Towards a Molecular-Level Understanding of Atmospheric Aerosols

MUOAA 2026

19–22 May 2026
Montréal, Canada

Conference venue: Otto Maass Chemistry Building
McGill University Downtown Campus

muoaa2026.sciencesconf.org

Conference Program

Schedule

All oral presentations will take place in Otto Maass 217. Poster sessions will take place in the lobby of the Otto Maass Chemistry Building.

	Tue 19-May	**Wed 20-May**	**Thu 21-May**	**Fri 22-May**
Session Chair	Nicole Riemer	Manabu Shiraiwa	Rachel O'Brien	Bryan Bzdek
Discussion Leader	**Viscosity - Cari Dutcher**	**SOA - Sergey Nizkorodov**	**BrC/BBOA - Alex Laskin**	**OA - Christian George**
8:50	Conference Intro			Future Plans
9:00	Theme Introduction	Theme Introduction	Theme Introduction	Theme Introduction
9:10	*Allan Bertram*	*Barbara Finlayson-Pitts*	*Nadine Borduas-Dedekind*	*Thomas Berkemeier*
9:50	*Veronique Perraud*	*Rachel O'Brien*	*Michael Cotterell*	*Lisa Wingen*
10:10	*Kristen Johnson*	*Kangwei Li*	*Stephanie Jones*	*Natasha Garner*
10:20		*Madeline Cooke*		
10:30	Break	Break	Break	Break
11:00	*Manabu Shiraiwa*	*ManNin Chan*	*Sergey Nizkorodov*	*Alex Laskin*
11:20	*Paul Ohno*	*Chris Kenseth*	*Zac Liang*	*Parisa Ariya*
11:30			*Fengxia Bao*	
11:40	Discussion	Discussion	Discussion	Discussion
12:00	Lunch	Lunch	Lunch	Lunch
Session Chair	Tara Kahan	Parisa Ariya	Chris Johnson	
Discussion Leader	**INP/Nuc - Miriam Freedman**	**Interfacial - Kevin Wilson**	**Trapping - Leisner**	
14:00	Theme Introduction	Theme Introduction	Theme Introduction	
14:10	*Ellie Browne*	*Markus Ammann*	*James Davies*	
14:50	*Chris Johnson*	*Cari Dutcher*	*Michael Jacobs*	
15:10	Break	Break	Break	
15:30	*Thomas Leisner*	*Tara Kahan*	*Paul Tumminello*	
15:40			*Nicolas Fauré*	
15:50	*Nicole Riemer*	*Christian George*	*Bryan Bzdek*	
16:10	*Celine Toubin*	*Patrick Hayes*	*Lexi Deal*	
16:30	Discussion	Discussion	Discussion	
16:50		Poster Intros	Poster Intros	
17:00		**Posters #1**	**Posters #2**	
18:00				
18:30	Dinner	Dinner	Dinner	

Contents

Welcome and Overview

Towards a Molecular-Level Understanding of Atmospheric Aerosols (MUOAA 2026) convenes scientists who study aerosols from the molecular scale to the global scale through laboratory experiments, field campaigns, and advanced modeling. The meeting highlights recent advances in new-particle formation; internal structure and phase behavior; heterogeneous and multiphase photochemistry; gas–surface interactions; ice and cloud nucleation; optical properties; and bioaerosols.

Program at a Glance

Date	Main activities
Tue., 19 May	Opening sessions; morning and afternoon theme sessions; discussion periods; dinner.
Wed., 20 May	Morning and afternoon theme sessions; poster introductions; Poster Session #1; dinner.
Thu., 21 May	Morning and afternoon theme sessions; poster introductions; Poster Session #2; dinner.
Fri., 22 May	Morning theme session; discussion; lunch and departure.

Invited Contributions and Session Format

Plenary speakers will have 35 minutes for their presentations, followed by 5 minutes for questions. Contributed talks by senior and early career researchers are planned for 15–20 minutes or 8–10 minutes (see Schedule). Session chairs and discussion leaders will structure each session to include theme introductions, plenary talks, contributed talks, and summary discussion periods.

Plenary Speakers

Speaker	Affiliation
Allan Bertram	University of British Columbia
Barbara Finlayson-Pitts	University of California, Irvine
Nadine Borduas-Dedekind	University of British Columbia
Thomas Berkemeier	Max Planck Institute for Chemistry, Mainz
Ellie Browne	University of Colorado Boulder
Markus Ammann	Paul Scherrer Institute, Switzerland
James F. Davies	University of California, Riverside

Discussion Leaders

Discussion leader	Affiliation
Cari S. Dutcher	University of Minnesota, Twin Cities
Sergey A. Nizkorodov	University of California, Irvine
Alex Laskin	Purdue University
Christian George	CNRS / IRCELYON, Université Lyon 1
Miriam Freedman	Pennsylvania State University
Kevin R. Wilson	Lawrence Berkeley National Laboratory
Thomas Leisner	Karlsruhe Institute of Technology

Session Chairs

Session chair	Affiliation
Nicole Riemer	University of Illinois at Urbana–Champaign
Manabu Shiraiwa	University of California, Irvine
Rachel O'Brien	University of Michigan
Bryan R. Bzdek	University of Bristol
Tara Kahan	University of Saskatchewan
Parisa Ariya	McGill University
Christopher J. Johnson	Stony Brook University

Poster Sessions

Date	Time	Activity
Wednesday, 20 May	16:50	Poster introductions
Wednesday, 20 May	17:00	Poster Session #1
Thursday, 21 May	16:50	Poster introductions
Thursday, 21 May	17:00	Poster Session #2

Poster boards support sizes up to 4 ft × 6 ft.

Organizing Committee

Name	Affiliation and contact
Miriam J. Freedman	Department of Chemistry, The Pennsylvania State University, University Park, PA, USA; maf43@psu.edu
Andrew B. Ault	Department of Chemistry, University of Michigan, Ann Arbor, MI, USA; aulta@umich.edu
Thomas C. Preston	Department of Chemistry and Department of Atmospheric & Oceanic Sciences, McGill University, Montréal, QC, Canada; thomas.preston@mcgill.ca
Andreas Zuend	Department of Atmospheric & Oceanic Sciences, McGill University, Montréal, QC, Canada; andreas.zuend@mcgill.ca

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Abstracts

Oral Presentation Abstracts

O-01 Viscosity, phase state, and tar ball characteristics of biomass burning organic aerosol

Tuesday, 19 May, 9:10 am

Presenter: Allan Bertram
Authors: Allan Bertram[1]

[1] University of British Columbia, Canada

Wildfires are a major source of atmospheric organic aerosol, commonly referred to as biomass burning organic aerosol (BBOA). The viscosity and phase state of BBOA strongly influence gas particle partitioning, heterogeneous chemistry, cloud interactions, and climate impacts, yet remain poorly constrained. Here, we quantify the viscosity of wildfire-derived BBOA using the poke flow technique, fluorescence recovery after photobleaching, and coalescence relaxation times measured with electron microscopy. We examine four classes of BBOA: primary BBOA, aged primary BBOA, secondary BBOA, and mixtures of aged primary and secondary BBOA. The viscosity of primary organic aerosol varies by more than seven orders of magnitude, depending on burn stage and whether leaves or wood are used as fuel. For pine wood BBOA, both UV-driven aging and OH oxidation increase viscosity by six or more orders of magnitude, transforming initially semisolid material into a glassy state after approximately 9 days and 5 days of atmospheric aging, respectively. Secondary BBOA generated via OH and O_3 oxidation exhibits high viscosity under dry conditions, whereas secondary BBOA generated via NO_3 radical chemistry remains highly viscous even at elevated relative humidities. We further show that secondary BBOA generated from NO_3 radicals meets key criteria for classification as tar balls. These particles are spherical, contain brown carbon, and exhibit viscosities exceeding 2×10^{11} Pa s under dry conditions, remaining above 2×10^{9} Pa s at elevated relative humidities. Chemical markers identified in laboratory-generated NO_3 BBOA are also observed in nighttime wildfire smoke samples. Together, these results demonstrate that aging processes and fuel-dependent combustion conditions strongly alter the physical state of BBOA, with possible implications for ice nucleation, gas-particle equilibration timescales, and brown carbon lifetimes.

Keywords: Biomass burning organic aerosol, viscosity, phase state, tar balls

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O-02 Elucidation of the composition and stability of methanesulfonic acid – amine nanoclusters using ion mobility mass spectrometry

Tuesday, 19 May, 9:50 am

Presenter: Véronique Perraud
Authors: Véronique Perraud[1]; Colleen Miller[1]; Paul Bauer[1]; Ivo Neefjes[2]; Dina Alfaouri[2]; Nanna Myllys[2]; James Smith[1]; Barbara Finlayson-Pitts[1]

[1] University of California, Irvine, United States
[2] University of Helsinki, Finland

New particle formation (NPF) from gaseous precursors has been recognized as a source of a large fraction of cloud condensation nuclei in ambient air. However, our understanding of the species and processes responsible for nucleation and the early stages of the growth of aerosol nanoclusters from 1 to 10 nm is still uncertain. One mechanism of interest is acid-base chemistry. While NPF has often been associated with H_2SO_4, there is growing evidence that methanesulfonic acid (MSA) can also play a key role. Ambient MSA concentrations can be 10-100% that of H_2SO_4 in air, and the relative contribution of MSA to NPF may increase in the future due to a decline in anthropogenic fossil-fuel derived SO_2 worldwide. In addition,

biogenic sources for MSA are expected to increase due to rising global sea water surface temperatures, leading to increases in phytoplankton activity and a higher frequency and intensity of wildfires, both of which are associated with a higher production of its precursor dimethyl sulfide. Previous flow reactor experiments showed that MSA can nucleate new particles efficiently with atmospherically relevant amines, especially if they have strong hydrogen bond-forming capability, e.g. primary amines and alkanolamines. The chemical composition of the nanoparticles was successfully determined down to 4 nm, showing in one case (i.e. methylamine) a size dependent acid-to-base molar ratio. However, smaller diameter aerosol nanoclusters were not accessible experimentally. To overcome this challenge, we generated methanesulfonic acid–amine aerosol nanoclusters using a different approach. A bipolar electrospray ion source coupled to a half-mini differential mobility analyzer (SEADMS) allowed the generation and classification of singly charged MSA-amine nanoclusters in the 1-2.5 nm range. Data include the size distribution of mobility-selected nanocluster ions using a Faraday cup electrometer and chemical composition using either a time-of-flight mass spectrometer (Tofwerk, ApiTOF-MS) or a high resolution Orbitrap mass spectrometer (ThermoScientific, Q Exactive Plus). Acid-base clusters from MSA with five different amines, including two alkylamines (methylamine and butylamine), two alkanolamines (monoethanolamine and 4-aminobutanol) and a diamine (1,4-diaminobutane) were probed. Additional in-source collision-induced fragmentation studies using an Orbitrap-MS provided data on the stability of these nanoclusters as a function of collision energy (0-100 eV). Both the importance of the experimental parameters (e.g. ion transmission and potential fragmentation artefacts) as well as the properties of the MSA-amine clusters will be discussed. These studies provide significant insights into our understanding of NPF from MSA-driven acid-base chemistry processes and their contribution to airborne particles and their impacts.

Keywords: ion mobility mass spectrometry, acid, base nanoclusters, methanesulfonic acid, amines

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O-03 Formation of Viscous and Polymerized Microdomains in Organic Aerosol Proxy Films: Consequences for Aerosol Phase Behavior and Aging

Tuesday, 19 May, 10:10 am

Presenter: Kristen Johnson
Authors: Khirujammon Sumon[1]; Emmanuella Ebinum[1]; Kristen Johnson[1]

[1] Tennessee Tech University, 1 William L Jones Dr, Cookeville, TN 38505, United States

Cooking emmissions account for a significant amount of organic aerosol particles in the urban environment and have been linked to an increase in organic content on the surfaces of urban particulates in general. There is evidence to suggest that self-assembly of molecules into densely packed domains within the particles from cooking emmisions result in decreased oxidation rates and therefore longer atmospheric lifetimes than are predicted by measured oxidation rates of the single component aersols. In this work, we use thin films with an eqimolar mixture of oleic acid and sodium oleate, shown to have lipid bilayer-like structure in ambient conditions, as a proxy system to investigate the relationship between physical properties of the film on the nanoscale to heteogeneous and multiphase reactions rates. We examine how reactions with common oxidants, including ozone and cleaning-related species such as hypochlorous acid, alter film composition and microstructure. Model films are exposed to controlled flows of reactant gases using an attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR) system to quantify heterogeneous reaction kinetics. Following exposure, the films are interrogated via atomic force microscopy (AFM) to resolve microscale morphological changes and identify the formation of highly viscous or polymerized domains. Ozonlysis rates and rates of reaction with HOCl of the mixed oleic acid sodium oleate film were found to be slower than the ozonlysis rate of oleic acid alone. The AFM imaging shows the transition from smooth film structure to structure dominated by aggregated particle-like structures. Overall, this work provides new insights into how gas–surface reactions transform organic films, with broader implications for understanding the evolution of atmospheric particles and improving both indoor and outdoor air-quality models.

Keywords: gas–surface interactions, heterogeneous chemistry, multiphase chemistry, phase behavior, cooking emissions

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O-04 Effective Mass Accommodation for Surface and Bulk Reactions in Particles with Varying Viscosities

Tuesday, 19 May, 11:00 am

Presenter: Manabu Shiraiwa
Authors: Manabu Shiraiwa[1]; Pascale Lakey[1]

[1] University of California, Irvine, United States

Kinetic multi-layer models explicitly treat mass transport and chemical reactions using fundamental kinetic parameters and have often been applied to understand the processes controlling uptake coefficients. These models are computationally expensive to run, so making simpler, computationally efficient equations that maintain accuracy highly desirable. For this purpose, the effective mass accommodation (αeff) equation was previously derived which simplifies bulk transport and reactions by treating an effective penetration depth. In this work the αeff equation is further developed by including reactions of adsorbed molecules at the surface. Surface reactions can often dominate over bulk reactions and may even lead to different products. The αeff equation is also updated by incorporating a bulk accommodation limitation. Systematic testing of the αeff method with a range of parameters demonstrates good agreement with benchmark kinetic multi-layer model simulations. The αeff method is also capable of accurately determining the fraction of molecules reacting at the particle surface compared to those reacting within the particle bulk. Deviations between the αeff method and the kinetic multi-layer model occur if quasi-equilibrium has not been achieved in the penetration depth or if the surface becomes depleted of a non-volatile reactant. If depletion at the surface occurs, agreement can still be achieved by removing the surface reaction. Comparisons have also been made with two other sets of equations which have previously been published in the literature.

Keywords: mass accommodation, kinetic modeling, reactive uptake, surface reactions

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O-05 In situ measurements of pH, viscosity, and phase state in submicron particles via aerosol fluorescent labeling

Tuesday, 19 May, 11:20 am

Presenter: Paul Ohno
Authors: Paul Ohno[1]

[1] Auburn University, Auburn, Alabama 36849, United States

Aerosol physicochemical properties have proven challenging to directly measure in situ due in part to small particle sizes and low number densities. Here, a general methodology for the volatilization and subsequent condensation of trace quantities of fluorophores into aerosols of interest is presented and shown to enable the in situ elucidation of aerosol pH, viscosity, and phase state. The phase state of secondary organic aerosols of varying precursors is discussed, as is the unexpected acidity of submicron inorganic particles of varying compositions. Finally, the outlook of this technique towards single submicron particle analysis and characterization of ambient aerosols is discussed.

