

# Atmospheric Chemical Mechanisms Conference

UC Davis Conference Center

*December 7-9, 2022*

*Presented By:*

**UC DAVIS**

**AIR QUALITY RESEARCH CENTER**

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**CALIFORNIA AIR RESOURCES BOARD**







# SCHEDULE AT A GLANCE

## WEDNESDAY, DECEMBER 7, 2022

7:00 AM	Registration & Breakfast
8:00 AM	Conference Welcome
8:15 AM	Keynote
9:15 AM	Break
10:00 AM	Fundamental Studies of Atmospheric Chemical Mechanisms Pt 1
11:40 AM	Lunch Break
12:40 PM	Fundamental Studies of Atmospheric Chemical Mechanisms Pt 2
2:20 PM	Break
2:50 PM	Fundamental Studies of Atmospheric Chemical Mechanisms Pt 3
4:30 PM	Lightning Talks
5:30 PM	Welcome Reception & Poster Review
7:30 PM	Reception Concludes

## THURSDAY, DECEMBER 08, 2022

7:30 AM	Registration & Breakfast
8:00 AM	Sulfur Oxidation Advancements – Improving mechanisms and modelling
9:15 AM	Break
10:00 AM	Mechanism Development and Reduction Pt 1
11:15 AM	Quick Stretch
11:25 AM	Mechanism Development and Reduction Pt 2
12:40 PM	Lunch
1:45 PM	Plenary
2:15 PM	Atmospheric Chemistry in Public Health and Regulatory Applications
3:30 PM	Break
4:15 PM	Chemical Regimes
5:30 PM	Sessions Close

## FRIDAY, DECEMBER 9, 2022

7:30 AM	Registration & Breakfast
8:00 AM	New and Emerging Air Pollutants (HAPs, VCPs, PFAS)
10:00 AM	Break
10:30 AM	Modeling at multiple scales of chemical complexity and spatial resolution
12:30 PM	Close

# CONFERENCE PROGRAM

WEDNESDAY, DECEMBER 7, 2022

- 7:30 AM **REGISTRATION AND BREAKFAST** *in Conference Center Lobby*
- 8:00 AM **OPENING REMARKS** *by Alex Archibald, University of Cambridge & Melissa Venecek, CARB*
- 8:10 AM **KEYNOTE: Considering Multiple Dimensions of Complexity in Atmospheric Chemistry Models**  
*By, Kelley Barsanti, University of California Riverside; National Center for Atmospheric Research*
- 9:15 AM **BREAK**  
Coffee and Refreshments in Lobby
- 10:00 AM **FUNDAMENTAL STUDIES OF ATMOSPHERIC CHEMICAL MECHANISMS (pt 1)**  
Hosted by Rebecca Caravan, *Argonne National Laboratory*, Sally Ng, *Georgia Institute of Technology*, Matti Rissanen, *Tampere University* & Max McGillen, *CNRS*  
**Speciated Monitoring of Organic Peroxy Radicals with Proton-Transfer Mass Spectrometry: First applications in the laboratory**  
*Barbara Noziere, KTH, Royal Institute of Technology*  
**Identification and Quantitation of Products Formed from the Reaction of Alkenoic Acids with OH Radicals in a Low NO<sub>x</sub> Environment**  
*Anna Ziola, University of Colorado Boulder*  
**Ring-opening yield and auto-oxidation rate of the first-generation hydroxy peroxy radical (C<sub>10</sub>H<sub>17</sub>O<sub>3</sub>) from OH-oxidation of  $\alpha$ -pinene and  $\beta$ -pinene**  
*Joel Thornton, University of Washington*  
**Recent Computational Results on RO<sub>2</sub> + R'O<sub>2</sub> Reactions**  
*Theo Kurtén, University of Helsinki*  
**Oxidation of naphthalene in atmosphere: A computational perspective**  
*Prasenjit Seal, Tampere University*
- 11:40 AM **LUNCH**  
Provided by Olive & Vine Catering
- 12:40 PM **FUNDAMENTAL STUDIES OF ATMOSPHERIC CHEMICAL MECHANISMS (pt 2)**  
Hosted by Rebecca Caravan, *Argonne National Laboratory*, Sally Ng, *Georgia Institute of Technology*, Matti Rissanen, *Tampere University* & Max McGillen, *CNRS*  
**Changes in composition and volatility of biogenic secondary organic aerosol from nitrate radical oxidation during night-to-day transition**  
*Claudia Mohr, Stockholm University*  
**Formation yields of organic nitrates in reactions of organic peroxy radicals with NO**  
*John Orlando, Atmospheric Chemistry Observations and Modeling (ACOM) Laboratory, NCAR*  
**SOA and volatile product formation from the nighttime oxidation of various terpenes, and the ICARUS database**  
*Tran Nguyen, UC Davis*  
**Investigating the Atmospheric Oxidation of Methylamine with Multiplexed Photoionization Mass Spectrometry: Insight into the Reactivity of C-centered and N-centered Radicals with O<sub>2</sub>**  
*Sommer Johansen, Sandia National Laboratories*  
**Reconciling Disparate Mechanisms for Oxidation of Hg(0) to Hg(II) in the Gas Phase**  
*Theodore Dibble, State University of New York - Environmental Science and Forestry*
- 2:20 PM **BREAK**  
Coffee and Refreshments in Lobby

