

An Atmospheric Aerosol Short Course for Early Career Scientists

James Mather, Susannah Burrows, Duli Chand, Nancy Hess,
Alexander Laskin, Allison McComiskey, Noopur Sharma, and John Shilling

The EMSL/ARM Aerosol Summer School

What: Early career scientists came together to learn about atmospheric aerosol science topics and related measurement and modeling techniques. The summer school was led by scientists from the Department of Energy's Environmental Molecular Sciences Laboratory and Atmospheric Radiation Measurement research facilities and the Atmospheric System Research program.

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Corresponding author: James Mather, jim.mather@pnnl.gov

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AFFILIATIONS: Mather, Burrows, Chand, Hess, Sharma, and Shilling—Pacific Northwest National Laboratory, Richland, Washington; Laskin—Purdue University, West Lafayette, Indiana; McComiskey—Brookhaven National Laboratory, Upton, New York

The first Department of Energy (DOE) Environmental Molecular Sciences Laboratory (EMSL)/Atmospheric Radiation Measurement (ARM) user-facility aerosol summer school was held in July 2019 at the EMSL user facility within the Pacific Northwest National Laboratory (PNNL) in Richland, Washington. The EMSL facility (Laskin et al. 2019; China et al. 2018) operates advanced instruments such as mass spectrometers and microscopes to achieve fundamental understanding and prediction of biological, Earth, and environmental systems. The ARM facility (McComiskey and Ferrare 2016) operates comprehensive atmospheric observatories in diverse climate regimes to improve the understanding of clouds, aerosols, and their interactions with Earth's surface. The school set out to give graduate students and early career scientists (within four years of receiving their Ph.D.) an overview of atmospheric aerosol science and an introduction to the measurement capabilities available through the EMSL and ARM user facilities.

Instructors for the course were drawn from scientists from the EMSL and ARM facilities as well as from the DOE Atmospheric System Research (ASR) program. Student support for the summer school was jointly provided by EMSL, ARM, and ASR. Students for the summer school were selected through a competitive process; 125 students submitted applications, including nomination letters and curricula vitae. This level of interest was a strong affirmation that a course of this type was needed in the atmospheric science community.

The school spanned five days, with each day covering a particular theme. Twenty-four students from 19 institutions attended morning lectures on aerosol composition, properties, theory, measurements, and modeling. During afternoons, the students explored instruments that collect and analyze aerosol samples at EMSL and PNNL's Atmospheric Measurements Laboratory. They also tested relevant computer modeling simulations and learned about NWChem, EMSL's open-source computational chemistry software suite.

Following are short descriptions of the daily themes covered during the summer school.

Day 1: Methods of aerosol characterization

Organized by Alex Laskin, Purdue University; topical presenters: Alla Zelenyuk-Imre, John Shilling, Zihua Zhu, Albert Rivas-Ubach, Eric Bylaska, and Edo Apra, all at PNNL.

The study of atmospheric aerosols is broad, including the characterization of physical and chemical properties, processes governing the life cycle of aerosol particles, and the impact of aerosols on cloud formation. Presentations on the first day focused on an introduction to atmospheric aerosols, different types of airborne particles, how they form, their impact on climate and weather, and how their chemical, physical, and optical properties are measured experimentally.

Obtaining comprehensive information on the chemical composition of atmospheric particles is challenging because no single method of analytical chemistry can provide the full range of needed information. Therefore, speakers discussed multimodal applications of complementary analytical methods in a context of providing comprehensive information ranging from microscopy-level details of individual particles to advanced molecular characterization of complex molecules that form particulate matter. Instructors gave specific attention to the application of a range of analytical techniques in various field studies of aerosol chemistry and physics pertinent to their impact on climate forcing.

Presentations illustrated how chemical and morphological particle microstructures affect physicochemical properties such as chemical reactivity, gas-particle partitioning, and hygroscopic and optical properties. Selected experimental and theoretical chemistry methods were discussed for studies of particles with different levels of elemental and molecular specificity. Presenters highlighted applications of these methods in recent studies and discussed their strengths, limitations, and potential future research directions.

Finally, presenters emphasized that future climate models would need to include dynamic

evolution of aerosol composition and properties for improved predictions of their atmospheric and climate impact.

Day 2: Secondary organic aerosols

Organized by John Shilling, PNNL; topical presenters: Rahul Zaveri, ManishKumar Shrivastava, and Xiao-Ying Yu, all at PNNL. Aerosol particles may either be emitted directly into the atmosphere (primary) or form as a result of condensation of gases (secondary). Among secondary aerosol sources, there is a great deal of interest in—and uncertainty associated with—secondary organic aerosols (SOA), which represent a significant fraction of the aerosol mass in most regions and are formed through complex chemical processes. Presentations on the second day focused on SOA, starting with an introduction that covered worldwide measurements of SOA composition and the role SOA plays in growing particles to cloud-condensing nuclei sizes.

