Rebecca Schwantes

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I desire to improve the description of chemistry in regional and global models in order to advance air quality prediction capability by more accurately simulated ozone and secondary organic aerosol. I gained a comprehensive and robust knowledge of atmospheric chemistry by performing laboratory chamber experiments during graduate school at Caltech. During my ASP postdoctoral work at NCAR, I am creating an updated and more comprehensive chemical scheme for isoprene and terpene oxidation. I have a strong record of publishing independent and collaborative work and am particularly interested in the development and promotion of NCAR community models (e.g., co-leading CAM-Chem wiki page development). Because of my unique background, I desire to better connect the experimental and modeling communities to ensure efficient and accurate progress on advancing our understanding of air quality.

EDUCATION

California Institute of Technology Pasadena, CA
PhD Environmental Science and Engineering June 2017
Thesis: Identifying Isoprene and Toluene Gas-Phase Oxidation Products to Better Constrain Ozone and Secondary Organic Aerosol Formation in the Atmosphere

University of Virginia Charlottesville, VA May 2009
B.S. in Chemistry with a specialization in Biochemistry
Distinguished Majors Program – Highest Distinction
B.A. in Mathematics

WORK HISTORY

National Center for Atmospheric Research Boulder, CO Nov 2016 to present
ASP Postdoctoral Fellow
Updating and optimizing chemistry (i.e., chemical mechanism, dry/wet deposition, and aerosol uptake of gas-phase compounds) in CAM-chem, a global chemical transport model, with a specific focus on improving simulated surface ozone.

California Institute of Technology Pasadena, CA Sept 2011 to Oct 2016
PhD Candidate
Conducted atmospheric chamber experiments under the supervision of Dr. John Seinfeld (primary advisor) and Dr. Paul Wennberg (secondary advisor) with a focus on identifying gas-phase oxidation products and secondary organic aerosol precursors using a CF_3O^- chemical ionization mass spectrometer.

Eastern Research Group, Inc. Chantilly, VA Aug 2009 – March 2011
Chemist
Worked as a technical contractor to the US Environmental Protection Agency to help develop a new rule that would better regulate wastewater discharges from steam electric power plants.

UVA Molecular Physiology and Biological Physics *Charlottesville, VA* Jan 2007 – May 2009
Undergraduate Research Assistant

Developed purification protocols for proteins associated with leukemia to better understand their structure and function.

SCIENTIFIC/TECHNICAL ACCOMPLISHMENTS

Chemical Mechanism Development

Currently developing a more complete chemical mechanism for isoprene and terpene oxidation to be used in regional or global models (Completion anticipated by Sept 2018). Future work will also include developing updated chemical mechanisms for other systems (e.g., alkanes and compounds emitted from biomass burning).

CAM-SE Regional Refinement Development

Helping to incorporate chemistry into the CAM-SE (spectral element) with regional refinement version of CAM-Chem, which includes emissions development and model evaluation.

CAM-Chem Wiki Page Development

Co-leading effort to create a concise, yet useful wiki page for CAM-Chem to attract new users and expand the CAM-Chem user community (Completion anticipated by Aug 2018).

Improved Understanding of Isoprene SOA Yields

New results using improved chamber experimental techniques and aerosol measurement data analysis suggest low-volatility nitrates and dinitrates are as important as 2-methyl glyceric acid for isoprene SOA formation under high-NO conditions (Completion anticipated by Aug 2018).

Improved Understanding of SOA Precursors from Cresol Oxidation

Identified important low-volatility cresol oxidation products that contribute appreciably to SOA formation, which ultimately advanced our mechanistic understanding of SOA formation from aromatic systems.

Improved Understanding of Isoprene + NO_3 Oxidation

Identified important first- and later-generation gas-phase oxidation products from isoprene nitrate radical (NO_3) oxidation. This study improves our understanding of organic nitrate formation and fate from isoprene NO_3 oxidation, which ultimately improves our understanding of O_3 formation.

Characterize Caltech New Chamber Facility

Characterized the new (2011) Caltech chamber facility to understand chamber volume, chamber particle and gas-phase wall losses, chamber mixing, chamber light distribution and intensity, chamber temperature capability, control experiments, etc.