# CONFERENCE PROGRAM

WEDNESDAY, DECEMBER 7, 2022

2:50 PM **FUNDAMENTAL STUDIES OF ATMOSPHERIC CHEMICAL MECHANISMS (pt 3)**

Hosted by Rebecca Caravan, *Argonne National Laboratory*, Sally Ng, *Georgia Institute of Technology*, Matti Rissanen, *Tampere University* & Max McGillen, *CNRS*

**Ozonolysis of  $\alpha$ -pinene and  $\Delta^3$ -carene – influence of molecular structure on aerosol formation and chemistry**

Marianne Glasius, *Aarhus University, Denmark*

**Particle-Phase Accretion Forms Dimer Esters in Pinene Secondary Organic Aerosol**

Christopher Kenseth, *University of Washington*

**Tunneling, Roaming, and Oligomerization Kinetics of Criegee Intermediates Elucidated through Theory and Experiment**

Stephen Klippenstein, *Argonne National Laboratory*

**Organic Aerosol Multiphase Aging: Rethinking the Chemical Mechanism under Atmospherically Relevant Conditions**

Haofei Zhang, *University of California, Riverside*

**Formation of Accretion Products in the Self-Reaction of Ethene-Derived Hydroxy Peroxy Radicals**

Sara Murphy, *California Institute of Technology*

4:30 PM **LIGHTNING TALKS** moderated by Havala Pye, *US EPA*

Poster Presenters will have 2-minutes 2-slides 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.

