

**UCDAVIS**

**AIR QUALITY RESEARCH CENTER**

**International**

**Aerosol**

**Modeling**

**Algorithms**

**Conference**

*December 6 - 8, 2023*

*University of California, Davis*

*Sponsored by*



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# Welcome to IAMA 2023!

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## Thank You to the 2023 Technical Program Committee

The 2023 IAMA Technical Program Committee has meticulously drawn from their extensive knowledge, experience, and dedication to craft a comprehensive program. Every effort has been made to ensure that the information presented is of the highest quality, relevance, and scientific accuracy. The UC Davis AQRC extends its profound gratitude to our committee members. Their invaluable knowledge and generous commitment of time have been pivotal in realizing this enriching educational conference. We deeply appreciate their support and contributions.

### *Committee Leads\**

**Jeremy Avise**

*CARB*

**Kelley Barsanti**

*NCAR*

**Thomas Berkemeier**

*Max Planck Institute for Chemistry*

**Chenxia Cai**

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**Chris Cappa**

*UC Davis*

**Daven Henze**

*University of Colorado, Boulder*

**Jim Kelly**

*US EPA*

**V. Faye McNeill\***

*Columbia University*

**Tinja Olenius**

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**Karine Sartelet**

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**Sam Silva**

*University of Southern California*

**Chris Tessum**

*University of Illinois*

**Knut Von Salzen**

*ECCC*

**Dan Westervelt**

*Columbia University*

**Andi Zuend\***

*McGill University*

## Notes

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# CONFERENCE INFORMATION

## Virtual Systems

### Pheedloop

The Pheedloop Virtual Platform and Phone App is the system that hosts information about the current schedule, updates on speaker changes, specialty announcements and the Conference live stream. Additionally, you can utilize Pheedloop set up in-person/virtual meet-ups with other attendees. Access the virtual portal by entering the website link below or by scanning the barcode to the right.

<https://pheedloop.com/iama2023/virtual/>

#### Use Pheedloop to:

- Connect with speakers and other attendees.
- View the event agenda
- Access handouts, video recordings, or articles uploaded by other participants



### Slido

Slido is the system we are using to moderate questions during the conference. Each session will have a personalized Slido "event" which you can post questions to. There are two ways to post a question.

1. You will visit the site below on your computer or phone and enter the specialty "event code" that shows up as listed on this print program AND on the sessions Q&A slides through out the conference.
2. You can directly click on the link within the Pheedloop Virtual Platform located in each session description from your phone or computer.

<https://www.slido.com/>

## Networking Highlights

### Early Career Networking in Downtown Davis

**Tuesday, December 5th**

Engaging early career and student registrants before the conference kicks off.

### Early Career Lunch Discussions

**Wednesday, December 6th**

Gain invaluable insights into various career pathways. You'll have the unique chance to move between tables, interacting with leaders in your field and engaging in meaningful conversations about advancing your career.

### Welcome Reception & Poster Review

**Wednesday, December 6th**

Optimal opportunity to network with scientists working on similar topics, build new connections, and say hello to fellow researchers whom you haven't seen in a while.

### Aerosol Model Benchmark Repositories and Standards (AMBRs) Brainstorming

**Wednesday, December 5th and Thursday, December 6th**

The activity will begin with a brief presentation on the background and objectives on Wednesday, followed by more in-depths discussions in smaller groups on Thursday.

# CONFERENCE PROGRAM

## Wednesday, December 6, 2023

- 7:00 AM Registration Opens & Continental Breakfast
- 8:00 AM Conference Welcome & Opening Remarks
- 8:10 AM **Keynote by Jeff Pierce: *Biomass Burning and Wildfire Aerosol Modeling***
- 9:15 AM Morning Break
- 9:45 AM **Session: Machine Learning and Data Science**
- 11:35 AM Lunch Break - Activity on Aerosol Modeling Testcases and Early Career Discussions
- 12:45 PM **Session: Air Quality Modeling for Health and Regulatory Assessments (Part 1)**
- 1:55 PM Afternoon Break
- 2:45 PM **Session: Air Quality Modeling for Health and Regulatory Assessments (Part 2)**
- 3:45 PM Transition
- 3:55 PM Lightning Talk Presentations
- 4:30 PM Welcome Reception and Poster Review
- 7:00 PM Conference Day 1 Concludes