Maintained Caltech Chamber CF_3O^- CIMS

Maintained, calibrated, and provided support to other lab members for the use and data analysis of a CF_3O^- chemical ionization mass spectrometer for 5 years during graduate school.

MENTORING, TEACHING, and SERVICE

NCAR Significant Opportunities in Atmospheric Research and Science Summer 2017 & 2018
Writing Mentor

Worked with undergraduate student to enhance writing and presentation skills.

Colorado Science and Engineering Fair Judge April 2017 & 2018

Judged senior division high school projects for state science fair competition.

Summer Undergraduate Research Fellowship Program Summer 2014

Mentor

Assisted undergraduate student in developing a project to better understand advected tracer transportation in GEOS-Chem, a global chemical transport model.

California Institute of Technology Spring 2013 & Spring 2014

Teaching Assistant

Atmospheric Chemistry and Introduction to Environmental Science and Engineering

Caltech Y Rise Program Oct 2011 – April 2013

Tutor

Tutored, as a volunteer, math and science to struggling students in middle and high school.

HONORS and AWARDS

NCAR Advanced Study Program (ASP) Postdoctoral Fellowship Nov 2016 – Nov 2018

PUBLICATIONS

Peer-Reviewed Journal Articles

Wennberg, P. O., K. H. Bates, J. D. Crounse, L. G. Dodson, R. C. McVay, L. A. Mertens, T. B. Nguyen, E. Praske, **R. H. Schwantes,** M. D. Smarte, J. M. St Clair, A. P. Teng, X. Zhang, J. H. Seinfeld, 2018: Gas-Phase Reactions of Isoprene and Its Major Oxidation Products. *Chem. Rev.*, 118, 3337-3390, https://doi.org/10.1021/acs.chemrev.7b00439.

Schwantes, RH., K. A. Schilling, R. C. McVay, H. Lignell, M. M. Coggon, X. Zhang, P.O. Wennberg, J. H. Seinfeld, 2017: Formation of Highly Oxygenated Low-Volatility Products from Cresol Oxidation. *Atmos. Chem. Phys.*, 17, 3453-3474, https://doi.org/10.5194/acp-17-3453-2017.

Kurten, T., K. H. Moller, T. B. Nguyen, **R. H. Schwantes,** P. K. Misztal, L. Su, P. O. Wennberg, J. L. Fry, H. G. Kjaergaard, 2017: Alkoxy Radical Bond Scissions Explain the Anomalously Low Secondary Organic Aerosol and Organonitrate Yields From α-Pinene + NO_3. *J. Phys. Chem. Lett.*, 8, 2826-2834, https://doi.org/10.1021/acs.jpclett.7b01038.

Ng, N. L., S. S. Brown, A. T. Archibald, E. Atlas, R. C. Cohen, J. N. Crowley, D. A. Day, N. M. Donahue, J. L. Fry, H. Fuchs, R. J. Griffin, M. I. Guzman, H. Herrmann, A. Hodzic, Y. Iinuma, J. L. Jimenez, A. Kiendler-Scharr, B. H. Lee, D. J. Luecken, J. Mao, R. McLaren, A. Mutze, H. D. Osthoff, B. Ouyang, B. Picquet-Varrault, U. Platt, H. O. T. Pye, Y. Rudich, **R. H. Schwantes,** M. Shiraiwa, J. Stutz, J. A. Thornton, A. Tilgner, B. J. Williams, R. A. Zaveri, 2017: Nitrate radicals and biogenic volatile organic compounds: oxidation, mechanisms, and organic aerosol. *Atmos. Chem. Phys.*, 17, 2103-2162, https://doi.org/10.5194/acp-17-2103-2017.

Nguyen, T. B., G. S. Tyndall, J. D. Crounse, A. P. Teng, K. H. Bates, **R. H. Schwantes,** M. M. Coggon, L. Zhang, P. Feiner, D. O. Miller, K. M. Skog, J. C. Rivera-Rios, M. Dorris, K. F. Olson, A. Koss, R. J. Wild, S. S. Brown, A. H. Goldstein, J. A. de Gouw, W. H. Brune, F. N. Keutsch, J. H. Seinfeld, P. O. Wennberg, 2016: Atmospheric Fates of Crigee Intermediates in the Ozonolysis of Isoprene. *Phys. Chem. Chem. Phys.*, 18, 10241-10254, https://doi.org/10.1039/C6CP00053C.