Thank you to our generous sponsor



# CONFERENCE PROGRAM

THURSDAY, DECEMBER 08, 2022

- 7:30 AM **REGISTRATION AND BREAKFAST** *in Conference Center Lobby*
- 8:00 AM **SULFUR OXIDATION ADVANCEMENTS - IMPROVING MECHANISMS AND MODELING**  
*Zongbo Shi, University of Birmingham*  
Assessing and improving the DMS oxidation mechanism in the MCM and CRI-Strat  
*Lorrie Jacob, University of Cambridge*  
Sulfur radical formation from the tropospheric irradiation of aqueous sulfate aerosols  
*Kelvin Bates, University of California, Davis*  
Chamber studies of the oxidation of DMS, DMDS, and DMSO: Mechanism and aerosol formation  
*Matthew Goss, Massachusetts Institute of Technology*  
Investigation of the OCS formation from the oxidation of DMS in marine-like conditions.  
*Anna Novelli, Institute of Energy and Climate Research, IEK-8: Troposphere, Forschungszentrum Jülich*
- 9:15 AM **BREAK**  
Coffee and Refreshments in Lobby
- 10:00 AM **MECHANISM DEVELOPMENT AND REDUCTION (pt 1)**  
*Hosted by Kelley Barsanti, University of California, Riverside & Tzung-May Fu, Southern University of Science and Technology*  
Comparing GECKO-A and MechGen as a basis for evaluation of simplified mechanisms  
*Julia Lee-Taylor, National Center for Atmospheric Research*  
Recent advances in SARs for the unimolecular chemistry of peroxy radicals  
*Luc Vereecken, Forschungszentrum Jülich GmbH*  
A Broad View of Structure-Activity Relationship Performance for Alkanes and Haloalkanes  
*Max McGillen, CNRS*  
Designing chemical mechanisms for ozone and secondary organic aerosol endpoints  
*Havala Pye, US EPA*
- 11:15 AM **TRANSITION BREAK**
- 11:25 AM **MECHANISM DEVELOPMENT AND REDUCTION (pt 2)**  
*Hosted by Kelley Barsanti, University of California, Riverside & Tzung-May Fu, Southern University of Science and Technology*  
Multi-phase chemistry surrogate modeling with a recurrent neural network  
*Xiaokai Yang, University of Illinois Urbana-Champaign*  
Detailed multiphase chemistry modelling of methylamines with CAPRAM  
*Erik Hoffmann, Leibniz Institute for Tropospheric Research (TROPOS)*  
An Online-Learned Neural Network Chemical Solver for Stable Long-Term Global Simulations of Atmospheric Chemistry  
*Makoto Kelp, Harvard University,*  
An adaptive auto-reduction solver for speeding up integration of chemical kinetics in atmospheric chemistry models: implementation and evaluation within the Kinetic Pre-Processor (KPP) version 3.0.0  
*Haipeng Lin, Harvard University,*
- 12:40 PM **LUNCH**  
Provided by Olive & Vine Catering
- 1:45 PM **PLENARY: Deeper insight into atmospheric reaction systems from the laboratory: RO2 isomerization and ROOOH formation**  
*By, Torsten Berndt, TROPOS Leipzig*

# CONFERENCE PROGRAM

THURSDAY, DECEMBER 08, 2022

2:15 PM **ATMOSPHERIC CHEMISTRY IN PUBLIC HEALTH AND REGULATORY APPLICATIONS**

Hosted by Melissa Venecek, *California Air Resources Board*, Jim Kelly, *US EPA*

Characterizing the impact of volatile chemical products (VCPs) and cooking on air quality in major US cities

Matthew Coggon, *National Oceanic and Atmospheric Administration*

Accounting for the chemistry of reactive toxic VOCs for community level modeling

Zhen Liu, *California Air Resources Board*

Long-term Trends of Impacts of Global Gasoline and Diesel Emissions on Air Quality and Human Health for 2000-2015

Ying Xiong, *Wayne State University*

Optimization of air pollutant control policy based on the nonlinearity of atmospheric chemistry

Jia Xing, *Tsinghua University*

3:30 PM **BREAK**

Coffee and Refreshments in Lobby

4:15 PM **NEW CHEMICAL REGIMES**

Hosted by Ellie Browne, *University of Colorado, Boulder* & James Lee, *University of York / NCAS*

Ozone photochemistry and free radical budgets in the Los Angeles basin: A comparison of ground-based observations in 2021 and 2010

Michael Robinson, *National Oceanic and Atmospheric Administration, Chemical Sciences Laboratory*

Chemistry of Reactive Organic Gases in Mega-cities of China: Insights from Vertical Gradient and Eddy Covariance Flux Measurements

Bin Yuan, *Jinan University*

An exploration of changing ozone production under new chemical regimes in three cities