Keywords: secondary organic aerosols, pH, acidity, viscosity, liquid, liquid phase separation

O-06 Vertical Gradients in New Particle Formation and Growth: Influence of Agricultural Emissions and Implications for Cloud Droplet Number

Tuesday, 19 May, 2:10 pm

Presenter: Eleanor Browne
Authors: Eleanor Browne[1]; Bri Dobson[1]; Daniel Katz[1]; Maxim Muter[1]; Maxwell Lee[1]; Mitchell Alton[2]; Harald Stark[2]; Tamanna Subba[3]; Douglas Worsnop[2]; Chongai Kuang[3]; Manjula Canagaratna[2]

[1] University of Colorado Boulder, United States
[2] Aerodyne Research Inc, United States
[3] Brookhaven National Laboratory, United States

Agricultural activities ranging from changing land and water use to the application of fertilizer have been a defining characteristic of the Anthropocene. Increased demands for food and biofuel as well as changes in environmental factors will alter agricultural emissions in the coming decades. How aerosol processes respond to such changes remains an open question with implications for future agricultural productivity and ecosystem and human health. To address these knowledge limitations, we have been investigating new particle formation and growth across multiple seasons at the United States Department of Energy Southern Great Plains research facility in Lamont, Oklahoma, an agriculturally intensive region. We use measurements of particle formation precursors (e.g., NH_3, amines, H_2SO_4, oxygenated organic molecules (OOMs)) at the surface, vertically resolved measurements of 1-3 nm aerosol-cluster concentration from the tethered balloon system, and WRF-Chem modeling. We have found that agricultural emissions of reactive nitrogen compounds, namely NH_3, amines, and nitrogen oxides play a central role in nucleation and growth processes. Due to the relatively high surface temperatures and low sulfuric acid concentrations, new particle formation is favored aloft. A notable exception occurs when amines are present, and cluster growth is observed at the surface. WRF-Chem results suggest that vertical mixing of NH_3 may play a defining role in determining the variability in boundary layer profiles of nucleation. High NO mixing ratios affect the formation of OOMs, specifically by depressing the formation of “dimer” molecules formed from peroxy radical cross reactions. As a result, sesquiterpene oxidation products rather than monoterpene oxidation products dominate the extremely low volatility compounds that contribute to growth, a finding consistent with emission factors from crops in the area. Using a 0D adiabatic cloud parcel number we show that these new particle formation and growth events increase the number of potential cloud droplets. Overall, these findings highlight that future prediction of aerosol processes in agricultural regions requires improved understanding of agricultural emissions.

O-07 Photochemical Processes During New Particle Formation Involving Iodic Acid and Iodine Oxides

Tuesday, 19 May, 2:50 pm

Presenter: Christopher J. Johnson
Authors: Christopher J. Johnson[1]

[1] Department of Chemistry, Stony Brook University, United States

Iodine oxide particles are likely to form and grow into climatically relevant aerosols in coastal and polar regions. While photochemical processing of iodine-containing molecules is relatively well established, the role of photochemistry in newly formed particles containing iodic acid and iodine oxides is only beginning to be explored. This presentation discusses the UV photolysis spectra of iodine oxide/iodic acid clusters and their relevance to new particle formation. We observe multiple photolysis products, most importantly atomic oxygen, I_2O_4, and I_2O_5, with absorption in the atmospherically relevant region (>300 nm) increasing with cluster size. Derived photolysis rates suggest that these processes can occur during daytime particle

formation events. We assign the chromophore as a covalent $I_3O_8^-$ molecule within the cluster. Atomic oxygen is likely produced in the triplet state, leaving a triplet-state cluster; both products may subsequently drive intraparticle chemistry.

O-08 The formation of icy clouds in upper planetary atmospheres

Tuesday, 19 May, 3:30 pm

Presenter: Thomas Leisner
Authors: Thomas Leisner[1,2]; Thomas Dresch[1]; Denis Duft[1]

[1] Institute of Meteorology and Climate Research, Atmospheric Aerosol Research, Karlsruhe Institute of Technology, Germany
[2] Institute of Environmental Physics, Heidelberg, Germany

Photochemically produced water molecules may nucleate on nanoparticles condensing from meteoric smoke to form ice clouds in the upper atmospheres in the inner solar system, including Venus, Earth and Mars. Here we report laboratory measurements on the heterogeneous ice nucleation and growth under mesopause conditions on small (r = 1 to 3 nm) iron silicate nanoparticles serving as meteoric smoke analogues Additionally, we investigate the influence of charges and nuclear spin statistics on the nucleation process and find that singly charged particles are favored as nucleation sites only at very small diameters below ~2nm.

Keywords: nanoparticles, nucleation, ice clouds, charge effects

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O-09 How aerosol mixing state controls immersion freezing: from particle heterogeneity to population response

Tuesday, 19 May, 3:50 pm

Presenter: Nicole Riemer
Authors: Nicole Riemer[1]; Wenhan Tang[1]; Sylwester Arabas[2]; Daniel Knopf[3]; Matthew West[1]

[1] University of Illinois at Urbana-Champaign, Urbana, United States
[2] AGH University of Science and Technology, Krakow, PL, Poland
[3] School of Marine and Atmospheric Sciences, Stony Brook, United States

Ice formation by atmospheric aerosols depends on the surface properties of ice-nucleating particles (INPs). However, predictions of ice production in clouds also depend on how ice-nucleating surfaces are distributed across entire aerosol populations. In particular, the same total amount of ice-active material can be arranged very differently among particles, raising a fundamental question: when does aerosol mixing state matter for ice formation, and why? Here, we present a combined theoretical analysis and particle-resolved Monte Carlo simulation framework that isolates the role of aerosol mixing state while controlling for particle size, surface area, and cooling conditions. Using classical nucleation theory and published aerosol-type-dependent ice nucleation rate coefficients, we show that internally and externally mixed ice-nucleating particle populations produce systematically different frozen fractions, even when their total ice-active surface area is identical. This difference arises from a nonlinear population effect: distributing small amounts of highly efficient ice-nucleating material across all particles is far more effective than concentrating it in a subset of particles. We identify regimes in which mixing state effects are negligible and regimes in which they dominate ice production, depending on particle size, aerosol-type-dependent freezing rates, and surface coverage. Particle-resolved simulations confirm these theoretical predictions for polydisperse aerosol populations and demonstrate how intermediate mixing states lead to bounded, but nontrivial, uncertainties in frozen fraction.

These results highlight aerosol mixing state as a structural source of uncertainty in ice formation predictions and provide a physically grounded link between INP material properties and cloud-scale ice formation.

Keywords: aerosol, ice nucleation, mixing state

O-10 Graph Theory–Driven Analysis with MD Simulations for Exploring Freezing in Aqueous Alcohols

Tuesday, 19 May, 4:10 pm

Presenter: Céline Toubin
Authors: Céline Toubin[1]; Rawan Abouhaidar[2]; Sana Bougueroua[2]; Denis Duflot[1]; Marie-Pierre Gaigeot[2]; Barbara Wyslouzil[3]

[1] PHLAM CNRS UMR 8523 - Université de Lille, Campus Cité scientifique - 59655 Villeneuve-d'Ascq, France
[2] Laboratoire Analyse, Modélisation et Matériaux pour la Biologie et l'Environnement, Bât. Maupertuis 1° étage bd François Mitterrand, 91025 EVRY CEDEX, France
[3] The Ohio State University, 281 W Lane Ave, Columbus, OH 43210, United States

Ice clouds in the upper troposphere are essential to Earth's climate, influencing both stratospheric humidity and radiative balance. The efficiency of heterogeneous ice nucleation—a key process in cloud formation—is largely dependent on the surface properties of aerosol particles, particularly the presence of functional groups capable of hydrogen bonding. Among the many surface-active organic compounds (SAOCs), short-chained alcohols such as 1-pentanol and 3-hexanol are of significant interest due to their tendency to accumulate at the liquid-vapor interface, modifying surface characteristics. While much attention has been given to the role of these alcohols in cloud condensation nuclei formation, their impact on freezing processes has been less explored. This study addresses this knowledge gap by investigating the behavior of linear and branched alcohols between the surface and bulk phases using classical molecular dynamics (MD) simulations, complementing existing experimental findings [1,2]. The MD simulations reveal that as temperature decreases from 283 K to 192 K, both the surface tension and solubility of 3-hexanol and 1-pentanol increase, indicating a temperature-dependent effect on ice formation. In addition to these macroscopic properties, graph theory [3] was employed to analyze the molecular-level influence of these alcohols on the hydrogen-bonding network of water at the interface. Our in-depth analysis shows that alcohol molecules are incorporated into the two-dimensional hydrogen-bonded network at the air-water interface, and during freezing, they form six-membered hydrogen-bonded rings, marking an early step in ice formation. References

[1] Sun, T.; Ben-Amotz, D.; Wyslouzil, B. E. Phys. Chem. Chem. Phys. 2021, 23 (16), 9991–10005. https://doi.org/10.1039/D0CP06131J.

[2] Sun, T.; Wyslouzil, B. E. J. Phys. Chem. B 2021, 125 (44), 12329–12343. https://doi.org/10.1021/acs.jpcb.1c06188.

[3] Bougueroua, S., Aboulfath, Y., Barth, D., & Gaigeot, M. P. (2023). Molecular Physics, 121(7–8). https://doi.org/10.1080/00268976.2022.2162456. [4] AbouHaidar, R., Bougueroua, S., Duflot, D., Gaigeot, M.P., Wyslouzil, B., Toubin C., Faraday Discussions 2025, Faraday Discuss., 2025,258, 396-418. DOI : 10.1039/D4FD00165F

Keywords: Molecular dynamics, alcohols, interface, H, bonds, freezing, ice

O-11 Developing a Predictive Model for Growth of Secondary Organic Aerosol Particles

Wednesday, 20 May, 9:10 am

Presenter: Barbara Finlayson-Pitts
Authors: Barbara Finlayson-Pitts[1]

[1] University of California, Irvine, United States

Low volatility organics formed from oxidation of volatile organic compounds in air are a significant component of airborne particulate matter. These secondary organic aerosol particles (SOA) are, under many atmospheric conditions, high viscosity materials where diffusion into the bulk is slow. This means that their growth via quasi-equilibrium with the gas phase as has been commonly assumed is severely restricted. Another growth mechanism we have proposed is a “burying mechanism” where an incoming gas molecule initially adsorbs to the particle surface. If the residence time on the surface is sufficiently long, it can be “buried” by an incoming species, and thus become incorporated into the particle to grow it. Evaluating the potential importance of this mechanism requires knowledge of the residence times for adsorbed species which is determined by their desorption energies to the surface. Experiments to measure the desorption energies of known organic gases to well-defined organic surfaces are being carried out using temperature-programmed desorption (TPD). Results for different combinations of polar/non-polar gases and polar/non-polar surfaces will be presented. The ultimate goal is to develop a parameterization of desorption energies/residence times as a function of the structural features of the gas and surface that can be incorporated into atmospheric models of SOA growth. .

Keywords: secondary organic aerosol, growth, temperature programmed desorption

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O-12 Functional groups with aerosol mass spectrometry: OA aging processes and properties

Wednesday, 20 May, 9:50 am

Presenter: Rachel E. O’Brien
Authors: Rachel E. O’Brien[1]; Manjula Canagaratna[2]; Xu He[1]; Janie (Yaeseul) Kim[1]; Willow Hwang[1]; Hannah Kenagy[3]; Chris Cappa[4]

[1] University of Michigan, United States
[2] Aerodyne Research Inc., United States
[3] University of Minnesota, United States
[4] University of California, Davis, United States

Organic aerosol (OA) contains thousands of different organic molecules which can transform in the atmosphere as a result of aging processes like photolysis and heterogeneous oxidation. Chemical properties like the average molecular weight and the functional group distribution of the mixture will impact the physical properties of the particles. Functional group distributions can be evaluated using offline methods like Fourier Transform Infrared Spectroscopy (FTIR), but this requires sample collection for offline analysis. Here, we have developed a novel method to quantify alkyl, aromatic, carboxylic acid, ketone, and alcohol functional groups directly from High Resolution-Time of Flight-Aerosol Mass Spectrometer (AMS) data sets. This method uses a grouping method termed delta analysis which also provides qualitative information about the chemical properties of the OA. We find that chamber studies of OA photolysis show an increase in the acid fraction and a decrease in the alkyl portion without a corresponding decrease in ketones. This is in contrast to photolysis aging on a filter in a flushed box where a decrease in ketone is observed. This highlights the potential role of the reservoir of semi-volatile organic carbon compounds in the chamber, but not in the flushed box. We also find that the composition of highly oxidized OA from ambient measurements is about 50% acid and 25% alcohol, with only a small fraction of ketone. Finally, we find that biomass burning OA can show variations in functional group shifts with aging dependent on the initial mixture.

Our ability to quantify functional groups directly from online data sets opens new doors for the analysis of OA formation and aging as well as an evaluation of the physical properties of OA.

Keywords: aerosol mass spectrometry, functional groups, delta analysis, photolysis

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O-13 Molecular Characterization of Organic Peroxides from Monoterpene-derived Secondary Organic Aerosol

Wednesday, 20 May, 10:10 am

Presenter: Kangwei Li
Authors: Kangwei Li[1]; Zhensen Zheng[2,3]; Markus Kalberer[1]

[1] Department of Environmental Sciences, University of Basel, Switzerland
[2] Institute of Ion Physics and Applied Physics, University of Innsbruck, Austria
[3] IONICON Analytik GmbH., Austria

Organic peroxides are health-relevant organic components in secondary organic aerosols (SOA), which is also a major compound class substantially contributing to SOA mass. However, their molecular identification and characterization in SOA is highly challenging and uncertain. Ozonolysis of alkenes is known to produce reactive intermediates - stabilized Criegee intermediates, and their subsequent bimolecular reactions with various carboxylic acids can form α-acyloxyalkyl hydroperoxides (AAHPs), which is considered a major class of organic peroxides in SOA. Here we use this knowledge to synthesize a number of atmospherically relevant AAHPs through liquid-phase ozonolysis from either α-pinene or 3-carene in the presence of ten different carboxylic acids. These AAHPs with diverse structures are identified individually by liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS). AAHPs were previously thought to decompose quickly in aqueous environment such as cloud droplets, but we demonstrate here that AAHPs hydrolysis rates are highly compound-dependent with rate constants differing by 2 orders of magnitude. Some synthesized AAHPs were further identified via targeted analysis in monoterpene SOA samples collected from laboratory flowtube experiments. Another focus of this study is to expand the molecular identification ability of organic peroxides in SOA, which aims to go beyond peroxide standards. Iodide is known to selectively react with organic peroxides, and the reaction kinetics should depend on the structure of each peroxide. We extrapolate this knowledge and develop a novel analytical approach for the molecular characterization of organic peroxides in α-pinene SOA, combining iodometry kinetic experiments with LC-HRMS. Through non-targeted analysis, we identify over 300 organic peroxides in α-pinene SOA, showing a wide range of reactivities with iodide, spanning four orders of magnitude. Our study improves the molecular-level identification and understanding of organic peroxides in SOA, offering numerous opportunities for further investigation into their formation chemistry, atmospheric transformation, and health impact.