Thomas, D. A., M. M. Coggon, H. Lignell, K. A. Schilling, X. Zhang, **R. H. Schwantes,** R. C. Flagan, J. H. Seinfeld, J. L. Beauchamp, 2016: Real-Time Studies of Iron Oxalate-Mediated Oxidation of Glycolaldehyde as a Model for Photochemical Aging of Aqueous Tropospheric Aerosols. *Environ. Sci. Technol.* 50, 12241-12249, https://doi.org/10.1021/acs.est.6b03588.

Schwantes, R. H., A. P. Teng, T. B. Nguyen, M. M. Coggon, J. D. Crounse, J. M. St. Clair, X. Zhang, K. A. Schilling, J. H. Seinfeld, P.O. Wennberg, 2015: Isoprene NO_3 Oxidation Products from the $RO_2 + HO_2$ Pathway. *J. Phys. Chem. A.*, 119, 10158-10171, https://doi.org/10.1021/acs.jpca.5b06355.

Zhang, X., **R. H. Schwantes,** R. C. McVay, H. Lignell, M. M. Coggon, R. C. Flagan, J. H. Seinfeld, 2015: Vapor Wall Deposition in Teflon Chambers. *Atmos. Chem. Phys.*, 15, 4197-4214, https://doi.org/10.5194/acp-15-4197-2015.

Nguyen, T. B., K. H. Bates, J. D. Crounse, **R. H. Schwantes,** X. Zhang, H. G. Kjaergaard, J. D. Surratt, P. Lin, A. Laskin, J. H. Seinfeld, P. O. Wennberg, 2015: Mechanism of the Hydroxyl Radical Oxidation of Methacryloyl Peroxynitrate (MPAN) and its Pathway toward Secondary Organic Aerosol Formation in the Atmosphere. *Phys. Chem. Chem. Phys.*, 17, 17914-17926, https://doi.org/10.1039/C5CP02001H.

Schilling Fahnestock, K. A., L. D. Yee, C. L. Loza, M. M. Coggon, **R. H. Schwantes,** X. Zhang, N. F. Dalleska, J. H. Seinfeld, 2015: Secondary Organic Aerosol Composition from C_{12} Alkanes. *J. Phys. Chem. A.*, 119 (19), 4281-4297, https://doi.org/10.1021/jp501779w.

Zhang, X., **R. H. Schwantes**, M. M. Coggon, C. L. Loza, K. A. Schilling, R. C. Flagan, J. H. Seinfeld, 2014: Role of Ozone in SOA Formation from Alkane Photooxidation. *Atmos. Chem. Phys.*, 14, 1733-1753, https://doi.org/10.5194/acp-14-1733-2014.

Nguyen, T. B., J. D. Crounse, **R. H. Schwantes,** A. P. Teng, K. H. Bates, X. Zhang, J. M. St. Clair, W. H. Brune, G. S. Tyndall, F. N. Keutsch, J. H. Seinfeld, P. O. Wennberg, 2014: Overview of the Focused Isoprene eXperiment at the California Institute of Technology (FIXCIT): Mechanistic Chamber Studies on the Oxidation of Biogenic Compounds. *Atmos. Chem. Phys.*, 14, 13531-13549, https://doi.org/10.5194/acp-14-13531-2014.

Nguyen, T. B., M. M. Coggon, K. H. Bates, X. Zhang, **R. H. Schwantes**, K. A. Schilling, C. L. Loza, R. C. Flagan, P. O. Wennberg, J. H. Seinfeld, 2014: Organic Aerosol Formation from the Reactive Uptake of Isoprene Epoxydiols (IEPOX) onto Non-Acidified Inorganic Seeds. *Atmos. Chem. Phys.,* 14, 3497-3510, https://doi.org/10.5194/acp-14-3497-2014.

