multiwavelength signals simultaneously. We present the motivation, design, construction, deployment, and refinement of the MIPN v2, focusing on specific upgrades made to the optoacoustic cavity and absorption sensors. Various quality-of-life upgrades to make the instrument more robust for field operation are also discussed within the context of results from the first deployment of the MIPN v1 to the field. A full characterization of the MIPN v2 will also be presented, and we will conclude with discussion on its use in future field campaigns.

12SW.2

Submicron Particle Composition and Acidity in Fire Plumes during FIREX-AQ Aircraft Study.

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During the Fire Influence on Regional to Global Environments and Air Quality (FIREX-AQ) aircraft study, the chemical composition of fire-emitted submicron particles was quantified with a High-Resolution Aerosol Mass Spectrometer (AMS). The western US wildfire particles show similar composition across the plumes and are overwhelmingly dominated by organic aerosol (OA). The agricultural fires sampled in the eastern US show larger variability in particle composition with a higher inorganic fraction, in particular Cl and K. Fast (up to 5Hz) measurements of K in fire plumes, which show excellent correlation with collocated IC filter measurements, allow a quantitative closure of the particle ion balance. Although lab experiments suggest variable AMS instrumental response of K for several K inorganic salts, field observations indicate a uniform response for fresh fire-emitted particles dominated by OA. AMS sulfate in some fresh biomass burning plumes had major contributions from organosulfur species, in contrast with typically a few percent in the regional background air. The AMS inorganic-only SO_4 agrees better with IC sulfate, as expected. The organosulfur appears to be dominantly primary for a similar aging profile with a PMF primary factor and the evidence from lab studies (FLAME-III). Ultrahigh-resolution analysis of FIREX-AQ filter samples is used to aid in the identification of the organosulfur species that include both organosulfonates and organosulfates. Lastly, we use thermodynamic models to estimate aerosol pH, an important lever on many particulate physical and chemical processes, based on AMS-quantified K, inorganic-only SO_4, NO_3, and collocated gas-phase NH_3 and HNO_3 measurements. The gas-particle partitioning was reasonably reproduced by the model. We find that fresh western biomass burning submicron particles had near-neutral pH (on average ~6-7), which was buffered by high levels of NH_3 and contrasts with regional background particles with moderate acidity (pH~2-3) and remote oceanic particles (pH~0).

12SW.3

A Bird's Eye View of Sampling Forest Fire Smoke: Using Drone-Based Measurements of Prescribed Burning to Help Close the Gap between Laboratory and Wild-Fire Smoke Studies. NATHAN KREISBERG, Deep Sengupta, Robert Weber, James D.A. Butler, Yutong Liang, Paul Van Rooy, Afsara Tasnia, Farrah Haeri, Coty Jen, Emre Ozen, Edward Gonzalez, Jason Kriesel, Kevin K. Schwarm, Daniel Foster, Rebecca A. Sugrue, Mitchell R. Spearrin, Thomas W. Kirchstetter, Kelley Barsanti, Allen Goldstein, *Aerosol Dynamics Inc.*

The incidence of forest fires in the western US is predicted to increase from ongoing changes in climate leading to an increased need to understand the atmospheric burden of biomass burning. The use of prescribed burns to reduce excess fuel loads is also likely to greatly increase to compensate for the historic preference to suppress fires of all sizes. Laboratory based studies to characterize the specific types of emissions from various fuel types (e.g., trees, shrubs and grasses) has led to inventories of chemical emission factors under small scale and necessarily simplified combustion conditions practicably achievable.

Prescribed burns can serve to help close the gap between somewhat artificial laboratory studies and uncontrolled wildfires if the differences in fuels and fire state (flame vs smolder) between them can be sufficiently characterized. A near perfect opportunity to explore this approach occurred at the Blodgett Forest Research Station where an ongoing forest management study involved the use of prescribed burns for comparison with alternative management techniques. Located in the Sierra foothills near the El Dorado National Forest, the Blodgett forest is mixed conifer forest that has not experienced fire for 100 years and thus fairly represents a large portion of the western US national and state forests.