Instructors provided an overview of gas-phase photochemistry leading to SOA formation, and simplified examples of the chemical mechanisms for volatile organic compounds reacting with atmospheric oxidants. Students learned about Raoult's law, the canonical approach for describing gas-particle partitioning and the theoretical basis for describing SOA formation in most models. From there, presentations transitioned into discussing SOA modeling across a variety of scales. Topics in this section included applications of nonequilibrium, kinetically driven approaches to describe partitioning in a box model and strategies for incorporating multiphase chemistry, SOA aging, and coupling biogenic and anthropogenic interactions in regional- and global-scale models. Instructors also reviewed results from recent modeling studies on SOA formation.

Following the review of theoretical and modeling applications, presenters covered laboratory studies of SOA formation, which form the basis for the parameterizations used in models. This module introduced the types of reaction chambers (e.g., flow reactors, Teflon chamber) used to investigate SOA formation, along with the advantages and disadvantages of each. Speakers discussed challenges and limitations of laboratory studies, such as dealing with gas- and particle-phase wall losses and simulating the solar spectrum. Finally, examples of recent knowledge advances derived from laboratory studies demonstrated the types of cutting-edge studies that can be conducted in simulation chambers. System for analysis at the liquid vacuum interface (SALVI) and in situ liquid secondary ion mass spectrometry (SIMS) were introduced as laboratory techniques to study aqueous-phase SOA formation and aging with and without photolysis from air–liquid interfacial reactions.

Day 3: Optical and cloud-forming properties of aerosols

Organized by Noopur Sharma and Duli Chand, both at PNNL; topical presenters: ManishKumar Shrivastava, Susannah Burrows, and Gourihar Kulkarni, all at PNNL; Jian Wang, Washington University in St. Louis; and Daniel Knopf, Stony Brook University. Aerosols contribute to Earth's radiation budget by direct (absorbing and/or scattering) or indirect (cloud formation) effects. Knowledge gaps in the understanding of these processes contribute to uncertainties in global climate models. This session sought to provide a fundamental understanding of the processes governing the optical and cloud-forming properties of aerosol particles, associated measurement techniques, and links between measurements and global climate models.

Instructors introduced techniques using filter- and non-filter-based methods for measuring aerosol absorption coefficients. Extensive and intensive optical properties of aerosols are largely determined by their composition, size, and number, so presenters focused on the refractive index and size parameters. They also discussed aerosol–light interactions in terms of aerosol chemistry and photolysis, and their influence on the lifetime and evolution

of aerosol particles. The speakers extended the discussion to the representation of aerosols in radiative transfer models. With the help of modeling results, presenters demonstrated sensitivity of direct radiative effects to hygroscopic growth of aerosols, impacts of photolysis rates on gas-phase chemistry, historical trends in aerosol emissions, and radiative forcing by black and brown carbon.

Aerosols are also responsible for indirect radiative effects through aerosol–cloud interactions. Instructors described the role of aerosols acting as cloud condensation nuclei and ice nucleating particles for warm and cold clouds, respectively. Speakers also discussed the dependence of cloud droplet diameter on supersaturation and composition using theoretical and experimental approaches. Discussion of ice nucleating particles included typical ice nucleation pathways (immersion freezing and deposition ice nucleation), the homogeneous freezing limit, the role of supersaturation, and derivation of ice nucleation rates, along with experimental techniques and field observations. Presenters explained current challenges in the understanding of ice cloud formation, as well as ongoing field campaigns to address those needs.

Day 4: ARM field measurements

Organized by Jim Mather, PNNL, and Allison McComiskey, Brookhaven National Laboratory; topical presenters: Janek Uin and Tom Watson, both at Brookhaven National Laboratory; Jason Tomlinson, Fan Mei, Jerome Fast, and Larry Berg, all at PNNL; and Jian Wang, Washington University in St. Louis. The ARM user facility provides measurements to support the study of aerosol, cloud, and precipitation processes, their impact on the atmospheric energy balance, and improvement of the representation of these processes in atmospheric models. ARM staff and data users provided an overview of ARM capabilities and services to the science community with an emphasis on aerosol measurements and data products.

ARM aerosol measurements include extensive suites of in situ measurements and remote sensors at six ground-based atmospheric observatories (McComiskey and Ferrare 2016). Instructors provided overviews of the in situ instrument suites, which at five of the observatories provide over a dozen instruments to measure a range of physical, chemical, and optical aerosol properties. These overviews included detailed operational considerations and challenges for the range of instruments deployed, as well as an emphasis on measurement uncertainty and the importance of its characterization for providing high-quality data for science. Presenters reviewed ARM remote sensing measurements, including lidars and shortwave spectral radiometers that provide information on aerosol properties in the atmospheric column for both column-integrated and profiling methods.