Keywords: organic peroxide, molecular characterization, secondary organic aerosol, high resolution mass spectrometry, nontargeted analysis

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O-14 Characterizing the emissions of gas-phase species associated with automotive brake wear at a molecular level using high resolution chemical ionization mass spectrometry

Wednesday, 20 May, 10:20 am

Presenter: Madeline Cooke
Authors: Madeline Cooke[1]; Michelia Dam[1]; Lisa Wingen[1]; Véronique Perraud[1]; Adam Thomas[1]; Berenice Rojas[1]; Sanjeevi Nagalingam[1]; Michael Ezell[1]; Samuel La Salle[1]; Paulus Bauer[1]; Barbara Finlayson-Pitts[1]; James Smith[1]

[1] University of California, Irvine, United States

Traffic emissions are a main source of air pollution in urban environments, comprising two categories: exhaust emissions, generated from combustion in the tailpipe, and non-tailpipe vehicular emissions, generated primarily from brake or tire wear. As our society transitions to a predominantly electric vehicular fleet, emissions from non-tailpipe sources will become increasingly important. While a large body of research has focused on characterizing the emission of particles from automotive braking, little attention has been paid to the emission of gas-phase species. In this work, we describe measurements of the molecular composition of gaseous emissions associated with automotive braking utilizing chemical ionization mass spectrometry (CIMS) equipped with nitrate (NO_3^-) or iodide (I-) reagent ion chemistry. Automotive braking was simulated in laboratory experiments using a custom-built dynamometer, which applied braking forces in a step-wise manner to replicate real-life braking torque and temperature conditions. Measurements using NO_3-CIMS detected the generation of sulfuric acid as well as numerous low-volatility oxidized organic compounds. Measurements with I-CIMS detected additional oxidized organic compounds as well as several inorganic reactive nitrogen species, including nitrous acid (HONO), nitryl chloride ($ClNO_2$), and dinitrogen pentoxide (N_2O_5). Of particular note is the detection of HONO, which is a predominant source of hydroxyl radicals in the atmosphere, and thus contributes substantially to atmospheric oxidation chemistry. Offline calibrations permitted the quantification of HONO during these experiments, revealing that substantial quantities of HONO were generated during the simulations of automotive braking, up to 26 parts per billion (ppb) measured. We propose that HONO is formed from reactions of NO_2 with organic compounds, which are emitted simultaneously in the hot plume emanating from the brake rotor. In support of this hypothesis, offline experiments were conducted using I-CIMS to react organic gases containing allylic and aldehydic hydrogens with NO_2 at ~70°C, resulting in the generation of substantial HONO. Overall, the emission of gas-phase species from automotive braking has important implications for urban air quality, becoming more important as vehicle electrification progresses globally and non-tailpipe emissions become an increasingly important source of atmospheric pollutants.

Keywords: Emerging contaminants, Braking, Nitrous Acid, Chemical Ionization Mass Spectrometry

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O-15 Beyond the Formation: Chemical Transformation of Organosulfates (OSs) and its Implications for Atmospheric Unidentified OSs and Sulfur Form

Wednesday, 20 May, 11:00 am

Presenter: ManNin Chan
Authors: ManNin Chan[1]

[1] The Chinese University of Hong Kong, Hong Kong SAR China

Organosulfates (OSs) have recently been recognized as important constituents of atmospheric aerosols, formed through reactions between inorganic sulfur species (e.g., SO_2, SO_4^{2-}) and organic compounds. Owing to their perceived chemical stability, OSs have been used as tracers for secondary organic aerosol (SOA) formation. However, recent work demonstrates that many OSs undergo rapid transformation via heterogeneous and aqueous-phase oxidation, generating a variety of new OSs, non-sulfated products and

inorganic sulfates. These reactions not only account for the formation of previously unidentified OSs in the atmosphere but also show that certain OSs can significantly regenerate inorganic sulfate (e.g., $SO_4{}^{2-}$), revealing a dynamic interconversion between organic and inorganic sulfur upon oxidation. This talk will discuss recent advances in OS oxidation chemistry (e.g. isoprene derived OSs). Based on state-of-the-art laboratory experiments and analytical techniques, I will discuss how OS structural factor influences reaction pathways and product formation, focusing on the generation of new OSs and inorganic sulfate. Together, this work highlights the need to re-evaluate the stability, formation, and transformation of atmospheric OSs, ultimately improving our ability to quantify their abundances and assess their properties and environmental impacts.

Keywords: organosulfate, inorganic sulfate, aerosol sulfur form, chemical transformation

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O-16 Particle-Phase Peroxides Form Carboxylic Acids in Pinene Secondary Organic Aerosol

Wednesday, 20 May, 11:20 am

Presenter: Christopher Kenseth
Authors: Christopher Kenseth[1,2]; Olivia Hakan[2]; Donterrio Moore[2]; Yuzhi Chen[3]; Vili-Taneli Salo[4]; Matthieu Riva[5]; Michael Kamrath[5]; John Shilling[3]; Henrik Kjaergaard[4]; Joel Thornton[2]

[1] University of Maryland, United States
[2] University of Washington, United States
[3] Pacific Northwest National Laboratory, United States
[4] University of Copenhagen, Denmark
[5] TOFWERK AG, Switzerland

Carboxylic acids are major components of atmospheric secondary organic aerosol (SOA), which plays a pivotal role in climate, air quality, and health. Their production is currently understood to occur predominantly through gas-phase chemistry. However, despite extensive study, the identities and thus the formation mechanisms of carboxylic acids in SOA remain largely unvalidated. In this work, we identify the most abundant carboxylic acids in SOA from ozonolysis of α-pinene and β-pinene—substantial global SOA sources—through independent synthesis of authentic standards. Based on targeted laboratory experiments featuring isotopically labeled compounds, tailored precursors, and isomer-resolved mass spectrometry, together with quantum chemical calculations of multigenerational peroxy and alkoxy radical chemistry, we show that these acids are formed in the particle phase through the decomposition of peroxyhemiacetals. These findings, together with past work on the formation of dimer esters in SOA, demonstrate that the particle-phase production of peroxyhemiacetals, and their subsequent conversion to carboxylic acids and dimer esters via Baeyer-Villiger decomposition and nucleophilic addition of alcohols, represents a key process in SOA formation.

O-17 General Assembly of Anions and Cations at the Aqueous Solution – Air Interface and the Advantage of Neutrals

Wednesday, 20 May, 2:10 pm

Presenter: Markus Ammann
Authors: Markus Ammann[1]

[1] Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland

Recently, several debates about the abundance or not of ions at the aqueous solution – air interface of atmospheric aerosol particles or cloud droplets have sparked significant interest in the role of ions or also neutral species in controlling surface tension, chemical reactivity and structure relevant for the impact of aerosols and clouds for atmospheric composition and climate. We have used X-ray photoelectron spectroscopy (XPS) on liquid jets of aqueous solutions with bromide, iodide, iodate and nitrate, as well as their mixtures with neutral or ionic surfactants to look at their interplay at the interface. These ions are all implicated in important multiphase chemical cycles in the atmosphere. I will review the potential and also limitations of XPS to unravel interfacial composition, acid-base exchange and details of density profiles of ions with depth into solution. I will also briefly address recent advances in electron spectroscopy allowing more sub-nanometer resolution information on the local environment of ions at the interface based on elastic scattering of photoelectrons.

Keywords: aerosol, interface, multiphase chemistry, photochemistry

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O-18 The Role of Interfacial Processes in Accelerated Reaction Kinetics in Aqueous Microdroplets

Wednesday, 20 May, 2:50 pm

Presenter: Cari Dutcher
Authors: Shu Yang[1]; Meng Li[2]; Justin Wang[2]; Vicki Grassian[2]; Satish Kumar[1]; Cari Dutcher[1]

[1] University of Minnesota, United States
[2] University of California, San Diego, United States

Aqueous microdroplets have been shown to exhibit enhanced chemical reactivity compared to bulk solutions, although the mechanisms for these enhancements are not completely understood. Here we combine experimental measurements and kinetic modeling to show the strong coupling of interfacial reactions and gas/droplet partitioning, with and without surface charge. Using a newly developed diffusion-adsorption-reaction-evaporation-electromigration model, we simulate the intricate kinetics where reactant diffuses and adsorbs to the surface of a microdroplet, where it can remain, react, desorb, or evaporate, while product formed at the surface desorbs and diffuses into the bulk. Tensiometry measurements are utilized to parameterize the adsorption kinetics in the Langmuir adsorption model. The model quantitatively predicts compositional changes during the condensation reaction, and provides insights into how microdroplet reactivity is controlled by coupled interfacial reactions and the gas-phase partitioning of the reactant and water. Moreover, the model can be generalized to systems where the interplay of reaction, adsorption, diffusion, and evaporation processes varies with droplet size, from nanometer to millimeter scales, or with different initial reactant concentrations, leading to diverse kinetic behaviors. Notably, we observe an intriguing competition between evaporation and reaction rates that determines the optimal droplet size. While smaller droplets exhibit faster reaction rates due to the dominance of surface reactions, they also experience higher reactant evaporation rates, leading to more reactants being consumed via evaporation rather than reaction. Recent results in the presence of an electric double layer at the surface will also be shown, highlighting the important coupling between evaporation and charge. These findings offer insights

into the complexity of microdroplet reaction kinetics, with interfacial processes playing a central role, and provide a universal mechanism for understanding reaction kinetics in aqueous nano- and microdroplets.

O-19 Spatial heterogeneity at atmospheric interfaces

Wednesday, 20 May, 3:30 pm

Presenter: Tara Kahan
Authors: Tara Kahan[1]

[1] University of Saskatchewan, Canada

Heterogeneous chemistry, including at aerosol surfaces, can greatly affect atmospheric composition. Highly variable physicochemical properties of atmospheric surfaces make predicting reactivity challenging. Further, standard surface-sensitive techniques such as X-ray spectroscopy are often unsuitable for studying volatile atmospheric particles.

We use micro-spectroscopic methods methods to investigate the spatially-resolved composition of atmospheric surfaces. Our results indicate that even “simple” systems, such as frozen aqueous NaCl solutions, demonstrate significant spatial heterogeneity, and that the spatial distribution of reactants can be very non-homogeneous. We use these observations, along with photochemical and bimolecular kinetics measurements, to propose mechanisms for important reactions at atmospheric interfaces. The insights gained from this work can inform the parameterization of chemical fate models.

O-20 Unveiling the Dual Role of Nitrate (NO_3^-) and Nitrite (NO_2^-) Anions at the Air-Water Interface of Atmospheric Droplets

Wednesday, 20 May, 3:50 pm

Presenter: Christian George
Authors: Christian George[1]; Yoan Carreira Mendes Da Silva[1]; Maria Angelaki[1]; Adrien Gandolfo[1]; D. James Donaldson[2]

[1] IRCELYON, 2, Av. Albert Einstein, F-69626 Villeurbanne Cedex, France
[2] University of Toronto at Scarborough, 1265 Military Trail, Scarborough, ON M1C 1A4, Canada

While numerous studies have documented the spontaneous generation of OH radicals and hydrogen peroxide (H_2O_2) at the air-water interface of aqueous droplets, the influence of nitrate (NO_3^-) and nitrite (NO_2^-) anions—key players in atmospheric chemistry—has remained unexplored. Our research fills this gap by investigating the spontaneous production of H_2O_2 in droplets containing NO_2^- or NO_3^- under dark conditions. We reveal a concentration-dependent dual effect: at low concentrations, these anions enhance H_2O_2 production by disrupting the interfacial water structure, whereas at higher concentrations, they inhibit it through specific interfacial chemistry, leading to the formation of gas-phase species such as HONO and NO_2. By monitoring H_2O_2 and other gas-phase products, we propose a mechanism to explain this unique interfacial reactivity. This chemistry, though potentially overshadowed by photolysis during the day, may have significant implications for nighttime atmospheric processes, influencing air quality and oxidative capacity.

O-21 Single Particle ICP-TOF-MS analysis of atmospheric aerosols

Wednesday, 20 May, 4:10 pm

Presenter: Patrick Hayes
Authors: Patrick Hayes[1]; Judith Boudrias[1]; Kevin Wilkinson[1]; Houssame-Eddine Ahabchane[1]; Aaron Goodman[2]

[1] Université de Montréal, Canada
[2] Colorado School of Mines, United States

Single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) provides quantitative measurements of the elemental composition of nano-and microparticles, as well as the capacity to measure thousands of particles in a minute. While SP-ICP-MS has been used extensively in water and other environmental matrices, relatively few studies have applied SP-ICP-MS to air. This unfulfilled potential is due to the need to develop robust sampling methods that can be used to capture airborne particles and transfer them to the SP-ICP-MS torch and sample introduction interface. This talk will present a number of recent developments of sampling of atmospheric aerosols for SP-ICP-MS analysis, including the use of filter sampling, Coriolis particle-into-liquid sampling, and direct aerosol injection via a gas exchange device (GED). Examples of field work that study high latitude mineral dust emissions (Kluane Lake, Yukon) and industrial emissions (Rouyn-Noranda, Quebec) will also be discussed. Particle-by-particle analysis with a ToF-MS detector provides detailed multi-elemental composition data that can be used in source apportionment studies.

Keywords: Aerosol, mineral dust, industrial emissions, trace elements, ICP, MS, SP, ICP, MS

O-22 The production of molecular singlet oxygen ($1O_2$*) from brown carbon-generating fuels during daytime and nighttime

Thursday, 21 May, 9:10 am

Presenter: Nadine Borduas-Dedekind
Authors: Nadine Borduas-Dedekind[1]; Claudia Sardena[1]

[1] University of British Columbia, Vancouver Campus, 2329 West Mall, Vancouver, BC, V6T 1Z4, Canada

The first excited state of molecular O_2 is molecular singlet state $1O_2$* and this oxidant can be formed in the atmosphere from chromophores present in brown carbon (BrC). To better constrain the role of $1O_2$* in atmospheric processing of BrC, we are interested in studying its sources and sinks throughout the lifetime of a BrC plume, for example in wildfire smoke. Most studies on $1O_2$* rely on water extractions, potentially overlooking water-insoluble chromophores that contribute to the photochemistry of BrC. We developed a new organic-solvent extraction method to probe water insoluble chromophores and their ability to sensitize $1O_2$* and its precursor triplet state organics, 3C*. Since aerosols are multi-phase and phase separate, we aimed to quantify $1O_2$* in acetonitrile and in water as a representation for multi-phase aerosols. We use particulate matter filter extracts from the combustion of beechwood, cow dung, straw and plastics to study the impact of the chemical composition on solubility and $1O_2$* quantum yields. We found that smoldering vs flaming conditions had a smaller effect than the original presence of N-containing compounds in the material. Next, we exposed the combustion aerosols to two different types of aging: photochemical aging through the production of hydroxyl radicals and dilution through the denuder. We find that dilution reduced $1O_2$* quantum yields, likely through the partitioning and removal of key $1O_2$* sensitizers. On the other hand, only photooxidized beechwood showed an increase in $1O_2$* quantum yield following light and hydroxyl radical exposure. These results indicate that, again, the original chemical composition and chromophores are dictating the sensitizing ability of BrC from different sources and after different atmospheric aging processes. Furthermore, we tested the nighttime processing of BrC through exposure to nitrate radicals and the formation of nitro-aromatic chromophores. These compounds are not water-soluble and could be accounting for an underappreciated source of sensitizers for $1O_2$*. Overall, these results are constraining our ability to predict $1O_2$* production in BrC, and linking this ability directly to the chemical composition of the BrC.

Keywords: photochemistry, molecular singlet oxygen, brown carbon, fuels, aging processes

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O-23 Optical Properties and Photobleaching of Brown Carbon Aerosol Particles using Laser Spectroscopy

Thursday, 21 May, 9:50 am

Presenter: Michael Cotterell
Authors: Michael Cotterell[1]; Aidan Rafferty[1]; Andrew Orr-Ewing[2]; Xu Zhang[2]; Jamie Knight[2]; Simon Chen[2]; Padraig Meehan[1]

[1] Department of Chemistry, University of Oxford, United Kingdom
[2] School of Chemistry, University of Bristol, United Kingdom

Brown carbon (BrC) aerosols remain a major source of uncertainty in aerosol radiative forcing because their optical properties vary strongly with wavelength, composition, phase state and atmospheric processing. This presentation summarizes results from our recent studies using laser spectroscopy to constrain the complex refractive index, m = n + ik, of representative BrC chromophores (nitroaromatics and imidazoles) and quantify how these properties evolve under atmospherically relevant conditions. We first discuss laser-based spectroscopy measurements on single, levitated aqueous droplets containing the abundant nitroaromatic chromophore 4-nitrocatechol. By combining single particle cavity ring-down spectroscopy at the 405 nm wavelength with bulk UV/Vis absorption spectra and a physically based refractive index mixing framework, we isolate contributions from protonated and deprotonated forms across a wide pH range. A Kramers–Kronig analysis of the bulk UV/Vis data, constrained by single-particle extinction and scattering measurements, yields wavelength-dependent complex refractive indices of the fully protonated and singly deprotonated 4-nitrocatechol species, enabling improved predictions of radiative properties for nitroaromatics in aerosol plumes and cloud water. We then turn to imine/imidazole-type BrC produced by aqueous glyoxal–nitrogen chemistry. Using size-selected dry particles (via an Aerodynamic Aerosol Classifier) coupled to cavity ring-down and photoacoustic spectroscopy, we retrieve n and k at the 405 nm wavelength with high precision while avoiding artefacts from multiply charged particles that can bias mobility-based selections. Absorption is observed primarily under basic precursor conditions and chromophore formation is enhanced by aerosolization and drying. We then demonstrate single-particle measurements of the photobleaching of imidazole chromophores. Levitated organic particles containing imidazole-2-carboxaldehyde are photolyzed at 405 nm while single particle cavity ring-down spectroscopy monitors the decay in k with exposure to the 405-nm photolysis light source. Comparing this data to a kinetic model coupled with Mie theory calculations yields a photobleaching quantum yield for imidazole-2-carboxaldehyde and a framework to predict bleaching timescales across particle sizes and actinic flux regimes, as well as highlighting important differences between bulk-solution and aerosol-phase behaviour. Finally, we summarize a new analytical approach for broadband light scattering that enables rapid retrieval of particle size and refractive index across the 380-800 nm wavelength range for single, levitated particles, validated against concurrent cavity ring-down spectroscopy extinction measurements. This development moves us toward accurate, precise, broadband characterisation of individual aerosol particles spanning the actinic spectrum, opening new opportunities to quantify BrC variability and processing in atmospherically relevant aerosol environments.