## Thursday, December 7, 2023

- 7:15 AM Registration Opens & Continental Breakfast Served
- 8:00 AM **Session: Development, Application, and Reduction of Gas- and/or Particle-Phase Chemical Mechanisms for Aerosol Predictions**
- 9:35 AM Morning Break
- 10:20 AM **Session: Fundamental Aerosol Processes from Nano- to Microscale**
- 11:40 AM Lunch Break and Activity on Aerosol Modeling Testcases
- 12:45 PM **Session: Process and Box Models of Aerosol Chemistry and Physics (Part 1)**
- 1:40 PM Transition
- 1:50 PM **Session: Process and Box Models of Aerosol Chemistry and Physics (Part 2)**
- 3:05 PM Afternoon Break
- 3:50 PM **Keynote by Ken Carslaw: *Modeling and Assessment of Aerosol–Cloud–Climate***
- 4:55 PM Conference Day 2 Concludes

## Friday, December 8, 2023

- 7:15 AM Continental Breakfast
- 8:00 AM **Session: Advances in Regional and Global Scale Aerosol Modeling (Part 1)**
- 9:25 AM Networking Break
- 10:15 AM **Session: Advances in Regional and Global Scale Aerosol Modeling (Part 2)**
- 11:30 AM Conference Concludes

# CONFERENCE PROGRAM

WEDNESDAY, DECEMBER 6, 2023

- 7:00 AM **REGISTRATION AND BREAKFAST** *in Conference Center Lobby*
- 8:00 AM **OPENING REMARKS** by Faye McNeill, *Columbia University* and Andreas Zuend, *McGill University*
- 8:10 AM **KEYNOTE: Biomass burning and wildfire aerosol modeling (SLIDO: 6836521)**  
By Jeff Pierce, *University of Leeds*
- 9:15 AM **BREAK**  
Coffee and Refreshments in Lobby
- 9:45 AM **Machine Learning and Data Science (SLIDO: 2860778)**  
*Hosted by Christopher Tessum, University of Illinois and Sam Silva, University of Southern California*
- Emulating Aerosol Optical Properties Using Machine Learning**  
*Andrew Geiss, Pacific Northwest National Laboratory*
- Physics-Constrained Learning of Aerosol Microphysics**  
*Paula Harder, Fraunhofer ITWM*
- Quantum Chemical Modelling of Atmospheric Molecular Clusters Enhanced by Machine Learning**  
*Jakub Kubecka, Aarhus University*
- Characterizing Atmospheric Molecules for Machine Learning**  
*Hilda Sandstrom, Aalto University*
- Combining Earth system modeling and machine learning to investigate volcanic sulfate deposition in polar ice cores**  
*Kostas Tsigaridis, Columbia University and NASA GISS*
- Data driven futures: From stakeholder development to model development**  
*David Topping, University of Manchester*
- 11:35 AM **LUNCH**  
Provided by Olive & Vine Catering
- 12:45 PM **Air Quality Modeling for Health and Regulatory Assessments Part 1 (SLIDO: 1916771)**  
*Hosted by Havala Pye, US EPA and James Kelly, US EPA*
- Integrating Earth-System Modeling and Multi-Scale Observations to Support Health Studies in California**  
*Minghui Diao, San Jose State University*
- Environmental Health, Racial/Ethnic Health Disparity, and Climate Impacts of Inter-Regional Freight Transport in the United States**  
*Maninder Thind, California Energy Commission/ Formerly University of Washington, Seattle*
- Health Impact Assessment of per Ton of Air Toxics and Its Regulatory Applications**  
*Xue (Sue) Meng, California Air Resources Board*
- The Impact of Air Pollution on the Health of Inhabitants in the City of Douala: CAMEROON**  
*Robert Mbiake, University of Douala*
- Particulate Matter (PM2.5) precursor emission sensitivities and the impact on human health in California**  
*Sarika Kulkarni, California Air Resources Board*
- 1:55 PM **BREAK**  
Coffee and Refreshments in Lobby