Continuous ground-based in situ and remote sensing measurements are further augmented with aerial measurements from ARM Aerial Facility aircraft and tethered balloons, and may also be complemented with enhanced observations during field campaigns through hosting guest instruments on the ground or in the air. A demonstration during the lecture introduced students to one of the aircraft measurement probes for observing aerosol size distributions.

The ARM field measurement session concluded with overviews of several aerosol-oriented ARM field campaigns by the lead investigators, who also presented considerations in designing field campaigns and some of the research findings.

Day 5: Aerosol modeling

Organized by Susannah Burrows, PNNL; topical presenters: Manabu Shiraiwa, University of California, Irvine; and ManishKumar Shrivastava and Hailong Wang, both at PNNL. DOE atmospheric aerosol research is aimed at advancing fundamental understanding and improving the representation of aerosol processes and properties in global Earth system

models. Presentations on the final day of the school focused on modeling the role of aerosols in the climate system. Ideally, models should be selected based on their appropriateness to the scientific question to be investigated. Considerations include the temporal and spatial scales of the processes under investigation, as well as the different degrees of process complexity represented in various models. This session sought to give students a general overview of the classes of models used to understand the climate impacts of aerosols, including their basic strengths and limitations.

Regional- and global-scale climate models can enable researchers to connect various aerosol sources to their atmospheric effects. Speakers discussed the processes included when modeling the transport, removal, and evolution of aerosols in the atmosphere, as well as their climate impacts. Process models, which describe chemical and physical processes at a detailed level, can be used to explain and understand laboratory experiments. When developed at an appropriate level of complexity, process models can be embedded into regional or global three-dimensional models to understand the atmospheric impacts of various chemical and physical processes.

Speakers shared recent findings regarding modeling of aerosol impacts on climate, including studies of the primary and secondary radiative impacts of aerosols. They introduced the Modal Aerosol Module (MAM) representation, which serves as the aerosol module within version 1 of DOE's Energy Exascale Earth System Model (E3SM). Recent studies on secondary organic aerosols and their radiative impacts were discussed, as well as the treatment of cloud-aerosol interactions. Presenters also described factors affecting radiative transfer in the atmosphere, such as the layering of aerosols and clouds.

Afternoon demonstrations

While the summer school focused on a particular science theme each morning in a classroom setting, in the afternoon, the students broke into groups to engage more directly with instructors and with some of the instruments and analysis techniques they studied in morning sessions. For the afternoon demonstrations, the students were divided into four groups. The four groups cycled through a total of 10 activities during the week. Students participated in seven instrument-oriented activities and three modeling-oriented activities. These activities ranged in length from 30 minutes to 2 hours.

Course organizers structured the instrument demonstrations, led by multiple scientists, to include time for questions and answers with the students. The demonstrations reinforced concepts introduced in the morning lectures and included a wide variety of instruments providing measurements of aerosol physical and chemical properties using bulk or single-particle analyses. Due to the limited space within the laboratories, the demonstration for a particular topic typically did not occur on the same day as the associated lecture topic.

The modeling activities were more conducive to hands-on engagement, and students engaged with model simulations in two of the modeling activities. The first of these hands-on modeling activities involved the use of the program NWChem to perform first-principles calculations of aerosol chemistry simulations. In the second modeling activity, students received an example dataset of simulation output from E3SM and a Jupyter Notebook, enabling them to visualize aerosol variables in the model output. Students explored the global and seasonal variations in simulated concentrations of different aerosol sizes and chemical species by visualizing global maps and local size distributions.

Feedback and future plans

A group discussion session of current and future research challenges ended each day. Students were encouraged to ask clarifying and follow-on questions of the presenters and provide feedback. An exit survey was also conducted. The overall response from both students and

instructors was positive, though there was feedback geared toward improving the course. The students felt that the mix of experimental and modeling topics balanced gaps in their academic curriculum or the focus of their research groups. The most common constructive feedback focused on the need to provide more hands-on activities and to more explicitly link them to the lecture material. The positive response has encouraged school organizers to consider hosting another school, perhaps every few years.

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References

China, S., and Coauthors, 2018: Fungal spores as a source of sodium salt particles in the Amazon basin. *Nat. Commun.*, **9**, 4793, <https://doi.org/10.1038/s41467-018-07066-4>.

Laskin, A., R. C. Moffet, and M. K. Gilles, 2019: Chemical imaging of atmospheric particles. *Acc. Chem. Res.*, **52**, 3419–3431, <https://doi.org/10.1021/ACS.ACCOUNTS.9B00396>.

McComiskey, A., and R. A. Ferrare, 2016: Aerosol physical and optical properties and processes in the ARM program. *The Atmospheric Radiation Measurement (ARM) Program: The First 20 Years*, Meteor. Monogr., No. 57, Amer. Meteor. Soc., <https://doi.org/10.1175/AMSMONOGRAPHS-D-15-0028.1>.