Keywords: Optical properties, Brown carbon, Laser spectroscopy, Single aerosol particles, Photochemistry, Photobleaching

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O-24 Photoaging of water-soluble wood smoke aerosol at low temperatures: impact on optical properties and chemical composition

Thursday, 21 May, 10:10 am

Presenter: Stephanie Jones
Authors: Stephanie Jones[1]; Emma Jaervinen[2]; Martin Schnaiter[2]; Yanxia Li[3]; Xuefeng Shi[3]; Harald Saathoff[3]; Robert Wagner[3]; Sonja Muelhopt[4]; Manuela Hauser[4]; Marco Mackert[4]

[1] York University, 4700 Keele Street, Toronto, ON, M3J 1P3, Canada
[2] Bergische Universität Wuppertal, Gaußstraße 20, 42119 Wuppertal, Germany
[3] Institut für Meteorologie und Klimaforschung - Atmosphärische Aerosol Forschung, Postfach 3640, 76021 Karlsruhe, Germany
[4] Karlsruhe Institute of Technology, P.O. Box 3640, 76021 Karlsruhe, Germany

The effect of biomass burning organic aerosol (BBOA) on the climate remains uncertain. With growing numbers of wildfires, it has become increasingly important to study aging of BBOA under atmospherically relevant conditions. Given the light absorbing nature of BBOA, it is necessary to study the effects of photoaging on the physicochemical and optical properties of BBOA. As BBOA can be transported to different heights within the troposphere and lower stratosphere, it is important to study photoaging at atmospherically relevant supercooled temperatures. An experimental campaign was performed in the Aerosol Interaction and Dynamics in the Atmosphere (AIDA) chamber at the Karlsruhe Institute of Technology, Germany, to study the photoaging of water-soluble wood smoke aerosol at temperatures representative of different atmospheric heights: 20°C, -25°C, and -50°C. Water-soluble wood smoke condensate samples were collected from the combustion of fir wood and beech briquettes and injected into the chamber under the three different temperature conditions. The aerosol was then equilibrated in the dark for several hours before being illuminated with LEDs simulating solar radiation for $\geq$ 17 hours. Continuous measurements of various aerosol physicochemical and optical properties were made throughout the experiments to determine any changes in the aerosol properties during illumination. In this presentation, I will focus on the aerosol optical properties determined using multiple wavelength photoacoustic spectrometers and a nephelometer and will also discuss Aerosol Mass Spectrometry data and potential links between the two. Photoaging of both types of wood smoke condensate aerosol was observed to cause changes in the optical properties and aerosol organic composition. The absorption coefficients at visible wavelengths (445 nm, 515 nm and 520 nm) were observed to increase with the onset of illumination followed by a gradual decrease with continued illumination. The O:C ratio was also observed to increase with the onset of illumination as well as the m/z 44/43 ratio suggestive of photo-induced oxidation of the aerosol. Temperature was observed to affect the magnitude of these changes, with lower temperatures resulting in smaller changes in the measured optical properties, O:C ratio, and m/z 44/43. A possible reason for the decreased magnitude of these changes could be a potential phase change in the aerosol at lower temperatures resulting in a reduced rate of photooxidation. These findings confirm the important role of temperature on aerosol properties during photoaging and could have important consequences for the contribution of BBOA to climate forcing.

Keywords: aerosol, biomass burning, photoaging, low temperature, simulation chamber, optical properties, chemical composition

O-25 Photochemical Evolution of Particulate Organics in Wildland–Urban Interface Fire Emissions

Thursday, 21 May, 11:00 am

Presenter: Sergey Nizkorodov

Authors: Sergey Nizkorodov[1]

[1] University of California Center for Hydrologic Modeling, Irvine, United States

The wildland–urban interface (WUI) is rapidly expanding and is increasingly impacted by fires that simultaneously combust vegetation and built infrastructure, generating smoke with chemical compositions and associated health and climate impacts that differ from those of traditional wildland fires. Despite rising concern over emissions from WUI fires, the molecular contributors of WUI-derived burning organic aerosol (BOA) to brown carbon formation and radiative forcing remain poorly constrained. This presentation centers on a detailed molecular-level interrogation of brown carbon in WUI BOA and its transformation during photochemical aging. BOA produced from controlled laboratory combustion of representative building materials was collected and exposed to photolysis. Bulk optical properties were linked to molecular composition through the combined use of UV–visible spectroscopy and high-resolution mass spectrometry, enabling identification of individual chromophoric species. The resulting molecular signatures reveal a chemically complex mixture arising from both lignocellulosic and synthetic sources. Across all materials examined, brown carbon was dominated by aromatic and highly functionalized molecular species consistent with the combustion of treated wood and composite materials. Unlike biomass burning organic aerosol, which frequently exhibits initial photoinduced enhancement followed by photobleaching, WUI BOA displayed predominantly monotonic photobleaching throughout the irradiation period. These findings indicate that WUI-derived brown carbon undergoes distinct molecular-scale photochemical evolution, with implications for its optical properties and radiative effects. Overall, this work advances a molecularly resolved understanding of chromophore evolution in WUI BOA and underscores the need to explicitly account for WUI fire emissions in atmospheric chemistry and climate models.

Keywords: wildland, urban interface, biomass burning, photodegradation, composition, brown carbon

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O-26 Multiphase uptake of N_2O_5 into Biomass Burning Organic Aerosol

Thursday, 21 May, 11:20 am

Presenter: Zac Liang

Authors: Zhancong Liang[1]; Jonathan Abbatt[1]

[1] Department of Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario M5S 3H6, Canada

The reactive uptake of N_2O_5 into aqueous aerosol particles has long been recognized as a critical sink for nitrogen oxides in the atmosphere. However, its interaction with organic aerosols remains less constrained, with reported uptake coefficients spanning a wide range. Here, we investigate the kinetics of N_2O_5 uptake into submicron biomass burning organic aerosol (BBOA) particles, an increasingly relevant substrate due to the rising frequency and intensity of global wildfires, using an aerosol flow tube reactor. Notably, significant uptake of the NO_3 radical was observed, particularly under low NO_2 concentrations where the NO_3/N_2O_5 ratio is elevated. Rapid NO_3 consumption facilitates N_2O_5 dissociation and enhances its apparent decay. Kinetic modeling shows that the N_2O_5 uptake coefficient (γ) increases from 1.8×10^{-4} to 1.4×10^{-3} as relative humidity (RH) rises from 25% to 71%, consistent with increasing particle water content. In contrast, $\gamma(NO_3)$ exhibits an inverse RH dependence, decreasing from close to a unity at 25% RH to ~0.25 at 71% RH. Mechanistic analysis based on kinetic data elucidates the relative roles of interfacial vs. bulk reactions. Together, our results provide insights into how N_2O_5 uptake onto BBOA particles may influence the reactive nitrogen budget and then the atmospheric oxidative capacity in a warming world.

Keywords: Multiphase reactions, Aerosol kinetics, Reactive nitrogen, Wildfire particles

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O-27 Brown carbon in biomass burning aerosol enhances HONO production

Thursday, 21 May, 11:30 am

Presenter: Fengxia Bao
Authors: Fengxia Bao[1]; Markus Ammann[1]

[1] Paul Scherrer Institute, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland

Nitrous acid (HONO) is an important source of hydroxyl radicals (·OH). ·OH drives ozone and aerosol formation, impacting air quality, health and climate. Elevated HONO concentrations have been observed in biomass burning (BB) plumes. However, the mechanism remains unclear, hindering parameterization and quantification of the impacts. Here, we conducted flow tube experiments with BB aerosol samples and proxies (3,4-dihydroxybenzaldehyde (DHB) and benzophenone (BP)) to investigate renoxification, a process that converts nitrate into HONO and NOx (NO and NO_2). We find that renoxification in BB aerosol is largely driven by brown carbon (BrC). We develop a parameterization to assess global impacts of the BrC-driven renoxification, which suggests that BrC enhances surface-level HONO production by one order of magnitude in BB-affected regions. Our findings establish BB aerosol as a critical, large-scale, yet previously underestimated source of HONO. By acting as a donor of eaq-, BrC enables BB aerosol to efficiently reduce nitrate into HONO while being oxidized itself. The subsequent photolysis of HONO leads to the production of ·OH and O_3, sustaining the oxidative capacity of the plume far downwind. Meanwhile, the oxidized BrC may undergo further aging processes, influencing aerosol aging and radiative forcing, which warrants future investigation. This mechanism resolves the paradox of persistent HONO production in aged plumes and redefines BB plumes as active photochemical reactors that couple reactive nitrogen recycling with aerosol aging. Apart from the immediate harmful impacts of fires, this work highlights their long-term effects on air quality and climate through the long-range transport of emissions and reactive species. Guided by this framework, we highlight that incorporating BrC-driven renoxification of BB aerosol into global atmospheric models is crucial for accurately predicting atmospheric chemistry, evaluating air quality and developing effective climate policies. This is particularly urgent as climate warming increases the frequency and intensity of fires, amplifying BrC-driven renoxification and aggravating its impacts.

Keywords: HONO, Brown carbon, nitrate, renoxification, NOx

O-28 Single-Particle Levitation as a Window into Aerosol Chemistry, Light Absorption, and Phase State

Thursday, 21 May, 2:10 pm

Presenter: James Davies
Authors: James Davies[1]

[1] UC Riverside, United States

Light-absorbing aerosol particles containing black and brown carbon are an important component of the atmosphere, particularly in regions impacted by wildfires. Although black carbon dominates light absorption across the solar spectrum, organic brown carbon can have significant contributions in the near-UV and visible wavlength range. The brown carbon chromophores responsible for light absorption coexist with a complex mixture of organic and inorganic species and are often highly sensitive to their chemical environment, including pH, water content, and ionic strength. In this talk, I will describe the development and application of a linear quadrupole electrodynamic balance for probing the physicochemical properties of individual light-absorbing aerosol particles. Using broadband light scattering, I will show how pH-dependent light absorption can be characterized for a range of common brown carbon chromophores. I will also demonstrate how single-particle mass spectrometry can be used to track chemical transformations that drive the evolution of aerosol optical properties. Finally, I will discuss how interactions between organic molecules and inorganic ions in aqueous particles can perturb the phase state, with important consequences for their heterogeneous and photochemical aging in the atmosphere.

Keywords: light absorption, phase state, heterogeneous reactions

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O-29 The Role of Partitioning and Bulk Depletion in the Apparent Surface pKa of Microdroplets

Thursday, 21 May, 2:50 pm

Presenter: Michael Jacobs
Authors: Michael Jacobs[1]; Rebika Tamang[1]; William Dean[1]; Jacob Twichell[1]; Christian Haich[1]

[1] Texas State University, 601 University Drive, San Marcos, Texas 78666-4684, United States

The chemical composition and acidity of the air-water interface are fundamental drivers of atmospheric processing of aerosol particles, yet their role in governing aerosol behavior remains a subject of intense debate. The reported ability of surface water to either accept or donate protons changes depending on how it is assessed, with some studies suggesting the surface is proton-rich, but others suggesting it is hydroxide ion-rich. Historically, to assess surface acidity, a 'surface pKa' has been defined for molecules that can be shifted by several units relative to their bulk pKa values. For example, medium and long chain alkyl acids can have a surface pKa > 7, indicating a proton-rich interface. However, the molecular origins of shifted surface pKa values remain unclear. Do they report on the acidity of surface water, or do they report on the different surface affinities of protonated/deprotonated species? Ultimately, an accurate, molecular-level understanding of surface acidity would inform both how surface chemistry can alter reaction kinetics in microdroplets and lead to a better understanding of surface tensions of atmospheric aerosol particles, which influences their ability to nucleate clouds. We use a single droplet levitation experiments to study how the unique physicochemical properties of microdroplets and aerosol particles can alter chemistry. Using model chemical systems, we measure the pH and surface tensions of levitated microdroplets to gain insight into the chemistry of the atmosphere. Here, we present recent experimental results aimed at understanding how the acidity of surface water changes molecular partitioning to the air-water interface and influences the pH of aerosol particles. Using macroscale surface tension measurements, we demonstrate that shifts in the apparent 'surface pKa' of alkyl acids can largely be explained by a simple partitioning model. However, in microdroplets, we find this value is further complicated by bulk-depletion effects. By measuring the surface tensions and pH of alkyl acid-laden microdroplets, we use our partitioning model to describe how changing surface pKa values can alter the pH and surface tensions of microdroplets. Ultimately, we find the surface concentrations of protonatable species in microdroplets are governed by droplet size, molecular concentration, and surface acidity. These results contribute to a fundamental understanding of how the unique chemical properties of the air-water interface can alter the chemical composition of microdroplets to promote a wide array of chemical reactions or change the atmospheric processing of aerosol particles.

Keywords: air, water interface, surface acidity, aerosol pH, microdroplets, surface tension

O-30 Detection of Controversial Microdroplet Assisted Degradation and Oxidation Products

Thursday, 21 May, 3:30 pm

Presenter: Paul Tumminello
Authors: Paul Tumminello[1]; Nathan Bays[1]; David Schafer[1]; Samantha Kruse[1]; Brynal Benally[1]; Jake Zenker[1]; Leonid Sheps[2]; Ryan Davis[1]

[1] Sandia National Laboratories, PO Box 5800, Albuquerque, NM 87185, United States
[2] Sandia National Laboratories, P.O. Box 969, Livermore, CA 94551-0969, United States

Observations of oxidation reactions occurring at the air-water-interface of aqueous microdroplets have recently generated significant interest and controversy among atmospheric chemists. Many of the reported reactions occurring in microdroplets are accelerated significantly when compared to the bulk, leading to remarkable implications for a variety of industrial and environmental processes. Some of the controversy stems from a lack of reproducibility within the community, wherein some observations have not yet been successfully replicated. Determining if these reactions are occurring and why only some researchers are observing them is paramount to advancing our understanding of microdroplet chemistry. In this work, we report efforts to replicate two surprising observations from the literature: Spray-based degradation of perfluorooctanoic acid (PFOA), a persistent organic pollutant, and oxidation of gaseous volatile organic carbon (VOC) compounds (e.g., methane and ethane). Aqueous microdroplets were generated via custom sprayers based on previously published designs. A combination of chromatography and mass spectrometry was used to quantify resulting degradation and oxidation products. Initial results indicated a higher occurrence of spray-based PFOA degradation, 3X more degradation than reported in the literature. In the case of VOC oxidation, however, we could not replicate previous reports without deviating significantly from published experimental design and detection methods. Observing VOC oxidation necessitated the use of an ultra-trace detection scheme, a cryogenic focusing gas chromatography mass spectrometer (Cryo-GCMS). The Cyro-GCMS detected oxidation products that were 5-6 orders of magnitude less concentrated than reported in the literature, well below the limit of detection for many commonly employed detection schemes. Ultimately, our observations suggest that microdroplet assisted oxidation does occur in sprays, albeit with dramatic variability between experimental setups and conditions.