# CONFERENCE PROGRAM

WEDNESDAY, DECEMBER 6, 2023

- 2:45 PM **Air Quality Modeling for Health and Regulatory Assessments Part 2 (SLIDO: 1275724)**  
Hosted by Havala Pye, *US EPA* and James Kelly, *US EPA*  
**Formation of Reactive Oxygen Species by Atmospheric Particulate Matter**  
*Manabu Shiraiwa, University of California, Irvine*  
**Comprehensive Accounting for Reactive Organic Carbon Emissions from Residential Wood Combustion Processes**  
*Benjamin Murphy, U.S. EPA*  
**Estimating Sector-Oriented Roadside Exposure to Ultrafine Particle Number Concentrations: An implication to covariates influences on the models performance**  
*Sultan Abdillah, Chung Yuan Christian University*  
**Understanding the evolution of reactive organic carbon in wildfire plumes**  
*Havala Pye, U.S. EPA*
- 3:55 PM **LIGHTNING TALKS**  
Poster Presenters will have 1-minute 1-slide to share with audience about their poster.
- 5:30 PM **WELCOME RECEPTION & POSTER DISCUSSIONS**  
Join us in the Lobby of the Conference Center for some light appetizers, drinks and great discussions on the poster displays and session topics.

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# CONFERENCE PROGRAM

THURSDAY, DECEMBER 07, 2023

- 7:30 AM **REGISTRATION AND BREAKFAST** *in Conference Center Lobby*  
**Development, Application, and Reduction of Gas- and/or Particle-Phase Chemical Mechanisms for Aerosol Predictions (SLIDO: 1379885)**  
Hosted by Karine Scarteleet, *Centre d'Enseignement et de Recherche en Environnement Atmosphérique* and Kelley Barsanti, *NCAR*  
Investigating Anthropogenic Emission Mitigation Effects on Biogenic SOA Formation using Simplified and GENOA-Generated Mechanisms in 3-D Modeling  
*Zhizhao Wang, CERE/INERIS*  
Evaluating an Isoprene SOA Kinetic Model Using Laboratory and Field Measurements  
*Haofei Zhang, University of California, Riverside*  
Machine Learning-Based Emulation of Secondary Organic Aerosol (SOA) Formation: An Overview of Ongoing Efforts  
*Alma Hodzic, NCAR*  
Modeling the seed-dependent particle growth via multiphase reactions with the particle-resolved model PartMC-CAMP  
*Yicen Liu, University of Illinois Urbana-Champaign*  
Atmospheric salt particle formation and hydration  
*Nanna Myllys, University of Helsinki*
- 9:35 AM **BREAK**  
Coffee and Refreshments in Lobby
- 10:20 AM **Fundamental aerosol processes from nano- to microscale (SLIDO: 2173011)**  
Hosted by Tinja Olenius, *Swedish Meteorological and Hydrological Institute (SMHI)*, Dan Westervelt, *Columbia University*, Zhongua Zeng, *Manchester University*  
Molecular mechanism of gas phase oxidation of select volatile vapors  
*Siddharth Iyer, Tampere University*  
The Effect of Atmospherically Relevant Ammonium Salts on Water Uptake  
*Noora Hyttinen, University of Jyväskylä*  
Modeling uncertainties of aerosol properties and processes  
*Kari Lehtinen, University of Eastern Finland*  
Assessing the impact of unresolved particle characteristics on climate-relevant aerosol properties  
*Laura Fierce, Pacific Northwest National Laboratory*
- 11:40 AM **LUNCH**  
Provided by Olive & Vine Catering

