PARTICULARS

The E-Newsletter of the American Association for Aerosol Research

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As always, we'd love any feedback or suggestions you may have for ***Particulars***.

Simply email **info@aaar.org** with the subject line ***'Particulars'***

Kristina Wagstrom, *Editor*

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President's Message

Dear Colleagues,

The year is running fast as we prepare for the **2018 International Aerosol Conference (IAC)** to be held **September 2-7** in **St. Louis**. With almost 1,700 abstracts submitted, we expect it to be the largest aerosol conference ever held. In comparison, our normal annual conference attracts about 700 abstracts and the last IAC four years ago had about 1,200. **Pratim Biswas**, **CY Wu**, and the rest of the organizing committee along with **Bill Carney** and his team at Drohan Management Group have done a great job responding and adjusting to such a large group. We are fortunate that the conference venue has plenty of space as the program will now include 9 parallel sessions.

For those of you attending, the IAC banquet will be held at the iconic Gateway Arch. Tickets are limited and first come, first serve so do not delay in registering for the conference if you would like to attend the banquet. Also, please consider booking your hotel room early as space at closest properties will likely fill up fast.

A very productive springboard of directors meeting was held February 24th at Drohan Management premises in Reston, Virginia. Many initiatives were started and just as importantly a good number were completed, I will touch on two items here:

— **Akua Asa-Awuku** presented a review of the results of her recent membership strategic survey. Our current strategic plan dates from 2009 and work on updating it has been ongoing for several years. In general, the membership approved of the basic values in the current plan but felt we needed to focus on attracting and retaining new members, acknowledge the increasing importance of environmental health and climate, and work harder on both outreach to groups

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outside the association—particularly industrial researchers—and also internal interaction between working groups. As a result of this discussion, there are plans to extend the working group chairs meeting at the conference to allow more interaction and an initiative was approved to generate a proposal for an **Indoor Air Symposium** to be held in **2019**.

- A name change was approved for the Health Related Aerosols working group to now be the **Health Effects of Aerosol**s working group. The group believes the new name will more closely align with researchers working with both aerosolized drug delivery and the human health effects of ambient aerosols, their two main focus areas. They felt that currently research in ambient aerosol health effects was somewhat randomly spread across several areas of the association and it would be beneficial to give it a clear home.

The association continues its strong financial position with unrestricted reserve funds in excess of 200% of our typical annual budgets (this year due to the IAC the budget is larger and unrestricted reserves are a little under 150% of budget). This financial strength has allowed us to invest in board directed strategic projects which this year includes over $40,000 in need based IAC travel grants for students and professionals who come from developing regions of the world and/or would not otherwise be able to attend the conference. This is very much in line with our mission to promote and communicate technical advances in the field of aerosol research and something we can all feel good about.

Finally, please take time to stop by the new AAAR booth at the IAC exhibition. It will be manned by directors and officers of the association who will be glad to answer questions or receive your feedback on how we are doing. *I look forward to seeing you in St. Louis!* ●

Tyler Beck, *AAAR President*

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AS&T Article Highlight

By Ben Murphy

"Ambient aerosol composition by infrared spectroscopy and partial least squares in the chemical speciation network: Multilevel modeling for elemental carbon"

https://doi.org/10.1080/02786826.2018.1439571

Detailed analyses of the carbon portion of atmospheric particles with Fourier-transform infrared spectroscopy (FTIR) techniques have yielded an impressive array of insights about the composition and source apportionment of these pollutants. To date, most studies using FTIR to analyze ambient particulate matter have focused efforts toward intensive field campaigns, in part because of the resources required to collect and analyze FTIR data as well as the availability of complementary detailed measurements to help interpret results. Meanwhile, application of FTIR techniques to routinely collected samples from ambient monitoring networks has the potential to offer additional composition detail to existing measurements as well as fill gaps where measurements are unavailable. The methods investigated by Weakley et al. are nondestructive to the analytes and can be cost-effective when implemented as a routine process. One major challenge, though, is how to connect the detailed compositional information made accessible by FTIR with the standard protocols for measuring particulate carbon constituents by mass. This paper is the most recent in a series of thoughtfully executed studies designed to meet that challenge—this time with a focus on urban and suburban elemental carbon (EC).

