Manjula Canagaratna & Nga Lee Ng on the Characterization of Organic Aerosol Particles

New Hot Paper Commentary, July 2011

L-R: Manjula Canagaratna & Nga Lee Ng.

Manjula Canagaratna & Nga Lee Ng talk with ScienceWatch.com and answer a few questions about this month's New Hot Paper in the field of Geosciences.

Why do you think your paper is highly cited? Does it describe a new discovery, methodology, or synthesis of knowledge?

SW:

The air we breathe contains micron-sized aerosol particles which impact air quality, human health, visibility, and even the radiative budget of the climate. Organic species constitute a large fraction of the observed aerosol particle mass, and there is a critical need for better characterization of their sources, processes, and composition.

Our paper is highly cited because it integrates organic aerosol measurements from 43 different ambient environments in the northern hemisphere to provide a holistic overview of how the chemical composition of organic particulate material evolves in the atmosphere. This synthesis provides critical information needed for constraining and developing simple, theoretically tractable parameterizations of ambient organic aerosol composition.

As part of this work, new mass spectral diagnostic tools were also developed for characterizing organic aerosol composition as a function of oxidation. These tools provide researchers with standardized methods for directly comparing, evaluating, and linking different field and laboratory measurements of organic aerosol particles.

Would you summarize the significance of your paper in layman's terms?

SW:

In recent years the Aerodyne aerosol mass spectrometer (AMS) has been widely used to characterize ambient organic aerosol composition. In this work we use a mathematical technique called factor

analysis to analyze AMS spectra and separate distinct groups of organic aerosol species emitted by combustion sources (i.e., vehicles, burning, cooking) from oxidized organic aerosol (OOA) species that are formed directly in the atmosphere via oxidation processes. OOA factors dominate the organic aerosol composition observed in all the sites studied in this work and we explore how their chemical composition varies with oxidation.

"Our research provides data needed for appropriately constraining theoretical predictions of the spatial and temporal evolution of key organic aerosol species."

Each OOA factor represents a lumped, bulk average of hundreds of similar oxidized organic molecules. We compare the bulk oxidation of OOA factors by plotting the normalized intensities of two tracer ions (m/z 44 and m/z 43) against each other. Each component provides a different "snapshot" of OOA species in the atmosphere, but by taking the components from multiple worldwide sites together, we are able to define and monitor the continuum of ambient OOA composition.

All ambient OOA factors are found to cluster in a well-defined triangular region in this plot. Less oxidized OOA factors occupy the base of the triangular region and differ more from each other than the more oxidized OOA factors, which are found at top of the triangle. This suggests that OOA species evolve towards similar end products regardless of their original sources and/or composition. This is a key result as it indicates that atmospheric oxidation of OOA species can be modeled in terms of a few common processes rather than explicit reactions of hundreds of individual organic molecules.

How did you become involved in this research, and how would you describe the particular SW: **challenges, setbacks, and successes that you've encountered along the way?**

I (Manjula) was first introduced to the field of aerosols and aerosol mass spectrometry when I began working for Aerodyne Research 10 years ago. At that time the AMS mass spectra were used to quantify and monitor mass concentrations of inorganic aerosol species and total organic aerosol. While the AMS organic spectra were too complex for detailed organic aerosol speciation, it was also clear that they did contain tracer ions that provided information about broad groups of organic aerosol species. The challenge was to try and extract this information from the complete organic mass spectra.

This led to a fruitful collaboration with several of our co-authors (Jose Jimenez and Ingrid Ulbrich from University of Colorado, Boulder, and Qi Zhang from University of California, Davis) on the applications of factor analysis methods to AMS spectra. Together we have applied these methods to AMS datasets from around the world and obtained a simple and uniquely useful characterization of organic aerosol in the atmosphere.

While my (Nga Lee) Ph.D. work at Caltech is primarily focused on laboratory experiments of secondary organic aerosol formation, at Aerodyne I got chances to participate in field measurements and instrument development. I first learned about factor analysis after coming to Aerodyne. A large amount of aerosol mass spectrometry datasets have been collected over the last 10 years or so and we decided to do an integrated analysis of the worldwide urban, rural, and remote aerosol mass spectrometry datasets. Because of my laboratory background, this also offered us a chance to compare the results from ambient measurements to those obtained in laboratory studies to gain more

insights into aerosol formation and composition.

I was completely new to this research area when I first joined Aerodyne—I did not even know the basics of the analysis software. The main challenge for me at the beginning was to learn how to use the software and learn how to perform factor analysis on AMS data. Also, since this work involves analysis of a total of 43 datasets, another big challenge was to make sure that we analyzed each dataset in a consistent way so as to be able to compare the results from one dataset to another.

Where do you see your research leading in the future?

SW:

The datasets analyzed in our manuscript were obtained from unit mass resolution AMS instruments. In recent years several high-resolution AMS datasets have also been obtained around the world. Factor analysis of these spectra provides even more detailed information about the elemental composition (hydrogen to carbon ratios, oxygen to carbon ratios) of the organic aerosol.

By extending our meta-analysis to include high resolution datasets, we will obtain more useful information about how the elemental composition of organic aerosol evolves in the atmosphere. Detailed inspection of the high resolution factor mass spectra may also provide us with unique information necessary to developing new diagnostic tools for evaluating and comparing worldwide AMS factors.

Do you foresee any social or political implications for your research?

SW:

Understanding aerosol formation and composition is imperative to assess the effects of particulate matter on climate and health. Both local air quality models as well as larger global models need to be able to model the evolution of aerosol composition if the impacts of aerosol particles are to be understood. Explicit modeling of chemical reactions is computationally prohibitive for large-scale models, and simpler parameterizations based on laboratory experiments do not reproduce the observed concentration or dynamic evolution of organic aerosol. Thus, there is a critical need for field observation data that can be used to accurately constrain and test parameterization that are used in model predictions.

Our research provides data needed for appropriately constraining theoretical predictions of the spatial and temporal evolution of key organic aerosol species. Observed AMS factor mass concentrations, and chemical composition trends, for example, can be directly compared with the outputs of models and used to refine the parameterizations used in the modeling framework. As models are able to reproduce observed aerosol properties and trends, then they can be used to more accurately assess the regulatory policies needed to control the detrimental effects of ambient aerosol particles.

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