# CONFERENCE PROGRAM

**THURSDAY, DECEMBER 07, 2023**

- 1:45 PM **Process and Box Models of Aerosol Chemistry and Physics Part 1 (SLIDO: 4788510)**  
Hosted by Nicole Riemer, *University of Illinois at Urbana-Champaign* and Thomas Berkemeier, *Max Planck Institute for Chemistry*  
Understanding the Formation of Organic Acids via Cloud Chemistry Box Modeling  
*Mary Barth, NCAR*  
Water activity and surface tension of aerosol nanoparticles composed of aqueous ammonium sulfate and D-glucose aqueous solution of aerosolized nanoparticles  
*Eugene Mikhailov, Saint-Petersburg state university*  
Investigating impact of surfactants on cloud condensation nuclei activity with a particle-resolved aerosol model  
*Xiaotian Xu, University of Illinois Urbana-Champaign*
- 1:50 PM **Process and Box Models of Aerosol Chemistry and Physics Part 2 (SLIDO: 4788510)**  
Hosted by Nicole Riemer, *University of Illinois at Urbana-Champaign* and Thomas Berkemeier, *Max Planck Institute for Chemistry*  
Process-Level, Kinetic Models to Study the Formation, Physicochemical Properties, and Experimental Artifacts for Secondary Organic Aerosol  
*Shantanu Jathar, Colorado State University*  
The Role of Interfacial Energy and Size-Dependent Morphology of Atmospheric Aerosol Particles  
*Ryan Schmedding, McGill University, Department of Atmospheric and Oceanic Sciences*  
PyPartMC: A Pythonic interface to a particle-resolved Monte Carlo aerosol simulation framework  
*Zach D'Aquino, University of Illinois Urbana-Champaign*  
MultilayerPy: a python package for creating and optimising multi-layer models of aerosol and film processes  
*Adam Milsom, University of Birmingham*
- 3:05 PM **BREAK**  
Coffee and Refreshments in Lobby
- 3:50 PM **Keynote: Perturbed parameter ensembles as a way to understand system behavior and improve models (SLIDO: 1981400)**  
By Ken Carslaw, *University of Leeds*
- 4:55 PM **End of Day Remarks**

Conference organized and hosted by

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# CONFERENCE PROGRAM

FRIDAY, DECEMBER 8, 2023

- 7:30 AM **REGISTRATION AND BREAKFAST** *in Conference Center Lobby*
- 8:00 AM **Advances in regional and global scale aerosol modeling Part 1 (SLIDO: 2017321)**  
Hosted by Daven Henze, *University of Colorado, Boulder* and Knut von Salzen, *Environment and Climate Change Canada (ECCC)*  
Comparison between a sectional and modal aerosol model in CESM2 for present-day and future aerosol injection experiments  
*Simone Tilmes, National Center for Atmospheric Research*  
Idealized particle-resolved large-eddy simulations to evaluate the impact of emissions spatial heterogeneity on CCN activity  
*Samuel Frederick, University of Illinois Urbana-Champaign*  
Impacts of aerosol dynamical processes on the early stage evolution of volcanic plumes  
*Julia Bruckert, Karlsruhe Institute of Technology (KIT Karlsruhe)*  
Application of the hyperdual-step method in the Community Multiscale Air Quality Model (CMAQ) for the assessment of aerosol formation from volatile chemical products (VCPs)  
*Jiachen Liu, Drexel University*  
Estimating the radiative effect and constraining the free parameter space of BrC aerosols in GISS ModelE  
*Maegan DeLessio, Columbia University/NASA GISS*
- 9:25 AM **BREAK**  
Coffee and Refreshments in Lobby
- 10:15 AM **Advances in regional and global scale aerosol modeling Part 2 (SLIDO: 2453193)**  
Hosted by Daven Henze, *University of Colorado, Boulder* and Knut von Salzen, *Environment and Climate Change Canada (ECCC)*  
Modeling constraints of aerosol layer height and night-time aerosol optical depth from space  
*Jun Wang, University of Iowa, UC Riverside*  
Developments and Applications of NOAA's UFS-Aerosols and UFS-Chem for Global Aerosol Forecasts  
*Li (Kate) Zhang, CIRES University of Colorado Boulder & NOAA GSL*  
AerChemMIP2 : Deciphering the role of aerosols and chemically reactive gases in climate change  
*Duncan Watson-Parris, University of California, San Diego*  
Temperature-dependent composition of summertime PM2.5 in observations and model predictions across the Eastern U.S.  
*Pietro Vannucci, University of California, Berkeley*
- 11:25 AM **CLOSING REMARKS** by Faye McNeill, *Columbia University* and Andreas Zuend, *McGill University*