Beth Nelson, *University of York*

The development of an isoprene mechanism for anoxic atmospheres

Alexander Archibald, *University of Cambridge & NCAS-Climate*

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# CONFERENCE PROGRAM

FRIDAY, DECEMBER 9, 2022

- 7:30 AM **REGISTRATION AND BREAKFAST** *in Conference Center Lobby*
- 8:00 AM **NEW AND EMERGING AIR POLLUTANTS (HAPs, VCPs, PFAs)**  
Hosted by Emma D'Ambro, *US EPA* & Matt Coggin, *Cooperative Institute for Research in Environmental Sciences / NOAA Chemical Sciences Laboratory*  
**Observations of Chlorinated Amines in an Urban Atmosphere in Summer and Winter**  
Jon Abbatt, *University of Toronto*  
**A Better Representation of VOC chemistry from VCP and Cooking emissions in WRF-Chem**  
Qindan Zhu, *Cooperative Institute for Research in Environmental Sciences and the NOAA Chemical Sciences Laboratory*  
**Chemical characteristics of indoor aerosol particles and surface films**  
Rachel O'Brien, *University of Michigan*  
**Volatile Organic Compounds inside Homes Impacted by Smoke from the Marshall Fire**  
Joost de Gouw, *University of Colorado, Boulder*  
**Personal care product VOC emissions: Indoor air quality impacts and estimated inhaled dosage from use**  
Amber Yeoman, *University of York*  
**Drivers of Perfluorocarboxylic Acid (PFCA) Gas-Particle Partitioning: Modeled Properties and Observational Constraints**  
Trevor VandenBoer, *York University*
- 10:00 AM **BREAK**  
Coffee and Refreshments in Lobby
- 10:30 AM **MODELING AT MULTIPLE SCALES OF CHEMICAL COMPLEITY AND SPATIAL RESOLUTION**  
Hosted by Kelvin Bates, *Harvard & UC Davis*, Louisa Emmons, *National Center for Atmospheric Research*  
**Developing a new ocean-atmosphere exchange model to calculate iodine emissions and better constrain their role in tropospheric chemistry**  
Ryan Pound, *University of York*  
**Urban and Remote cheMistry modELLing with the new chemical mechnaism URMELL**  
Marie Luttkus, *Leibniz Institute for Tropospheric Research (TROPOS)*  
**Climate forcing from vegetation emissions strongly influenced by the chemical mechanism employed.**  
James Weber, *University of Sheffield*  
**Modeling the multiphase chemistry of isoprene-related organic hydroxy hydroperoxides and epoxides with MCM/CAPRAM**  
Andreas Tilgner, *Leibniz Institute for Tropospheric Research (TROPOS)*  
**Plans For Enhanced Research Capabilities for Atmospheric Chemistry within NOAA's Unified Forecasting System**  
Rebecca Schwantes, *National Oceanic and Atmospheric Administration, Chemical Sciences Laboratory*
- 12:30 PM **CLOSING REMARKS** *by Carl Percival, NASA JPL & Alex Archibald, University of Cambridge*



# LIGHTNING TALKS

## LIGHTNING TALKS

**30 Atmospheric Photolysis of CF<sub>3</sub>CHO: A Source of HFC-23?**

Mads Sulbaek Anderson, *California State University*

**45 Development and evaluation of an improved mechanism for the oxidation of dimethyl sulfide in the UKCA model**

Alexander Archibald, *University of Cambridge*

**42 Volatile Chemical Product Contributions to the Urban Secondary Organic Aerosol Burden in the United States**

Shantanu Jathar, *Colorado State University*

**31 Use of OH/VOC 'site-specific' rate coefficient data to test, train and constrain structure-activity relationships.**

John Orlando, *Atmospheric Chemistry Observations and Modeling Laboratory, NCAR*

**20 Investigating fundamental structures in atmospheric chemical reaction mechanisms**

Sam Silva, *The University of Southern California*

**32 Reduction strategies for the automatic generation of SOA mechanism using GENOA**

Zhizhao Wang, *CEREA, ENPC*

## POSTER COMPETITION - LIGHTNING TALKS

We are excited to welcome our first participants in the ACM Poster Competition! This group of students and early career researchers represents an outstanding group of scientists that were selected by our judges for this first competition. Please join the team in supporting their continued development as researchers by listening to their lightning talks and asking questions of their work.