Loza, C. L., J. S. Craven, L. D. Yee, M. M. Coggon, **R. H. Schwantes**, M. Shiraiwa, X. Zhang, K. A. Schilling, N. L. Ng, M. R. Canagaratna, P. J. Ziemann, R. C. Flagan, J. H. Seinfeld, 2014: Secondary Organic Aerosol Yields of 12-carbon Alkanes. *Atmos. Chem. Phys.*, 14, 1423-1439, https://doi.org/10.5194/acp-14-1423-2014.

Book Chapters

Schwantes, R. H., R. C. McVay, X. Zhang, M. M. Coggon, H. Lignell, R. C. Flagan, P.O. Wennberg, J. H. Seinfeld, 2017: Chapter 1: Science of the Environmental Chamber. *Advances in Atmospheric Chemistry: Vol 1* In J. R. Barker, A. L. Steiner, & T. J. Wallington Eds., Singapore: World Scientific Publishing Co. Pte. Ltd., 1-93.

In Preparation

Schwantes, R. H., S. M. Charan, Y. Huang, K. H. Bates, T. B. Nguyen, H. Mai, W. Kong, R. C. Flagan, J. H. Seinfeld: Low-volatility compounds contribute significantly to isoprene SOA under high-NO conditions. *Atmos. Chem. Phys*. (In preparation).

Schwantes, R. H., L. K. Emmons, J. J. Orlando, G. S. Tyndall, M. C. Barth, S. R. Hall, K. Ullman et al.: Comprehensive Terpene Chemistry Is Necessary for Accurately Simulating Surface Ozone in the Southeastern U.S. in CAM-Chem. (In preparation).

SELECTED PRESENTATIONS

Schwantes, R. H., et al.: The Impact of Aerosol Uptake of Organic Nitrates on Simulated Surface Ozone in CAM-chem. Oral Presentation, International Aerosol Conference (IAC), St. Louis, Missouri, USA, 2018.

Schwantes, R. H., et al.: Comprehensive Monoterpene Chemistry is Necessary for Accurately Simulating Surface Ozone in the Southeastern U.S. in CAM-Chem. Oral Presentation, Gordon Research Seminar (Early Career Portion of GRC) and Gordon Research Conference (GRC): Biogenic Hydrocarbons and the Atmosphere, Les Diablerets, Switzerland, 2018.

Guenther, A. and **R. H. Schwantes**: Atmosphere-Surface Exchange Overview. Oral Presentation, NSF-ATC and NCAR Atmospheric Chemistry Workshop, Boulder, Colorado, USA, 2018.

Schwantes, R. H., et al.: The Impact of Updating Isoprene and Monoterpene Chemistry on Simulated Surface Ozone in CAM-Chem. Oral Presentation, Winter CESM Chemistry Climate Working Group Meeting, Boulder, Colorado, USA, 2018.

Schwantes, R. H., et al.: The Impact of Chemical Mechanism Design on Simulated Ozone in CAM-Chem. Oral Presentation, American Geophysical Union, New Orleans, Louisiana, USA, 2017.

Schwantes, R. H., et al.: The Impact of Chemical Mechanism Design on Simulated Ozone in CAM-Chem. Poster Presentation, Gordon Research Conference – Atmospheric Chemistry, Newry, Maine, USA, 2017.

Schwantes, R. H.; et al.: Secondary Organic Aerosol Yields from Isoprene under High NO Conditions. Oral Presentation, 34th American Association for Aerosol Research, Minneapolis, Minnesota, USA, 2015.

Schwantes R. H.; et al.: Isoprene NO_3 Oxidation Products from the $RO_2 + HO_2$ Pathway. Oral Presentation, Workshop on Nitrate Radicals and Biogenic Volatile Organic Compounds: Oxidation, Mechanisms and Organic Aerosol, Georgia Institute of Technology, Atlanta, GA, USA, 2015.

Schwantes R. H.; et al.: The Formation and Aerosol Uptake of Isoprene Nitrooxyhydroxyepoxide (INHE), a Newly Identified Product from the $RO_2 + HO_2$ Pathway of Isoprene NO_3 Oxidation. Oral Presentation, American Geophysical Union, San Francisco, CA, USA, 2014.