Keywords: microdroplet, gc, ms, pfoa, methane, ethane, voc

O-31 Spontaneous chlorate formation on sea salt crystal surfaces upon surface solvation

Thursday, 21 May, 3:40 pm

Presenter: Nicolas Fauré
Authors: Nicolas Fauré[1]; Ivan Gladich[2]; Luis Escusa Dos Santos[3]; Andrey Shavorskiy[4]; Luca Artiglia[5]; Xiangrui Kong[1]; Erik Thomson[1]

[1] University of Gothenburg, Sweden
[2] University of Urbino, Italy
[3] Chalmers University of Technology, Sweden
[4] MAX IV Laboratory, Sweden
[5] Paul Scherrer Institute, Switzerland

Surfaces expose chemical entities to unique environments, such as strong localized electric fields and domains of partial solvation, which can alter both the thermodynamics and kinetics of chemical reactions. Redox pathways that are absent in bulk solutions have been reported to occur spontaneously on surfaces, primarily based on studies of aqueous solution surfaces. Surfaces of solid materials, like salts, may begin to solvate at relative humidities (RHs) well below their deliquescence points. Similar to aqueous solution surfaces, solvating salt surfaces may exhibit unique chemical reactivities, yet such systems remain largely unexplored.

Here, we investigate surfaces of crystallized sea salt, formed by evaporating droplets of Arctic Ocean water, across a range of RH conditions from dry (0%) to 18.9%, using two surface-sensitive techniques: Ambient Pressure X-ray Photoelectron Spectroscopy (APXPS) and Auger-Meitner electron yield Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy. We observe unexpected spontaneous oxidation of surface chloride (Cl^-) to chlorate ($ClO_3{}^-$) upon exposure to water vapor. The oxidation pathway appears to occur in/on solvated magnesium chloride domains at the sea salt surface. Depth-resolved measurements reveal that $ClO_3{}^-$ is further enriched at the topmost surface of these domains. Beam-induced oxidation is ruled out by monitoring the evolution of $ClO_3{}^-/Cl^-$ molar ratio as a function of X-ray exposure time and shows that the ratio decreases under the beam rather than growing. Together, these results underscore the unique chemical reactivity of solvated surfaces on salt crystals. On Earth, chlorate has been detected in minerals, lakes, snow and aerosols in various arid environments. Although ozone oxidation is generally considered to be the dominant formation pathway, discrepancies between modelled and observed chlorate concentrations persist. This previously unrecognised surface-mediated pathway for chlorate formation may help to resolve the observed discrepancies

Keywords: Sea Salt Particles, Surface Chemistry, Chlorate, Arctic, APXPS

O-32 Development and Application of Novel Tools for Exploring Accelerated Chemical Reactivity in Aerosol Droplets

Thursday, 21 May, 3:50 pm

Presenter: Bryan Bzdek
Authors: Bryan Bzdek[1]

[1] University of Bristol, Bristol, United Kingdom

Recent observations of chemistry being accelerated up to 10^7-fold in microscopic droplets could revolutionise chemical synthesis and transform our understanding of aerosols, with the potential impacts extending to fields like atmospheric chemistry and the origin of life. However, these observations simultaneously pose a direct challenge to our basic understanding of chemistry. Aerosols magnify the importance of interfacial chemistry and allow access to supersaturated solute states because of their high surface area-to-volume (S/V) ratios, providing routes to catalyse chemical change in ways impossible in macroscopic systems. Disentangling the competing contributions to accelerated reactivity is challenging due to the complex coupling between physical and chemical processes in aerosols and the unique environment of the droplet-air interface. This presentation will describe novel approaches developed in our lab to explore chemical reactivity in aerosol droplets from picolitre to zeptolitre droplet volumes. These approaches will be applied to different chemical systems where chemical reactivity is anticipated to be catalysed by the high S/V ratio environment of the droplet, namely an esterification reaction between an alcohol and a carboxylic acid and a protein digestion reaction. Lastly, an approach to controllably modify the electric field strength at the droplet-air interface will be presented, along with its potential applications to studies of accelerated reactivity.

Keywords: accelerated reactivity, picolitre droplets, nanoparticles, mass spectrometry

O-33 Anomalous surface-activities of doubly charged sulfur oxyanions in submicron aerosols

Thursday, 21 May, 4:10 pm

Presenter: Alexandra Deal
Authors: Alexandra Deal[1]; Sorren Warkander[2]; Sean Boyce[1]; Madison Foreman[2,3]; Dan Neumark[3,2]; Musa Ahmed[2]; Kevin Wilson[2]

[1] University of Michigan, Michigan, United States
[2] Lawrence Berkeley National Laboratory, 1 Cyclotron Rd. MS 50A-1148, Berkeley, CA 94720, United States
[3] University of California, Berkeley, CA, United States

Quantitative understandings of ion surface-activities are crucial for understanding their physicochemical impacts on aerosols and microdroplets. Of particular interest are aqueous sulfur oxyanions, which can have significant contributions to atmospheric chemistry and climate via the concentration and distribution of S(VI). We have investigated the surface-activities of five aqueous sulfur axions with aerosol X-ray photoelectron spectroscopy, a surface-specific spectroscopic technique recently proven to detect solute surface-activities in submicron aerosols with quantitative accuracy. We find that sulfate (SO_4^{2-}) and sulfite (SO_3^{2-}) are repelled from the interface (with Langmuir equilibrium constants, K_L, of 7×10^{-4} M^{-1} and 4×10^{-4} M^{-1}, respectively), but thiosulfate ($S_2O_3^{2-}$), persulfate ($S_2O_8^{2-}$), and tetrathionate ($S_4O_6^{2-}$), have significant surface-activities (K_L = 4.4 M^{-1}, TBD, and 11 M^{-1}). Here, we will discuss potential drivers for these varied surface-activities including solvation structure, polarity, and size.

O-34 Interplay of phase state and multiphase chemistry in nanoparticle growth and evaporation of secondary organic aerosol

Friday, 22 May, 9:10 am

Presenter: Thomas Berkemeier
Authors: Thomas Berkemeier[1]; Hyun Kang[2]; Zhiqiang Zhang[2]; Maja Radecka[2]; Masayuki Takeuchi[3,4]; Nga L. Ng[3]; Ulrich Pöschl[2]

[1] Max Planck Institute for Chemistry, Germany
[2] Max Planck Institute for Chemistry, Germany
[3] Georgia Institute of Technology, United States
[4] University of Colorado Boulder, United States

Recent studies have shown that evaporation rates of secondary organic aerosol (SOA) particles may be slower than expected (Vaden et al. 2011; Berkemeier et al. 2020) and that growth rates of ambient SOA nanoparticles show surprisingly little dependency on condensable vapors in the gas phase (Kulmala et al., 2022). A large fraction of SOA may exist in oligomerized form, which might alter their condensation and evaporation. Additionally, SOA can be highly viscous, which leads to kinetic limitations in evaporation, slowing of particle-phase chemistry, and non-equilibrium partitioning. The effects of composition, oligomerization, and slow diffusion are inherently coupled, as high concentrations of low-volatility compounds or products of accretion reactions can cause high viscosity. We use a kinetic multi-layer model to estimate the kinetic limitations affecting SOA formation and fate in laboratory experiments and the ambient atmosphere. The model explicitly considers gas- and particle-phase chemistry, kinetic gas-particle partitioning, and composition-dependent bulk diffusivity. We re-analyze data from laboratory chamber experiments with mixtures of terpenes as SOA precursors (Berkemeier et al. 2020) as well as published field and laboratory chamber data of nanoparticle growth (Stolzenburg et al., 2025) to find pronounced effects of multiphase chemistry and particle phase state under these conditions. Especially the partitioning of semi and low-volatile organic compounds (SVOC/LVOC) is strongly affected by these processes in the model, while the partitioning of extremely- and ultra-low volatility organic compounds (ELVOC/ULVOC) is less affected. We discuss the possible effect of growth limitation through bulk accommodation in models

that follow monolayer adsorption schemes versus models that allow the "burying" of surface-adsorbed molecules through multi-layer adsorption. The model predicts that, during particle evaporation, particles may be radially heterogeneous with respect to composition and diffusivity: higher volatility chemical species evaporate more quickly than oligomers or lower volatility species, leaving behind a near-surface layer crust of more viscous material that presents a barrier for further evaporation. The results highlight gaps in our knowledge about the physical and chemical properties of SOA and their interactions. References Berkemeier, T., Takeuchi, M., Eris, G., Ng, N. L. Atmos. Chem. Phys. 20, 15513-15535 (2020). Kulmala, M., Cai, R., Stolzenburg, D., et al. Environ. Sci.: Atmos. 2, 352-361 (2022). Stolzenburg, D., Sarnela, N., Bianchi, F. et al. npj Clim Atmos Sci 8, 75 (2025). Vaden, T. D., Imre, D., Beranek, J., et al. P. Natl. Sci. Acad. USA 108, 2190–2195 (2011).

Keywords: Secondary Organic Aerosol, Phase State, Diffusion, Volatility, Modelling

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O-35 Detection of Highly Oxidized Molecules from Ethylbenzene Oxidation Using Matrix Assisted Ionization in Vacuum - Mass Spectrometry

Friday, 22 May, 9:50 am

Presenter: Lisa Wingen
Authors: Lisa Wingen[1]; Elizabeth Wingen[1]; Yiming Qin[2]; Michelia Dam[3]; James Smith[1]; Barbara Finlayson-Pitts[1]

[1] University of California, Irvine, United States
[2] City University of Hong Kong, 83 Tat Chee Avenue, Kowloon-Hong Kong, Hong Kong SAR China
[3] California Air Resources Board, 1001 I Street, Sacramento, CA 95814, United States

Aerosol particles are central to many atmospheric processes that affect human health, air quality, and climate. Aromatic compounds are a significant precursor of secondary organic aerosol (SOA), especially in urban regions. Pathways for oxidation of aromatic compounds involve the formation of highly oxidized molecules (HOM), but mechanisms are not fully understood. In addition, it is not clear which HOM formation pathways participate in the growth of existing particles and nucleation of new particles. Matrix assisted ionization in vacuum – mass spectrometry (MAIV-MS) was used to measure HOM generated from OH oxidation of ethylbenzene (C_8H_{10}) that are scavenged to matrix particles. The use of solid glutaric acid particles as a matrix allows matrix ions along with co-adsorbed species to be spontaneously emitted from the surface and detected in the absence of an ionization source. The soft ionization and mild thermal conditions in the MS inlet facilitate the detection of HOM, including thermally labile peroxides. Matrix particles provided a large condensation surface area for gas phase HOM to condense, allowing detection of a series of ethylbenzene HOM products having up to 16 carbon atoms and 12 oxygen atoms. Measurements using nitrate chemical ionization mass spectrometry (NO_3-CIMS) provided a comparison of products remaining in the gas phase to those scavenged to the particle surface measured with MAIV. MAIV intensities for ROOR (C_{16}) products were much higher than those for ROOH (C_8) compared to CIMS. The results suggest that ROOR are more likely to grow particles and participate in nucleation of new particles. Optimizing the surface area of the matrix particles to increase the HOM condensation sink confirmed this observation and led to insights on which HOM products are most involved in growing particles and nucleating new ones. Insights on which pathways form these products will also be presented.

Keywords: secondary organic aerosol (SOA), aromatics, highly oxidized molecules (HOM), particles, nucleation

O-36 Photo-Fenton reactions drive mass loss and volatility decrease in Fe-containing α-pinene secondary organic aerosol

Friday, 22 May, 10:10 am

Presenter: Natasha Garner
Authors: Natasha Garner[1,2]; Jens Top[1]; Fabian Mahrt[1,3]; Sabine Lüchtrath[4]; Sacha Fallah[1]; Katie Kolozsvari[5]; Andrew Ault[5]; Andreas Held[4]; Imad El-Haddad[1]; Markus Ammann[1]; David Bell[1]

[1] Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland
[2] University of Leeds, Woodhouse Lane, Leeds LS2 9JT, United Kingdom
[3] Aarhus University, Nordre Ringgade 1, DK-8000 Aarhus C, Denmark
[4] Technical University of Berlin / Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany
[5] University of Michigan, 500 Church Street, Ann Arbor, MI 48109-1090, United States

Secondary organic aerosol (SOA) play a key role for air pollution, health and climate. They often comprise the majority of submicron particles by mass, and can become internally mixed with inorganic particles such as mineral dust. When transition metals like Fe are present, they can initiate aging processes that alter physical and chemical SOA properties. Furthermore, they can facilitate dissolution of minerals and form Fe-organic complexes, which are common in atmospheric particles. They can further generate reactive oxygen species within particles through dark peroxide and photochemical reactions (Fenton chemistry), leading to further aging of SOA by functionalization or fragmentation of organic species. Given the chemical complexity of SOA, a detailed understanding of these aerosol-aging processes and the subsequent impact they have on air quality, health and climate is lacking. Here, we present data on the molecular-level chemical composition of Fe-containing SOA and how it evolves over time. Particles were produced by forming SOA via α-pinene ozonolysis on both ($(NH_4)2SO_4$ or Fe-containing seed particles in an atmospheric simulation chamber under dark conditions at low and high relative humidities (RH). This allowed us to probe the impact of dark e.g., peroxide, reactions on aerosol aging with varying aerosol mixing states. Additionally, the impact of photochemically driven Fenton chemistry was studied by irradiating particles with UV light. Aerosol bulk composition was determined using extractive electrospray ionization mass spectrometry, allowing for high chemical and temporal identification of oxidation products, i.e., monomers and dimers. At low RH, all particles were found to contain a higher fraction of monomers, compared to dimers. In contrast, at high RH the monomer/dimer ratio was smaller when Fe was present due to rapid condensed-phase oligomerization reactions. This increased gas-particle partitioning of semi- and low-volatility species, increasing SOA mass. As Fe-containing SOA aged, the monomer/dimer ratio remained small; however, the composition shifted towards lower carbon number monomers and dimers likely from Fe-driven fragmentation reactions. Following irradiation, significant aerosol mass loss - driven through photo-Fenton radical production, and enhanced fragmentation and functionalization reactions - was observed for Fe-containing particles under high RH conditions. This included loss of many higher volatility species, resulting in a composition and volatility shift in particles' remaining organic fraction. The same trend was not observed at low RH, highlighting that internal aerosol mixing state is critical for the formation of photochemically active Fe-organic complexes. Furthermore, trends in the timeseries for individual monomers and dimers provide potential insight into the identity of these Fe-complexes and mechanisms at play. These results suggests that Fe-catalyzed reactions (both under dark and light conditions) affect the composition of SOA, particularly at higher RH, as is common in many regions of the troposphere.