**24 NO<sub>3</sub> Initiated Oxidation of Furan Compounds: Rate Coefficients, Gas-Phase Chemical Mechanisms and SOA Formation**

Fatima Al Ali, *Université du Littoral Côte d'Opale*

**5 Atmospheric Chemical Reaction Mechanism Dependence on the Environment and Stellar Radiation**

Alexandra Deal, *University of Colorado, Boulder / CIRES*

**29 Investigation of nighttime chemistry of trans-2-hexene in the atmospheric simulation chamber SAPHIR**

Michelle Färber, *Forschungszentrum Jülich*

**27 Unimolecular reactions of hydroxy-substituted Criegee Intermediates**

Lauri Franzone, *University of Helsinki*

**22 Atmospheric oxidation of imine derivative of piperazine initiated by OH radical**

Thomas Golin Almeida, *University of Helsinki*

**37 Chemical surrogate modeling with uncertainty quantification using a Bayesian Neural ODE**

Lin Guo, *University of Illinois at Urbana-Champaign (UIUC)*

**13 Computational Investigation of the Reaction Routes for 3(RO...OR') Intermediates Formed in Peroxy Radical Self- and Cross-Reactions**

Galib Hasan, *University of Helsinki*

**34 Comparison of Common Vapor Pressure Estimation Methods through Modeling of Alkene OH/NO<sub>x</sub> Systems**

Emmaline Longnecker, *University of Colorado, Boulder - Chemistry Department*

**28 Structure-activity relationship to predict Arrhenius parameters of OH addition to unsaturated volatile organic compounds under atmospheric conditions**