For decades, the **Chemical Speciation Network (CSN)** and **Interagency Monitoring of PROtected Visual Environments (IMPROVE)** network have measured and catalogued organic carbon (OC) and EC mass with thermal/optical methods, relying on operational definitions (e.g. the temperature at which the carbon evolved from a quartz filter) to distinguish among carbon classes. As the authors discuss, previous studies have successfully demonstrated that partial least squares statistical models can be built to predict OC and EC mass (measured by Thermal Optical Reflectance; TOR) from FTIR spectra collected from polytetrafluoroethylene (PTFE; or Teflon) filters. Importantly, the models for OC applied one 'global' calibration and found that OC mass was well-reproduced across all sites, seasons, and years for both CSN and IMPROVE data. However, performance for EC mass was enhanced for IMPROVE data when high and low concentrations were calibrated separately. For EC data from CSN on the other hand, it became clear that some samples, from one site in particular (Elizabeth, NJ), exhibited

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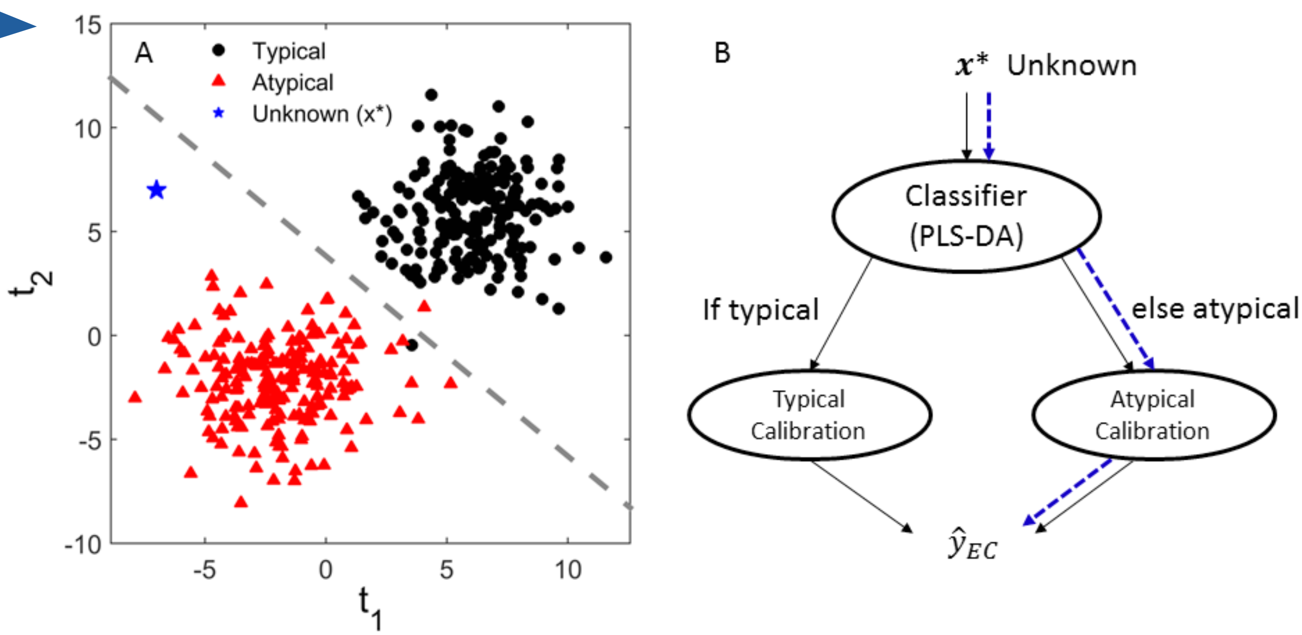
different features from the bulk of the measurements. This suggested that the existing statistical model could have difficulty accommodating samples abnormally influenced by nearby sources.

The authors address this issue directly in this paper by developing a multi-level model whereby all of the available spectra from 10 CSN sites in 2013 are first classified into "typical" and "atypical" classes ***(Fig. 1)***. After this preliminary classification, separate regression parameters are derived for the "typical" and "atypical" classes. A comparison of this two-model approach with the single-model approach (without preliminary classification) shows substantial improvements in bias, error and correlation metrics. But in addition to highlighting statistical performance, the authors lay out the quantitative procedure for how "atypical" classes can be detected and segregated in future datasets, thereby improving the feasibility of using FTIR spectra from Teflon filters to estimate TOR EC and other quantities of interest when quartz filter samples are not available.

As mentioned before, the application of FTIR spectra allow deeper interpretation of the EC composition and thus the root causes for differences between the "typical" and "atypical" samples. For this dataset, the sample spectra from Elizabeth, NJ are chosen since they exhibited "atypical" features compared to the other sites. By comparing the classes' representative spectra and spectral features used for calibration, the authors are able to identify the role of organic nitrogen in the "atypical" samples, and connect that finding to potential influence of enhanced diesel particulate matter at the Elizabeth site. Moreover, the "atypical" samples show little influence of OH and NH groups as well as C=C stretches, suggesting to the authors that they are possibly less oxidized than the "typical" samples. This paper thus demonstrates, at least preliminarily, the exceptional added value that FTIR analysis may contribute to the traditional mass-based metrics for routine observations. ●

Figure 1. *(Fig. 2 in paper)*

Example of classifying an unknown spectrum (x) as either atypical or typical using PLS-DA (a). In this context, the PLS scores (t_1 and t_2) may be thought of as transformed FT-IR spectra where each point represents a spectrum, distinguished here according to class label. For the purpose of this illustration, 200 atypical and typical samples were simulated from two Gaussian distributions with a mean of (-2, -2) and (6, 6), respectively. Simulated class variances are equal ($\sigma 2_{ii} = 4$, $\sigma 2_{ij} = 0$). Estimating the mean of each class and pooled-covariance matrix defines the boundary used to classify and then allocate an unknown test spectrum (star; a) to the appropriate FT-IR calibration (dashed path; b).*



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Aerosol Scientist Spotlight:

By Jason D. Surratt

Featured Scientist | **Andrew Ault** | University of Michigan

1.) How did you get involved in the aerosol science community? This could include past educational or research experiences.