O-37 Matrix Effects Reshape Organic Aerosol Volatility and Atmospheric Persistence

Friday, 22 May, 11:00 am

Presenter: Alexander Laskin
Authors: Qiaorong Xie[1]; Abigail M. Smith[1]; Sara C. Botero-Carrizosa[1]; Steven A. L. Sharpe[1]; Gali Dekel[3]; Nicole A. June[4]; Manish Shrivastava[4]; Yuqing Dai[5]; Kevin Ridgway[6]; Christian L'Orange[6]; Shantanu H. Jathar[6]; Katherine S. Hopstock[7]; Sergey A. Nizkorodov[7]; Yinon Rudich[3]; Alexander Laskin[1,2]

[1] Department of Chemistry, Purdue University, West Lafayette, Indiana 47907, United States
[2] Department of Earth, Atmospheric, and Planetary Sciences, Purdue University, West Lafayette, Indiana 47907, United States
[3] Department of Earth and Planetary Sciences, Weizmann Institute of Science, Rehovot 76100, Israel
[4] Atmospheric, Climate, and Earth Sciences Division, Pacific Northwest National Laboratory, Richland, Washington 99352, United States
[5] School of Geography, Earth and Environmental Science, University of Birmingham, Birmingham B15 2TT, United Kingdom
[6] Department of Mechanical Engineering, Colorado State University, Fort Collins, Colorado 80523, United States
[7] Department of Chemistry, University of California, Irvine, California 92697, United States

Matrix effects in chemically complex organic aerosol (OA) mixtures markedly suppress the apparent volatility of individual species, causing substantial deviations from intrinsic, pure-compound-based volatility assumptions. When implemented in chemical transport modeling, these reduced volatilities lead to large increases in predicted biomass-burning OA mass loadings, extended atmospheric lifetimes, and enhanced regional transport. The results demonstrate that neglecting matrix effects can systematically underestimate OA burdens and their climate and air-quality impacts. Incorporating mixture-dependent volatility parameterizations is therefore essential for improving predictions by regional and global atmospheric models. Herein, we systematically investigate component-resolved, mixture-specific volatility for more than 1,500 individual species across 33 proxies and chemically complex mixtures representative of selected organic aerosol types. The results show that species in simplified proxies and reference mixtures with limited components follow a higher-volatility trend that approaches their intrinsic values, whereas species present in ambient and biomass-burning organic aerosols exhibit the opposite behavior, with systematically reduced apparent volatility attributable to matrix effects. Using levoglucosan (LG), a representative biomass-burning tracer, as an illustrative example, we find that its volatility in complex organic mixtures is reduced by 1–4 orders of magnitude relative to its intrinsic volatility in pure LG. This pronounced reduction underscores strong matrix effects that substantially suppress the apparent volatility of individual species in mixed systems. Machine-learning analysis further indicates that mixture-dependent molecular metrics are more predictive of apparent volatility than compound-specific molecular properties that define intrinsic volatility. Collectively, these findings highlight the critical role of intermolecular interactions in governing gas-particle partitioning in multicomponent systems. This study provides strong evidence that matrix effects significantly influence the apparent volatility of individual species in aerosols and other environmental organic mixtures and should be explicitly considered in volatility prediction frameworks and aerosol transport models.

O-38 Advancing multidimensional physicochemical processes and AI-assisted detection at interfaces

Friday, 22 May, 11:20 am

Presenter: Parisa Ariya
Authors: Parisa Ariya[1]

[1] McGill University, Canada

Understanding the multidimensional physicochemical processes that govern particles and interfaces is central to predicting their environmental and health impacts. Aerosols—small particles suspended in air, play a critical role in climate forcing and contribute to millions of premature deaths annually. Our research advances fundamental knowledge of the formation and transformation of radicals, atoms, and particles across a broad range of sizes and compositions, with relevance to nanoplastics, black and brown carbon, radiation chemistry, medical diagnostics, and sustainable technologies. This presentation highlights three pillars if this talk. (1) We develop real-time methods to characterize interfacial and surface physicochemical properties, enabling direct observation of transient processes. (2) We pioneer the study of nano-ice nucleation and microphysical pathways that drive cloud formation and influence atmospheric chemistry. (3) We leverage natural nanoparticle surfaces to reduce air pollution, using novel spectroscopy approaches that catalyze sustainable, nature-based reaction pathways. We will discuss the broader scientific and technological impacts of this work, including its relevance to global climate processes, environmental health, and emerging opportunities enabled by AI-assisted detection. Challenges and future research directions will also be presented.

Poster Abstracts

P-01 Pop It Like It’s Hot: Probing Organic Aerosol Viscosity One Particle at a Time

Wednesday poster presentation

Presenter: Andrew Ault
Authors: Andrew Ault[1]; Katherine Kolozsvari[2]; Cara Waters[2]; David Bell[3]; Natasha Garner[3,4]; Jin Yan[5]; N. Armstrong[5]; Madeline Cooke[2]; Alison Fankhauser[2]; Yao Xiao[2]; Rebecca Parham[2]; Jens Top[3]; Markus Ammann[3]; Jason Surratt[5]

[1] University of Michigan, United States
[2] University of Michigan, Ann Arbor, United States
[3] Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland
[4] University of Leeds, Woodhouse Lane, Leeds LS2 9JT, United Kingdom
[5] University of North Carolina, Chapel Hill, United States

The phase state and viscosity of organic aerosol are critical determinants of mixing time scales within individual particles, which impacts heterogeneous reaction kinetics and product formation. Both secondary organic aerosol (SOA) and biomass burning organic aerosol (BBOA) are often mixed with inorganic species, which makes it difficult to predict their individual particle phase state based on ensemble average measurements, such as digital scanning calorimetry. Herein, we use nanothermal analysis (NanoTA), which uses a heated atomic force microscopy (AFM) tip to probe the melting temperature of individual particles. We use NanoTA to probe three important organic aerosol systems: isoprene epoxydiol (IEPOX) SOA, α-pinene + ozone SOA, and biomass burning. These measurements are then compared to established models converting bulk mass spectrometry data to viscosities and mixing time scales. For IEPOX SOA we show that at high relative humidity (RH) measurements and models agree well, but that below 50% RH models overpredict viscosity of the organic material. For α-pinene ozonolysis SOA we show that the presence of seed aerosol (no seed, ammonium sulfate, and Fe(II) ammonium sulfate) strongly impact the amount and composition of SOA forming, as well as the glass transition temperature. After UV aging, the viscosities converge towards a consistent and viscous state. Lastly, biomass burning aerosol with and without aging by ·OH radical show that ·OH oxidation leads to more viscous SOA. Together these results provide insight into the physicochemical changes that result for different important forms of organic aerosol, which has important implications for understanding their atmospheric behavior and impacts.

Keywords: Aerosol Phase State, Secondary Organic Aerosol, Biomass Burning Organic Aerosol, Viscosity, Mixing Time Scales

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P-02 Estimating the Composition of Biomass Burning Primary Organic Aerosol

Thursday poster presentation

Presenter: Dan Barthaux
Authors: Dan Barthaux[1]; Andreas Zuend[1]

[1] McGill University, Department of Atmospheric and Oceanic Sciences, Montreal, Québec, H3A 0B9, Canada

Biomass burning is a major emission source of organic aerosols (OA). We compiled a dataset of measured emission ratios for 691 compounds and expressed their concentrations as functions of total emitted volatile organic compounds and pyrolysis temperature. We performed gas–particle partitioning calculations using the Aerosol Inorganic–Organic Mixture Functional groups Activity Coefficients (AIOMFAC) thermodynamic model to attain the corresponding compound-resolved OA composition and mass concentration. Initial comparisons of partitioning predictions to laboratory and field data suggested that a pool of intermediate- or semi-volatile organic compounds with large oxygen-to-carbon (O:C) and hydrogen-to-carbon (H:C) ratios

was missing from the speciated measurements. To match these measurements, we inserted a surrogate IVOC compound and increased concentrations of compounds with high H:C ratios. This adjustment resulted in better general agreement with measured OA mass concentrations and average O:C and H:C ratios. Analysis using Latin hypercube sampling revealed that wildfire smoke plume mass concentrations were consistently above the predicted range, possibly serving as an indicator for the rapid formation of secondary organic aerosol.

Keywords: wildfire, biomass, burning, primary, POA, partitioning, emissions, organic

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P-03 Individual Quantification of Organic Peroxides in Aerosols Using HPLC In-Column Derivatisation with Chemiluminescence Detection

Wednesday poster presentation

Presenter: Julia Bechter
Authors: Julia Bechter[1]; Julian Resch[1]; Kangwei Li[1]; Arianne Soliven[2,3]; Andrew Shalliker[3,4]; Markus Kalberer[1]

[1] University of Basel, 4056 Basel, Switzerland
[2] Avantor, Theale, Reading RG7 4PE, United Kingdom
[3] Western Sydney University, South Parramatta Campus, NSW 2151, Australia
[4] Chromaspeed Pty Ltd., Tonsley, SA 5042, Australia

Secondary organic aerosols (SOA) are formed by the oxidation of volatile organic compounds in the atmosphere and have been the subject of numerous studies due to their impact on human health and the Earth's climate. A significant fraction of SOA is composed of organic peroxides, which are considered to have a major impact especially on aerosol-health effects due to their high reactivity and oxidation potential. The majority of peroxide quantification methods described in literature are employed for the determination of the total peroxide concentration of samples and are based on UV-Vis spectroscopic detection such as iodometric titration. However, this technique lacks the ability to quantify individual organic peroxides in complex mixtures such as aerosols and usually requires a reaction time of several hours. In addition, chemical structures of most peroxides in aerosols are unknown and therefore commercial standards are not available. In order to overcome these limitations, we developed a high-performance liquid chromatography (HPLC) in-column derivatisation method with chemiluminescent detection to separate and quantify individual organic peroxides with varying peroxide functional groups. We adapted a detection method from Calandra et al., (2015), in which the cytochrome c-catalysed luminol reaction was used for derivatisation after chromatographic separation. Due to the fast reaction time and reactivity towards a wide range of peroxides, including hydroperoxides, peroxyacids and diacyl peroxides, this reaction is optimally suited for post-column derivatisation. A novel in-column derivatisation (ICD) fitting (Manwaring et al., 2023) was utilised to minimise the dead volume and optimise the mixing to avoid loss of chromatographic separation performance during post-column derivatisation. Iodometric titration with UV-Vis detection was employed to validate the system. We optimised various HPLC parameters including the eluent flow rate, the column temperature, the mixing ratio of the HPLC and derivatisation reagent, and the concentrations of luminol and cytochrome c as well as the pH of the buffer solution. Subsequently, we used a mixture of different commercially available peroxide standards for the calibration of the system. Complex samples containing mixtures of peroxides using liquid-phase ozonolysis (Li et al., 2024) of α-pinene and 3-carene, and laboratory generated SOA, using an oxidation flow reactor (Keller et al., 2022), from α-pinene, 3-carene, and naphthalene were prepared. A similar signal response was observed for peroxides with varying peroxide functional groups at concentrations below 100 µM, with quantification possible down to 25 pmol for individual peroxides. In liquid-phase ozonolysis of terpenes, large amounts of hydrogen peroxide and up to 10 different small peroxides were quantified. The analysis of SOA samples revealed strongly varying peroxide profiles across the biogenic and anthropogenic precursors. Comparisons between the total peak area obtained through

HPLC chemiluminescent detection (HPLC-CL) and the peroxide concentration obtained through iodometric titration revealed a clear correlation. This confirms the broad quantitative capability of the novel HPLC-CL method developed here for a wide range of peroxides.

Keywords: aerosol peroxides, quantification, hydroperoxides, chemiluminescence, luminol, in, column derivatisation

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P-04 Influence of Amino Acids and Surfactants on Aerosol Phase Transitions

Thursday poster presentation

Presenter: Miriam Freedman
Authors: Miriam Freedman[1]; Kiran Pitta[1]; Reena Jaglan[1]

[1] The Pennsylvania State University, University Park, PA 16802, United States

The fate of aerosol particles in the atmosphere depends on their composition, morphology, and phase state. These chemical and physical properties of aerosol particles impact heterogeneous chemistry, cloud formation, and optical properties. In this poster, we show two recent projects investigating the impact of organonitrogen compounds and surfactants on aerosol phase transitions, focusing on liquid-liquid phase separation. Results from micrometer size aerosol particles are determined using optical, fluorescence, and Raman microscopies. Results for submicron aerosol particles are acquired from cryogenic-transmission electron microscopy.

Studies of aerosol phase transitions have focused on aerosol particles with organic compounds consisting of C, H, and O atoms, although a substantial fraction of organic compounds contain heteroatoms such as sulfur and nitrogen. In this study, non-polar amino acids were used to study the effect of organonitrogen compounds on the phase transitions of model aerosol particles. The ternary internal mixtures used were composed of ammonium sulfate, a non-polar amino acid, and either 2-methylglutaric acid or 1,2,6-hexanetriol (model oxidized organic compounds). A suppression of the separation relative humidity was observed when the concentration of amino acid was more than 50% of the organic component by weight for micrometer droplets. For some systems, the amino acid crystallizes, while the oxidized organic compounds and ammonium sulfate undergo liquid-liquid phase separation, yielding a three-phase system. Trends in the efflorescence relative humidity depend on the solubility of the amino acid. These studies are important in understanding the impact of organic-organic interactions as well as organonitrogen compounds on the phase transitions of aerosol particles, which have consequences for heterogeneous chemistry and cloud droplet nucleation in the atmosphere.

The role of surfactants in controlling the phase state and morphology of phase separated aerosols remains unclear. We have investigated the effects of various hydrocarbon surfactants on the phase transitions and morphology of model secondary organic aerosol particles composed of ammonium sulfate and either 2-methylglutaric acid or 1,2,6-hexanetriol. Distinct morphologies were observed depending on surfactant type, concentration, and relative humidity (RH). At higher surfactant concentrations, in anionic surfactant systems, the ammonium sulfate migrates towards the particle-air interface. Cationic surfactants displayed varied morphology depending on the organic compound. For aerosol particles containing neutral surfactants, two sequential LLPS transitions were observed during the dehumidification cycle. These morphological transitions are primarily controlled by the balance of interfacial and surface energies. Our findings provide a detailed understanding of how different types of surfactants drive phase transitions and morphological evolution in internally mixed aerosols and their potential influence on aerosol-cloud interactions.

P-05 Analytical Techniques to Interrogate the Molecular-Level Details of Emerging Environmental Pollutants in Atmospheric Aerosol

Wednesday poster presentation

Presenter: Samantha Kruse
Authors: Samantha Kruse[1]; Corey Carlos[1]; Mohammad Shohel[1]; David Schafer[1]; Ryan Tumminello[1]; Trinity Griffus[1]; Nathan Bays[1]; Andre Benally[1]; Steve Storch[1]; Jake Zenker[1]; Andres Sanchez[1]; Jess Kustas[1]; Ryan Davis[1]

[1] Sandia National Laboratories, United States

Atmospheric aerosol composition is significantly impacted by human activity, from the increasing presence of microplastics from tire wear and trash burning, to the chemical contamination of water sources that generate spray aerosol. As these aerosols persist in the atmosphere, they transform chemically through both surface and bulk reactions with oxidants and other volatile organic compounds as well as photoaging. There is an increasing need to better understand the interfacial chemistry that is both transforming what humans are exposed to and how it may be removing these pollutants from the environment. In this work, we present two major focuses, (1) developing a 3-D chemical profile of microplastic composition, and (2) exploring accelerated degradation of perfluoroalkyl substances (PFAS) in microdroplets. In the first focus, we have utilized matrix-assisted laser desorption ionization mass spectrometry to create depth profiles of microplastic composition. While this technique typically suffers from high variability in ionization across a sample, we show how machine learning can help categorize spectra in a way that enables a high level of precision and knowledge of the sampling depth within the particle. In the second focus, we discuss how microdroplet-assisted degradation of PFAS can lead to degradation rates of up to 97% without the inclusion of environmentally hazardous catalysts. The influences of particle size as well as PFAS carbon chain length will be explored. By investigating these two areas of atmospheric chemistry, we can better understand the mechanisms behind these chemical changes and the unique chemistry that can occur in aerosol environments. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

Keywords: PFAS, Microplastics, Microdroplet, Mass Spectrometry

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P-06 Nanoscale effects on CCN activation of insoluble particles

Thursday poster presentation

Presenter: Ari Laaksonen
Authors: Ari Laaksonen[1,2]; Ana Piedehierro[1]; Linnea Mustonen[1]; Yrjö Viisanen[1]; Golnaz Roudsari[1]; André Welti[1]

[1] Finnish Meteorological Institute, Finland
[2] University of Eastern Finland, Finland

Understanding the interaction energies of atoms and molecules with the surfaces of nanoparticles having complex surface structures is important for technological processes like heterogeneous catalysis, but also in atmospheric science. The adsorption of water molecules onto insoluble aerosol particles such as various minerals enables them to become nuclei for cloud droplets. Mineral particles play an important role in weather and climate by triggering the freezing of cloud droplets, thereby initiating precipitation. Hitherto, the theoretical description of the cloud condensation efficiency of insoluble particles has suffered from a closure problem because predictions based on water adsorption measurements have not been in agreement with laboratory experiments of cloud drop formation. Here we show that the closure is obtained for a wide range of 50-800 nm sized metal oxide and mineral particles by accounting for two nanoscale factors influencing the adsorption energies of water molecules: the fractal heterogeneities of the surfaces and the particle size. We derive a theoretical formula for the particle size effect and show that it becomes

very pronounced at adsorption layer thicknesses of hundreds of water layers, which are typical during the activation of cloud nuclei but difficult to detect in standard adsorption experiments. Our discovery resolves the closure problem in cloud drop formation and improves understanding of gas and vapor adsorption on nanoparticles in general.