Lisa Michelat, *ICARE-CNRS Orleans*

**38 Developing methods for efficient transport and chemistry calculations in forecasting applications**

Obin Sturm, *NASA GMAO / University of Southern California*

**48 Kinetic Studies of the Pressure and Temperature Dependence of OH+SO<sub>2</sub> in the Presence of Water Vapor**

Megan Woods, *California Institute of Technology*

**16 Low-pressure yields of stabilized Criegee intermediates produced from ozonolysis of a series of alkenes**

Lei Yang, *UC Riverside*

# POSTER PRESENTATIONS

## POSTER DISPLAYS

- 23 Secondary Organic Aerosol (SOA) formation from the gas-phase reaction of guaiacol with NO<sub>3</sub> radicals  
Fatima Al Ali, *Université du Littoral Côte d'Opale*
- 6 Trace H<sub>2</sub>S Promotes Organic Aerosol Production and Organosulfur Compound Formation in Planetary Haze Photochemistry Experiments  
Eleanor Browne, *University of Colorado Boulder & Cooperative Institute for Research in Environmental Sciences*
- 9 First Direct Kinetic Studies of Four-Carbon, Resonance-Stabilized Criegee Intermediates Formed from Isoprene Ozonolysis  
Rebecca Caravan, *Argonne National Laboratory*
- 40 Modeling the atmospheric fate of Per- and Polyfluoroalkyl Substances (PFAS)  
Emma D'Ambro, *US EPA, Office of Research and Development*
- 33 Multi-day Evolution of Organic Aerosol Mass and Composition from Biomass Burning Emissions  
Abraham Dearden, *Colorado State University*
- 35 Multi-scale modeling of air quality and mechanism comparison with MUSICA  
Louisa Emmons, *National Center for Atmospheric Research*
- 8 Detection of Ambient Concentrations of Hydroxyl Radical using Broadband Cavity-Enhanced Absorption Spectroscopy  
Callum Flowerday, *Brigham Young University*
- 11 Acetonyl peroxy and hydro peroxy self- and cross- reactions: Temperature-dependent kinetics parameters, branching fractions, and chaperone effects  
Fred Grieman, *Jet Propulsion Laboratory, California Institute of Technology*
- 36 Impacts of Low-Level Jets on Surface Temperature  
Jonathan Hale, *University of California, Davis*
- 41 Influence of application method on disinfection byproduct formation during indoor cleaning: an example of phenol chlorination during bleach cleaning  
Leif Jahn, *University of Texas at Austin*
- 15 Ions diffuse slower than water in mixed organic/inorganic aerosol particles  
Liviana Klein, *ETH Zurich*
- 18 WiFEX: Walk into the warm fog over Indo Gangetic Plain region  
Rachana Kulkarni, *Independent Researcher*
- 12 Decoding VOC Photooxidation on a Molecular Level – A Novel Ensemble of Methods to Generate, Analyze, and Characterize Multifunctional Oxidation Products in the Gas and Particle Phase  
Finja Löher, *University of Bayreuth*
- 44 Investigating the Chemistry of Isoprene Nitrates and Nitrooxyorganosulfates Under Polluted Urban Conditions  
Alfred Mayhew, *University of York*
- 1 Atmospheric Chemistry Classics: Exploring Recent Trends in Surface Ozone  
Anke C. Noelscher, *University of Bayreuth*
- 14 Vibrational Photochemistry and Dissociation of Peroxyformic Acid Initiated by Visible Light  
Josue Perez, *University of California San Diego*
- 7 Nonisothermal nucleation in the gas phase is driven by cool subcritical clusters  
Bernhard Reischl, *University of Helsinki*

# POSTER PRESENTATIONS

## POSTER DISPLAYS

**39 Explicit and reduced chemical mechanisms for indoor air quality models**

Roberto Sommariva, *University of Birmingham*

**26 Chekimomi: a tool for enabling FAIR kinetic models**

Luc Vereecken, *Forschungszentrum Jülich GmbH*

**19 The gas-phase formation mechanism of iodic acid: a catalytic role of iodine in particle formation**

Rainer Volkamer, *University of Colorado, Boulder*

**10 New Measurements of Glyoxal Yields from Acetaldehyde Oxidation**

James Warman, *University of Leeds*

**46 Probing the DMS Oxidation Mechanism Through Measurements of the OH Radical**

Frank Winiberg, *Jet Propulsion Laboratory*

**25 Automated Mechanism Reduction Algorithm Applied to Isoprene Chemistry**

Forwood Wiser, *Columbia University*

**17 Understanding How Representative Laboratory Simulation is for Ambient Chemical Processes through a Compound-Specific Approach**

Lindsay Yee, *University of California, Berkeley*

**43 High time resolution ambient measurements of gas- and particle-phase perfluorocarboxylic acids (PFCAs): Implications for sources and fate**

Cora Young, *York University*

The 2022 conference committee has dedicated their knowledge, experience and time to designing a well thought out program and have taken the time to ensure all information presented is of the highest quality, as well as relevant and scientifically accurate. We are grateful for their support and contributions!

## Technical Planning Committee

Alex Archibald, *University of Cambridge*

Max McGillen, *CNRS*

Ellie Browne, *CU Boulder*

Melissa Venecek, *CARB*

Emma D'Ambro, *U.S. EPA*

Patrick Veres, *NOAA CSL*

Havala Pye, *U.S. EPA*

Rebecca Caravan, *Argonne National Laboratory*

James Lee, *University of York*

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Kelvin Bates, *Harvard University & UCD*

Sally NG, *Georgia Institute of Technology*

Louisa Emmons, *NCAR*

Tzung-May Fu, *Peking University*

Matthew Coggon, *NOAA CSL*