## POSTER PRESENTATIONS

- Assessing the value of each instrumented CMAQ model for addressing aerosol-related policy questions  
*Shannon Caps, Drexel University*  
A three-dimensional particle-resolved model for quantifying error in CCN and optical properties under common simplifying aerosol mixing state assumptions  
*Jeffrey Curs, University of Illinois*  
Investigating the Long-Term Temporal and Spatial Variations in Aerosol Optical Depth (550 nm) across Major Indian Cities with MODIS Terra and Aqua Satellite Data  
*PRIYANSHU GUPs, BANARAS HINDU UNIVERSITY BHU*

# POSTER PRESENTATIONS

## POSTER PRESENTATIONS

Global simulations of secondary organic aerosol phase state with GEOS-Chem

*Regina Luus, University of California Irvine*

Long-term Air Quality and Health Effects of Dairy Digesters in the Future San Joaquin Valley

*Jia Jias, UC Davis*

3-D Simulations of toluene SOA formation at regional and street scales

*Karine Sars, CERECA Ecole des Ponts*

Amore 2.0: A New and Improved Algorithm for the Reduction of Atmospheric Oxidation Mechanisms

*Forwood (Woods) Wiss, Department of Chemical Engineering Columbia University*

Ab initio Simulations of Nitrate Anion Photolysis in an Aqueous Solution

*Kam-Tung Chas, University of California Davis*

Parametric and structural uncertainties in modeling dry deposition of atmospheric aerosol particles

*Zachary D'As, University of Illinois Urbana Champaign*

Influence of dust storms on the aerosol properties over the northern region Kanpur

*Ranjitkumar Sols, Sardar Vallabhbhai National Institute of the Technology*

A kinetic compass for the design of experiments to determine kinetic parameters

*Thomas Bers, Max Planck Institute for Chemistry*

A Novel Computational Framework for Optimal Experimental Design to improve Climate Prediction

*Zhongjing Jias, Brookhaven National Laboratory*

Machine Learning Classification Model to Label Sources Derived from Factor Analysis Receptor Models for Source Apportionment

*Vikas Kums, Indian Institute of Technology Bombay*

Assessing the Spatial Transferability of Calibration Models across a Low-cost Sensors Network

*Vasudev Mals, Indian Institute of Technology Bombay*

Reducing the computational expense of aerosol transport modeling using a machine-learned advection operator

*Manho Pars, University of Illinois Urbana Champaign*

A Machine Learning Approach for Determining the Pure Component Surface Tensions of Aerosol Particle Species

*Ryan Schs, McGill University Department of Atmospheric and Oceanic Sciences*

Automated Machine Learning to Evaluate the Information Content of Tropospheric Trace Gas Columns for Fine Particle Estimates Over India: A Modeling Testbed

*Zhonghua Zhes, The University of Manchester*

Effects of volatility, viscosity, and non-ideality on particle-particle mixing timescales of SOA

*Meredith Schs, University of California Irvine*

Recent progresses in simulating the thermal desorption of filter-collected aerosol for chemical ionization mass spectrometry

*Siegfried Schs, University of Eastern Finland*

Understanding volatility basis set feedback in relative-humidity-sensitive gas-particle partitioning of organic aerosols

*Camilo Sers, Department of Atmospheric and Oceanic Sciences McGill University*

Immersion freezing simulation of multi-species ice-nucleating particles using PartMC

*Wenhan Tans, Department of Atmospheric Science University of Illinois at Urbana Champaign*

Thank you to our researchers who have shared their work as Poster Displays and Lightning Talks!

# Thank You for Attending!

*We hope you enjoyed the 2023 IAMA Conference*

## UC DAVIS

### AIR QUALITY RESEARCH CENTER

Our mission at the AQRC is to facilitate research on the scientific, engineering, health, social, and economic aspects of gaseous and particulate atmospheric pollutants. The best way for us to facilitate the research and education of the world is through educational conferences like this. We thank you, as our attendees, for joining us to learn about new science and technology and for sharing your experiences and knowledge with the world.

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