Keywords: CCN activation, adsorption, insoluble aerosol, surface fractal dimension

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P-07 Single-particle spectroscopy of photochemical and ice-nucleation processes in aerosols

Wednesday poster presentation

Presenter: Alexander Logozzo
Authors: Alexander Logozzo[1]; Nadine Borduas-Dedekind[1]; Russ Algar[1]; Thomas Preston[2]; Allan Bertram[1]

[1] Department of Chemistry, University of British Columbia, Vancouver, Canada
[2] Department of Chemistry, McGill University, Canada

Single particle spectroscopy allows for aerosol droplets to be studied in-situ, avoiding ensemble averaging and capturing molecular processes that are often obscured in bulk measurements. This has enabled the investigation of metastable phase states, which influence cloud formation, ice nucleation, and atmospheric aging processes. We have developed a temperature-controlled dual-beam optical trap capable of suspending individual aerosol particles in a contact-free environment. Using Raman spectroscopy, we monitored photochemical transformations in highly concentrated aqueous amino acid and monosaccharide droplets. Under intense visible-light excitation (32 MW cm^{-2}), we found that weakly absorbing organics underwent photochemical reactions at wavelengths (473 - 532 nm) exceeding their core electronic transitions. To determine whether bulk or surface reactions were dominant, we developed a photochemical model that captured the size-dependent autocatalytic behavior of these reactions and attributed the absorption to excitation of the low-energy tail. Future work is focused on developing burst analysis spectroscopy to investigate the aggregation of InaZ, an efficient ice-nucleating protein (INP). Through a combination of single-particle experiments and nanoparticle-protein functionalization, these studied aim to develop a mechanistic understanding of ice nucleation by INPs.

P-08 Photochemical Prebiotic Peptide Formation from HCN-Derived Condensing Agents in Aerosol Microdroplets

Thursday poster presentation

Presenter: Devan Macdonald , Thomas Preston
Authors: Devan Macdonald[1]; Thomas Preston[1]

[1] Department of Chemistry, McGill University, Canada

Peptide bond formation from amino acids is a fundamental step in protein synthesis and a key process of prebiotic chemistry, providing insight on the origins of life. This project explores the significance of hydrogen cyanide (HCN) polymerization on prebiotic earth and uses its derivatives to facilitate dipeptide formation from amino acids. Dicyandiamide and sodium dicyanamide act as condensing reagents within aerosol droplets to promote peptide reactions relevant to early Earth conditions. Using single-particle levitation and cavity-enhanced Raman spectroscopy, the role of atmospheric aerosols as micro-reactors and their efficient molecular interactions at air-water interfaces can be investigated in a surface-free environment, while also allowing for the photochemical processes that form amide bonds between amino acids to be observed. However, photochemical autocatalysis within these condensing reagents limits peptide formation, so the addition of hygroscopic compounds such as sodium chloride (NaCl) help to stabilize these reactions. A significant concentration dependence is explored within this project, by examining how increased salt

levels extend droplet lifetimes and assist in driving dipeptide formation forward. These findings emphasize the potential of atmospheric aerosol micro-droplets as chemical reactors for prebiotic peptide synthesis, with implications for understanding reaction pathways that may have contributed to the origins of life.

Keywords: Prebiotic Chemistry, Optical Trapping, Single, particle Levitation

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P-09 Single-Particle Analysis of Atmospheric Sulfate Aerosol Gels and Phase State Evolution

Wednesday poster presentation

Presenter: Aleksandr Odelskii
Authors: Aleksandr Odelskii[1]; Svitlana Malashevych[2]; Thomas Preston[1,2]

[1] Department of Chemistry, McGill University, Canada
[2] Department of Atmospheric and Oceanic Sciences, McGill University, Canada

Understanding the microphysical properties of atmospheric sulfate aerosols is essential for accurate climate predictions and aerosol–cloud interaction modelling. Under the temperature and humidity conditions characteristic of the upper troposphere and lower stratosphere, these particles undergo complex phase transitions that significantly alter their atmospheric behaviour, yet detailed single-particle measurements remain scarce.

We present a novel experimental approach combining dual-beam optical levitation with cavity-enhanced Raman spectroscopy to investigate the real-time evolution of individual sulfate aerosol particles under controlled atmospheric conditions. Our method enables precise manipulation of temperature, from 220–300 K, and relative humidity, from 10–95%, while maintaining particle isolation, allowing direct observation of phase-state changes and viscosity increases that occur during atmospheric aging processes.

Preliminary results demonstrate the formation of highly viscous, semi-solid states in levitated sulfate droplets under simulated upper-atmospheric conditions. These transitions occur at lower relative humidity than previously predicted, suggesting enhanced particle stability and altered water-uptake kinetics. Raman spectral analysis reveals structural reorganization accompanying the liquid-to-gel transition, with implications for heterogeneous chemistry rates and optical properties.

This work contributes to improved parameterizations of aerosol microphysics in global climate simulations and enhances our understanding of aerosol–climate feedback mechanisms. Furthermore, the obtained data on sulfate aerosol phase behaviour and optical properties under stratospheric conditions can serve as a foundational basis for evaluating the effectiveness and environmental impact of sulfate-based solar radiation management strategies.

Keywords: atmospheric sulfate aerosol, optical trapping, aerosol phase state

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P-10 Surfactant Partitioning: Dynamic Surface Tension Measurements of Picoliter Droplets over Microsecond to Millisecond Timescales

Thursday poster presentation

Presenter: Isabel Quant
Authors: Isabel Quant[1]; Alison Bain[2]; Jim Walker[1]; Bryan Bzdek[1]

[1] University of Bristol, United Kingdom
[2] Oregon State University, United States

Aerosols are microcompartments with high surface area-to-volume ratios. Mounting evidence indicates chemical reactions in aerosols can be accelerated by many orders of magnitude relative to bulk solutions. Because of their high S/V ratios, interfacial chemistry is often implicated in explaining observations of accelerated chemistry. Such interfacial chemistry would be strongly influenced by the interplay between physical (e.g. diffusion, adsorption, evaporation) and chemical (e.g. reaction) steps, highlighting that knowledge about the dynamics of interfacial composition and structure is essential. In the atmosphere, outcomes of this accelerated chemistry can impact atmospheric aerosol composition and air quality. Due to their size and high surface area, aerosol interfaces are highly sensitive to partitioning equilibria, subsequently affecting chemical reactions that can occur and their timescales. Surfactants are important components of atmospheric aerosol composition, mainly from natural sources like sea spray. The dynamic partitioning of surfactants in aerosols can impact interfacial aerosol composition and reaction outcomes. Additionally, the presence of surfactants in atmospheric aerosols can lower the aerosol surface tension with respect to that of water, impacting the formation of cloud droplets. Resolving how surfactants partition to the droplet-air interface is essential both to understand cloud droplet activation and to explain observations of highly accelerated chemical reactions in microcompartments.

One method of measuring dynamic changes to aerosol interfaces in the presence of surfactants is through monitoring dynamic surface tension. The dynamic surface tensions of microscopic droplets can be explored through stroboscopic imaging of a stream of monodisperse picoliter (30 μm diameter) droplets. Ejected droplets undergo characteristic time-dependent shape oscillations, the frequency of which permits retrieval of droplet surface tension as a function of surface age. Although initial studies permit exploration of dynamic surface tensions over several hundred microseconds after droplet generation, such timescales are insufficient to fully characterize surfactant partitioning to the droplet surface, which can take >1 ms. By coalescing two droplets, surface oscillations can be re-excited, allowing access to even longer droplet ages (~500 – 1200 μs after droplet generation).

This contribution presents the results of experiments designed to characterise the dynamic surface tensions of surfactant-laden droplets beyond 1 ms surface age. A novel experimental method was developed where two microdroplet dispensers were positioned such that the droplets they generate coalesce in a controlled and reproducible manner, with the resulting re-excited shape oscillations visualised through stroboscopic imaging. Droplets whose surface tensions span a wide range (e.g. containing water, ethanol, or organic acids) were investigated to validate the developed method, with retrieved surface tensions agreeing with expectations. This new method was then applied to measure dynamic changes in surfactant systems at varying concentrations, expanding previously accessible timescales for this method from~400 μs to up to surface ages of 1.2 ms, tripling original measurement timescales limits. Surface tension results from the surfactant droplets agreed well with an existing diffusion limited kinetic model of surfactant partitioning. This new technique allows for further detailed exploration of kinetic barriers to surfactant adsorption in aerosol surfaces, necessary to understand the impact of surfactants on atmospheric chemistry and cloud formation.

Keywords: dynamic surface tension, aerosol, coalescence, microdroplet

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P-11 Accurate retrieval of single aerosol particle radius and real refractive index using broadband light scattering spectroscopy

Wednesday poster presentation

Presenter: Aidan Rafferty
Authors: Aidan Rafferty[1,2]; Jonathan Reid[3]; Andrew Orr-Ewing[4]; Michael Cotterell[5]

[1] McGill University, Canada
[2] University of Oxford, United Kingdom
[3] University of Bristol, Bristol, United Kingdom
[4] University of Bristol, Cantock's Close, United Kingdom
[5] Department of Chemistry, University of Oxford, United Kingdom

Improved measurements of the refractive index of aerosol particles are essential to improve the accuracy of current climate models. A potentially powerful technique to make such measurements is broadband light scattering (BLS) spectroscopy, which measures the variation in light scattering intensity over a broad range of wavelengths. However, analysis of full BLS spectra is a time-consuming endeavor due to the need to simulate large numbers of synthetic spectra. We introduce a new approach to fitting BLS spectra that addresses this issue by minimizing the number of spectra that need to be calculated. The new method is tested by comparison with concurrent cavity ring-down spectroscopy (CRDS) measurements on two benchmark systems, namely 1,2,6-hexanetriol (a proxy for evaporating semivolatile organic aerosol) and aqueous ammonium sulfate (a proxy for hygroscopic inorganic aerosol). The accuracy of the new method is tested by comparison with the CRDS measurements and comparison of measured BLS spectra against those generated by retrieved parameters. In addition to demonstrating accuracy, we show that radii of particles spanning 0.8-2.5 microns are retrieved with a typical precision of 1.5 nm, and the real part of the refractive index is retrieved with a precision of order 0.001 across the measured wavelength range of 380-800 nm.

Keywords: Optical Trapping, Spectroscopy, Light Scattering

P-12 Oxidation of alkenes by bicarbonate activated peroxide in microdroplets

Thursday poster presentation

Presenter: Mythreyi Rayaluru
Authors: Mythreyi Rayaluru[1]; Kevin Wilson[1]

[1] Lawrence Berkeley Laboratory, United States

Studying mixed phase chemical reactions in microdroplets helps us understand aerosol chemistry in the atmosphere. To this end, we are currently looking at reactions between H_2O_2, a trace atmospheric gas, in the gas phase, and alkenes in microdroplets. The ongoing work aims to understand the kinetics of these reactions in microdroplets and follows closely with some of the work done previously by the group, including the study of multiphase reactions between O_3 and and a number of compounds in the aqueous phase in microdroplets. The current work has been primarily inspired by studies that have shown enhanced oxidizing efficiency of H_2O_2 in the presence of bicarbonate, which acts as a catalyst, thus resulting in a "bicarbonate activated peroxide" or BAP. In the bulk, BAP has shown to efficiently oxidize sulfides and alkenes with conversion efficiencies reaching up to ~ 99%. Additionally, the reported timescales for these reactions in the bulk are considerably long reaching up to 15 hours in the case of alkenes. Preliminary studies are currently being performed using a quadrupole electrodynamic trap to trap droplets containing mixtures of a water-soluble alkene, sodium 4-vinyl benzene sulfonate, and $NaHCO_3$ in microdroplets while using the open-port sampling interface to analyze these droplets in a mass spectrometer. Next immediate experiments involve studying reactions in droplets and using accurate kinetic models to help us better understand the kinetics and mechanism of these reactions.

P-13 Concentration dependence of the Hofmeister series in the droplet phase

Wednesday poster presentation

Presenter: Vahid Shahabadi
Authors: Vahid Shahabadi[1]; Thomas Preston[2]

[1] McGill University, 845 Sherbrooke Street West, Montreal, Quebec H3A 0G4, Canada
[2] McGill University, 845 Sherbrooke Street West, Montreal, Quebec H3A 0G4, Canada

The Hofmeister series ranks cations and anions according to their hydration strength and their ability to structure surrounding water molecules. These ion-specific interactions govern a wide range of physicochemical properties of electrolyte solutions, including solubility, hygroscopic growth, water activity, and surface tension. A defining manifestation of Hofmeister effects is interfacial ion partitioning: strongly hydrated ions preferentially remain in the bulk aqueous phase, whereas their counterions exhibit enhanced propensity for the air–liquid interface, thereby influencing surface composition and electrostatic potential. In this work, we investigate how ion partitioning evolves as a function of concentration using optically levitated microdroplets containing selected electrolytes. By systematically reducing the ambient relative humidity, droplets are driven into metastable, highly supersaturated regimes where ionic concentrations far exceed those achievable in bulk equilibrium solutions. Surface tension measurements, along with Raman spectroscopy under these conditions, are used as a proxy for interfacial composition. This approach enables us to probe how extreme confinement and supersaturation modulate Hofmeister-driven surface segregation and to assess whether conventional dilute-solution trends remain valid at ultrahigh ionic strengths.

Keywords: Hofmeister series, Optical trapping, Raman spectroscopy, Aerosols

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P-14 A Coupled Kinetic–Thermodynamic Aerosol Model Resolving Phase-specific Viscosity and Diffusivities in Simulations

Thursday poster presentation

Presenter: Zixuan Shen
Authors: Zixuan Shen[1]; Andreas Zuend[1]; Manabu Shiraiwa[2]; Meredith Scherwish[2]; Ying Li[3]

[1] McGill University, Department of Atmospheric and Oceanic Sciences, 845 Sherbrooke St W, Montreal, Quebec H3A 0G4, Canada
[2] University of California, Irvine, Department of Chemistry, Irvine, CA 92697, United States
[3] Chinese Academy of Sciences, Institute of Atmospheric Physics, 52 Sanlihe Rd, Xicheng District, Beijing, 100045, China

The chemical and physical properties of ambient aerosol particles, both in outdoor and indoor settings, evolve over a range of timescales due to thermodynamic mixing effects and the kinetics of mass transfer and chemical transformations. At a detailed level, advancing the understanding of aerosol particle behavior in relation to the surrounding gas phase requires a coupled kinetic–thermodynamic modeling approach. The ONION model is a powerful multilayer aerosol box model, developed for dynamic gas–particle partitioning simulations accounting for molecular gas- and bulk-phase diffusion, particle-internal and external interfaces, and dynamic phase separation in aerosol systems. Developed since 2019, ONION simulations have been applied to explore the behavior of multicomponent, multiphase aerosol particles representing either particle systems of interest in comparison to laboratory studies or particle populations to represent ambient conditions. In recent work, this model's numerical robustness, efficiency, and accuracy have been tested under a variety of conditions. These include simulations of particles responding to rapid changes in gas-phase relative humidity (RH), generating steep diffusion gradients, and how RH changes affect the onset or suppression of liquid–liquid phase separation, including as a function of submicron particle size. We will showcase applications of the fractional Stokes–Einstein relation, and explore its limitations in

describing component-specific diffusivity within distinct particle layers by comparing experimental data of different systems. This approach enables detailed tracking of the molecular species distribution and their evolution over time. Moreover, we will investigate how rapid evaporation induces substantial temperature gradients between the gas phase and the aerosol particle surface, and how aerosol particles respond to these gradients. Furthermore, we will demonstrate how ONION simulations facilitate the study of the size- and time-dependent effects of phase separation, alongside the concurrent time-evolution of particle surface tension. With our recent model improvements, the ONION model enables the simulation of multicomponent, multiphase aerosols in a more precise way, offering a pathway to understand the micro-level changes in aerosols that are challenging to measure.