A sample collection and sensor laden drone package was designed, built, and deployed between April 20th and 23rd, 2021 as part of the scheduled prescribed burns. A unique aspect of this study is the pre- and post-burn fuel inventory conducted by UCB that offers the prospect of tying specific smoke plumes sampled with known fuel types consumed by fire. Both particulate and gas samples were acquired in conjunction with real-time gas (CO2, CO and NO) and BC measurements gathered at 1Hz throughout each flight. The samples will be analyzed by multi-dimensional GCMS while the real-time measurements provide a means of estimating specific emission factors for individual compounds while also providing insights into the plume structures themselves. Supplemental visual/thermal and high temporal resolution CO measurements were conducted on two additional drones. Initial findings of this multi-drone sampling strategy will be reported with examples of the real-time sensor and imaging data.

12SW.4

Size Distributions of Biomass Burning Aerosol as a Function of Age and Comparisons to Models. GREGORY SCHILL, Karl D. Froyd, Daniel Murphy, Charles Brock, Christina Williamson, Agnieszka Kupc, Eric Ray, Huisheng Bian, Mian Chin, Peter Colarco, *NOAA ESRL and CIRES, University of Colorado Boulder*

We have recently developed a new technique to couple single-particle mass spectrometry data with concurrently measured quantitative size distributions. This allows us to determine the size distribution of different particle types (e.g., sea salt, dust, biomass burning). Using data from the NASA ATmospheric tomography missions (ATom), Studies of Emissions, Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC4RS), Deep Convective Clouds and Chemistry Project (DC3), and Mid-latitude Airborne Cirrus Properties Experiment (MACPEX) field missions, we present size distributions of biomass burning aerosol as a function of age. Missions were chosen to represent fresh wildfire plumes, background continental air, remote tropospheric air, and stratospheric air.

We employ several metrics of age including gas phase tracers, their ratios, and back trajectory products. Additionally, subcomponents of biomass burning aerosol, including organic-to-sulfate mass ratios, were analyzed as a function of size and age. These results are then compared to output from global chemistry/climate models with aerosol modules, including the Goddard Earth Observing System Model (GEOS) coupled to the Goddard Chemistry Aerosol Radiation and Transport (GOCART) aerosol module or the 7-mode Modal Aerosol Model (MAM7). In particular, the shape of the measured size distributions will be compared to parameters prescribed or output by the model. Additionally direct comparisons of extinction calculated in the model and it situ measurements of biomass burning only extinction are compared as a function of age for both dry and wet conditions.

12SW.6
Mixing State of Urban Aerosol under the Influences of Biomass Burning and Transboundary Smoke Haze in Southeast Asia. LAURA-HELENA RIVELLINI, Nethmi Kasthuriarachchi, Mutian Ma, Alex Lee, *National University of Singapore*

Biomass burning (BB) emissions from forest and tropical peat lands strongly impact air quality in Southeast Asia. BB emissions can mix with urban pollutants and undergo atmospheric aging, leading to a complex mixture of transboundary haze. Advanced understanding on aerosol mixing state can provide insight into resolving aging processes that can significantly impact the aerosol properties of BB emissions. In this study, a soot-particle aerosol mass spectrometer (SP-AMS) was deployed in Singapore during the northeast (NEM) and southwest (SWM) monsoons in 2019. The SP-AMS was operated with dual vaporizers to measure chemical composition and size distribution of non-refractory (inorganic and organic) and refractory (black carbon and metals) particulate matter in bulk and single-particle scales. Positive matrix factorization (PMF) of bulk organic aerosol (OA) data evidences the occasional influences of relatively fresh biomass burning OA (BBOA) during the NEM. Single particle characterization shows that potassium-rich (i.e. an indicator of flaming fire emissions) and a few types of OA-rich particles (e.g. Heavy molecular weight, hydrocarbon-like and cooking OA) had moderate correlations with BBOA factor identified by PMF. In particular, the diel cycles of these OA-rich particles depict higher concentrations with BBOA between 2am and 6am, suggesting a potential mixing of BB emissions on urban primary OA. The intense transboundary smoke haze caused by Indonesian wildfires during the SWM period resulted in high concentrations of highly oxygenated haze-related OA factor, and two major types of sulfate and OA internally mixed particles were observed. The first composed of a higher OA content (~50wt%, SO4~30wt%) and had moderate correlations with the haze-related OAs, highlighting the importance of sulfate chemistry on aging of regional peat fires emissions. In contrast, the second had a higher sulfate content (~50wt%, OA~25wt%) with a smaller peak diameter, which is probably formed locally by oxidation of mixed biogenic and industrial emissions.