Keywords: liquid–liquid phase separation, multiphase chemistry, gas–particle partitioning, thermodynamic modeling

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P-15 Atmospheric Transformation of Clomazone by OH Radicals: Mechanistic and Kinetic Insights into Gas and Aqueous Phases Oxidation

Wednesday poster presentation

Presenter: Céline Toubin
Authors: Céline Toubin[1]; Madhumita Chakraborty[2]; Sonia Taamalli[2]; Duy Quang Dao[3]; Michal Pitoňák[4]; Florent Louis[2]

[1] Laboratoire de Physique des Lasers, Atomes et Molécules - UMR 8523, Campus Cité Scientifique - Bât. P5 - 2 Avenue Jean Perrin - 59655 Villeneuve d'Ascq cedex, France

[2] Physicochimie des Processus de Combustion et de l'Atmosphère - UMR 8522, Cité Scientifique - Bâtiment C11 - 59655 Villeneuve d'Ascq Cedex, France

[3] Institute of Research and Development, Duy Tan University, Da Nang, Vietnam

[4] Comenius University in Bratislava, Univerzita Komenského v Bratislave, Šafárikovo námestie 6, 814 99 Bratislava, Slovakia

Abstract: Clomazone ($C_{12}H_{14}ClNO_2$), a widely used pre-emergent herbicide in agricultural practices, is highly reactive and has been frequently detected as a persistent organic pollutant in both atmospheric and aquatic environments, reflecting its volatilization, transport, and environmental persistence. Understanding its degradation pathways in both the gas and aqueous phases is essential for assessing its environmental fate, atmospheric lifetime, and potential impacts on air and water quality. In this study, we present a comprehensive theoretical investigation of clomazone degradation with a focus on its oxidation by hydroxyl radicals. Density functional theory (DFT) calculations were performed at the M06-2X/6-311++G(3df,3pd)//M06-2X/6-311++G(d,p) level to systematically explore reaction mechanisms involving both hydrogen abstraction and addition processes. Thermochemical properties and kinetic parameters were computed to evaluate the feasibility and competitiveness of each reaction channel. Among the possible pathways, hydrogen abstraction from the methyl side chains of clomazone was found to be energetically favorable for both the gas and aqueous phase. The most stable degradation products were identified, and further oxidation reactions with OH, O_2, and NOx were considered to generate additional secondary oxidation products. The ecotoxicity of the primary and secondary degradation products in the aqueous phase was assessed using ECOSAR for fish, daphnia, and algae.

Keywords: clomazone, environment, contaminants, reaction mechanisms, kinetics, ecotoxicity, molecular simulations

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P-16 UV Photochemistry of Cysteine in Single Trapped Aqueous Droplets: Reduced-Sulfur Prebiotic Microreactors

Thursday poster presentation

Presenter: Nina Warren
Authors: Nina Warren[1]; Thomas Preston[2]; Aidan Rafferty[3,4]; James Davies[5]

[1] Department of Chemistry, McGill University, Canada
[2] Department of Chemistry, McGill University, Canada
[3] McGill University, Canada
[4] University of Oxford, United Kingdom
[5] UC Riverside, United States

Ultraviolet (UV) radiation is widely considered a major energetic driver of prebiotic chemistry on early Earth, capable of both promoting synthesis and imposing photochemical selection on organic molecules. In particular, reduced sulfur compounds are of interest in the origins of life scenarios due to their rich radical reduction-oxidation (redox) chemistry under UV exposure. However, most experimental investigations of sulfur photochemistry have been conducted in bulk aqueous solutions that may obscure behavior in localized and transient heterogeneous prebiotic environments. Here, we investigate the UV driven photochemistry of the amino acid cysteine within single optically trapped aqueous microdroplets using in situ Raman spectroscopy to monitor real-time chemical evolution. Individual droplets serve as isolated microreactors, allowing direct observation of reduced-sulfur speciation and reaction kinetics under controlled relative humidity and ultraviolet irradiation at 250 nm (UVC) and 285 nm (UVB). Mixtures of cysteine were prepared just below the solubility limit. Measurements of droplet radius and morphology dependent resonances (MDRs) shifts provide insight into concentration-driven confinement effects. Preliminary observations indicate an increase in Raman features associated with S-S bond formation over the course of irradiation, suggesting that UV exposure may contribute to cystine formation beginning the confirmation of more complex molecule generation. This single droplet approach links UV wavelength, chemical composition, and micro-environmental confinement to reduced sulfur photochemical behavior, offering mechanistic insight into how heterogeneous aqueous microenvironments may have shaped chemical selection and molecular survivability under early-Earth surface UV conditions.

Keywords: Prebiotic Microreactors, UV Photochemistry, Cysteine, Microdroplets, Raman Spectroscopy

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P-17 Stereoselectivity in Liquid Aerosols Through Epoxide Ring-Opening Reactions

Wednesday poster presentation

Presenter: Cara Waters
Authors: Cara Waters[1]; Madeline Cooke[2]; N. Cazimir Armstrong[3]; Qiyuan Zhao[1]; Michael Gatazka[1,4]; Yuzhi Chen[3]; Scarlet Aguilar-Martinez[1]; Joshua Kammeraad[1]; Ziying Lei[1]; Anel Alfonso[5]; Luis A. Ladino[5]; Zhenfa Zhang[3]; Avram Gold[3]; Corinna Schindler[4,6]; Paul Zimmerman[1]; Jason Surratt[3]; Andrew Ault[1]

[1] University of Michigan, 500 Church Street, Ann Arbor, MI 48109-1090, United States
[2] University of California, Irvine, CA 92697, United States
[3] University of North Carolina, Chapel Hill, United States
[4] University of British Columbia, 2036 Main Mall, Vancouver, BC V6T 1Z1, Canada
[5] Centro de Ciencias de la Atmósfera, Universidad Nacional Autónoma de México, Ciudad Universitaria, Coyoacán. Ciudad de México. CP 04510. México, Mexico
[6] BC Cancer Research Institute, 675 West 10th Avenue, Vancouver, BC, V5Z 1L3, Canada

Stereoisomers are assumed to be present in equal concentrations as aqueous atmospheric aerosols are most commonly mixtures of simple inorganic salts with a range of organic species that lack obvious pathways

to induce stereoselectivity. Further, since submicron aerosols are highly acidic (pH ~0-3), acid-driven nucleophilic attacks are a crucial pathway for forming key condensed-phase products. Here, we show strong diastereoselectivity during the ring-opening reaction of trans-β-isoprene epoxydiol (trans-β-IEPOX) and cis-β-IEPOX by sulfate to form methyltetrol sulfates (MTS, e.g., 1,3,4-trihydroxy-2-methylbutan-2-yl sulfate) in acidic aqueous particles. These key epoxides are formed from isoprene (2-methyl-1,3-butadiene) oxidation and subsequent reactive uptake to aerosols forming condensed-phase species (i.e., secondary organic aerosol, SOA). Diastereomers and regioisomers were quantified using hydrophilic interaction liquid chromatography coupled with high-resolution tandem mass spectrometry. Acid-driven concerted attack of sulfate at the tertiary site of the epoxide ring was the dominant pathway (~93%) for MTS formation, while other pathways – acid-driven stepwise substitution and concerted addition at the secondary carbon – contributed

Keywords: secondary organic aerosol, stereochemistry, mechanism

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P-18 A multilayer simulation framework for dynamic phase separation in aerosols

Thursday poster presentation

Presenter: Andreas Zuend
Authors: Andreas Zuend[1]; Zixuan Shen[1]; Manabu Shiraiwa[2]

[1] Department of Atmospheric and Oceanic Sciences, McGill University, Montréal, Québec, Canada
[2] University of California, Irvine, Irvine, California, United States

The interactions of molecules of diverse polarities, shapes and sizes within aerosol particles affect mutual solubility and drive morphological changes, including liquid–liquid phase separation (LLPS) and bulk–surface partitioning. Such mixing effects have impacts on size-dependent particle morphology, hygroscopicity, heterogeneous reactions, and phase viscosities. Molecular diffusion due to chemical potential gradients and interfacial effects in aerosols drive the dynamic formation or dissolution of multiphase configurations. We will introduce a new approach for simulating the time-resolved, diffusion-driven liquid–liquid phase separation dynamics in particles of various sizes exposed to changing environmental conditions. Our simulations make use of the so-called ONION box model. ONION is an advanced, multicomponent multilayer kinetic model based on a sound coupling of the kinetic multilayer gas–aerosol partitioning (KM-GAP) framework and the AIOMFAC model for chemical mixing thermodynamics. We show that composition-dependent interfacial tension between different liquid phases as well as the surface tension of particles need to be considered to model realistic core–shell LLPS configurations that dynamically emerge through spinodal decomposition during drying – or dissolve during humidification cycles. We will discuss such simulations and provide insights into dynamic aerosol growth features due to molecular-level mixing effects.

Keywords: liquid, liquid phase separation, multilayer aerosol model, kinetics, thermodynamics

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P-19 Ultrafine Particle Formation and Growth in the Upper Troposphere during the Deep Convective Clouds and Chemistry (DC3) Campaign

Wednesday poster presentation

Presenter: Madeline E. Cooke
Authors: Madeline E. Cooke[1]; John Ortega[1]; Eric C. Apel[1]; Rebecca S. Hornbrook[1]; Roy L. Mauldin III[1]; Lewis Gregory Huey[1]; James N. Smith[1]

[1] University of California, Irvine, United States

Ultrafine particles impact climate and weather as a main source of cloud condensation nuclei. The vertical transport of boundary layer pollutants to the upper troposphere during convection drives new particle formation. During midlatitude summers, atmospheric convection occurs frequently. However, the extent to which convection influences upper tropospheric particle formation remains unclear. Herein, we report measurements of ultrafine particles in the upper troposphere during the Deep Convective Clouds and Chemistry (DC3) campaign. Across 21 flights tracking convective outflow, several flights exhibited elevated concentrations of particles with diameters of less than 100 nm ($N_{100\,\mathrm{nm}}$), often exceeding 1000 cm^{-3}. One particular flight followed and intersected a plume downwind several times, showing an ultrafine particle growth rate of 1.4 ± 0.1 nm h^{-1} due to photochemical aging. Condensation of sulfuric acid can only explain a small fraction of this growth. Gas-phase measurements indicate that oxidized organic vapors likely contribute to particle growth in this region. Future measurements are needed to constrain these processes in atmospheric models, particularly of the molecular speciation of gas-phase precursors. Upper tropospheric ultrafine particles in this region may become more important as climate models project increasing frequency of atmospheric convection in the future.

Maps


MOUNT ROYAL
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METRO
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HÔPITAL GÉNÉRAL DE MONTRÉAL
P.E. TRUDEAU AIRPORT
AV DES PINS
McGILL ATHLETICS
AV DU PARC
SCHWARTZ'S DELI
MUSÉE DES BEAUX ARTS
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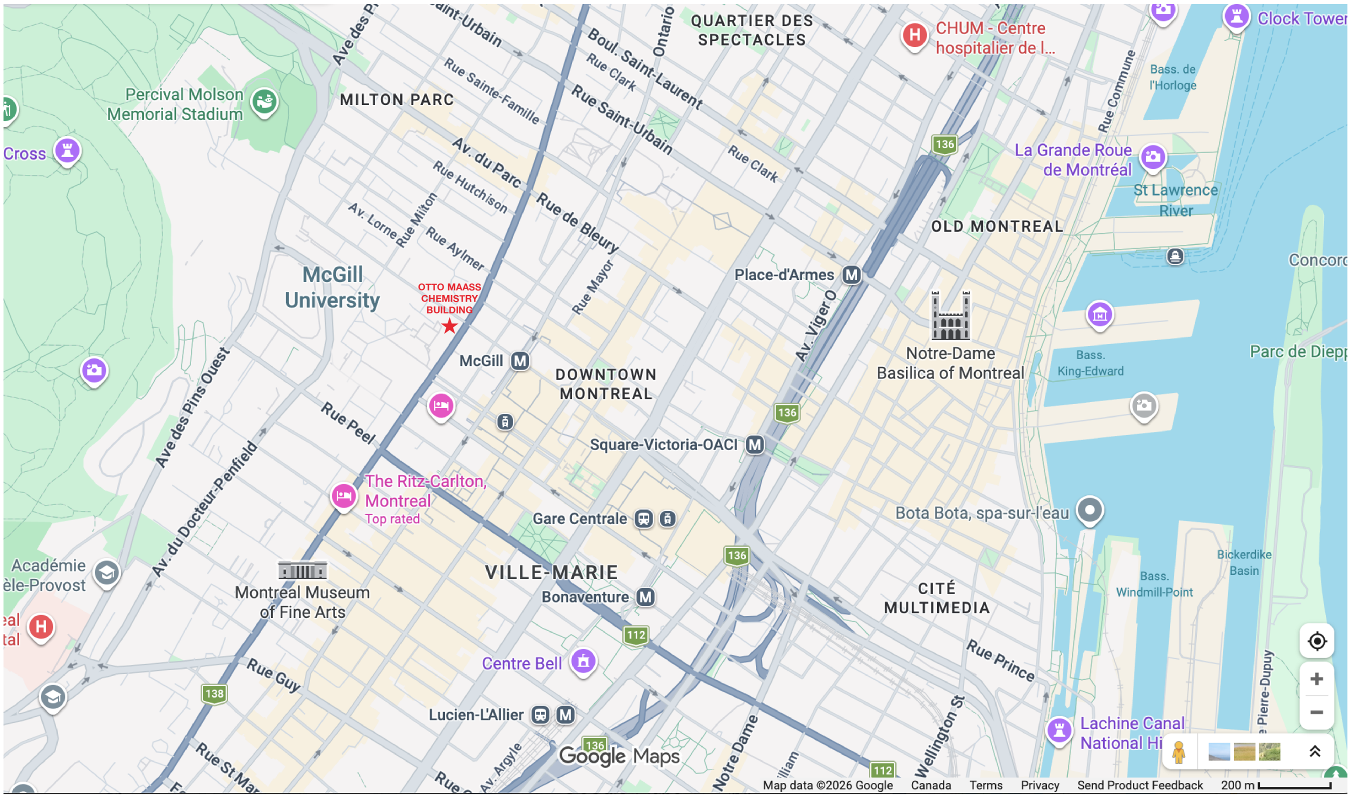
RUE UNIVERSITY
RUE CRESCENT
OTTO MAASS
CHEMISTRY
BUILDING
TIME OUT
MARKET
EATON
SHOPPING DISTRICT
BELL CENTRE
UQÀM
RUE SHERBROOKE
RUE PEEL
GARE CENTRALE
PLACE DES ARTS
BOUL. ST-LAURENT
BOULEVARD RENÉ-LÉVESQUE
RUE SAINTE-CATHERINE
CHINA
TOWN
UQÀM
RUE DE BLEURY
BOULEVARD ROBERT-BOURASSA
BASILIQUE NOTRE-DAME
VIEUX-MONTRÉAL
(OLD MONTRÉAL)
ST LAWRENCE RIVER



Note: The interactive Google Map can be found here: https://maps.app.goo.gl/hYAjQM2AfvtTigNu7.