I first knew that aerosol research was something I'd want to do for a long time when I was in the process of fixing an aerosol time-of-flight mass spectrometer (ATOFMS) in a barn in rural Wisconsin as a junior at Carleton College. I was doing summer research with **Prof. Deborah Gross** in the Chemistry Department as part of a collaboration with **Prof. Jamie Schauer** and hadn't realized that chemists could go outside the lab and make a these complicated measurements in the real world. Watching the different mass spectra flash by on the screen every second as the instrument measured aerosols in real time and trying to guess what they were made of felt like playing a scientific video game. I remember being in awe of how something so small could be so complex and wanting to know more about these things that are always floating in the air around us. Having now made aerosol measurements all over the U.S. and beyond, there is still a special excitement when you get into the field and see that first particle, size distribution, etc. getting collected and it's something I get excited about sharing with students each time we leave the lab.

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2.) Which people in our field have been most influential to you and your career?

I have been fortunate to have gotten to work with great mentors at each stage of my career, who have all helped me in different ways, and all have been involved with AAAR over the years. At Carleton, Prof. Deborah Gross really got me hooked on aerosols. At UCSD, my Ph.D. advisor **Prof. Kim Prather** has an infectious enthusiasm for science and understanding aerosols. If things weren't going well in the lab or the field, Kim always had a knack for cutting through whatever the challenges were and recharging my excitement for the project. At the end of the day, to do the challenging work of aerosol measurements, you have to have passion for what you are studying, and seeing Kim's passion for whatever challenge she is trying to tackle is motivating and inspiring. At Iowa, my postdoc advisor **Prof. Vicki Grassian** (now at UCSD) taught me so much about how to think about challenging scientific questions and be an innovative scientist. She has an amazing sense at the very early stages of a project about how to put the pieces together in ways that lead to a compelling result. I really appreciate how Vicki is always thinking about how a new type of experiment or new instrument or new method could let us address questions that we didn't have the tools to previously. She and Kim have both been extremely supportive as I've gotten started as a faculty member. I have also gotten to work with too many amazing collaborators over the years to list, but who have all helped do some fun and exciting science. Lastly, the overall collaborative and supportive nature of the AAAR community is something I've appreciated since my first meeting a decade ago.

3.) What are, in your opinion, the most interesting or important research contributions you've made so far?

I'd like to highlight two contributions that I'm really proud of from my group so far. The first is coming up with methods for measuring of pH of an individual particle (Rindelaub et al. 2016 *J. Phys. Chem.—A* and Craig et al. 2017 *J. Phys. Chem.—A*). The acidity of aerosols is incredibly important for so many processes, including: secondary organic aerosol (SOA) product, metals dissolution, and heterogeneous/multiphase chemistry, but we haven't had methods available to measure it. Particularly as others have shown poorly proxy methods represent acidity in many cases, we need new tools to use in tandem with thermodynamic models. We have more methods for measuring pH on the way, and I can't wait to share them with the community!

The second thing, I'm proud of is our work pushing the lower size limit of particles we can analyze with vibrational spectroscopy. Raman and infrared (IR) spectroscopy have so much to offer

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studies of aerosols in terms of detailed measurements of species, local environments, and reactions, but have traditionally been limited to larger sizes by the diffraction limit of light and way larger than the number size mode in the atmosphere. We published the first paper on surface enhanced Raman spectroscopy (SERS) of atmospheric aerosol particles (Craig et al. Anal. Chem. 2015), which took our Raman analysis below one micron and have since pushed this all the way to 150 nm. We've also used atomic force microscopy with photothermal infrared (AFM-IR) spectroscopy to get IR spectra of particles down to ~100 nm. I think these spectroscopic tools (SERS and AFM-IR) and others will enable us to study aerosol chemistry coupled with physical properties in a whole new light!

4.) What future research questions do you hope to address?

I am fascinated by how complex aerosols are in terms of chemistry, but also, as we are learning more and more, in terms of physical properties (viscosity, phase separations, surface tension, etc.). We are seeing that in so many ways that aerosols often are not simply little, dilute water droplets floating around, but that they have complex shapes, structures, surfaces, phases, etc. I want to understand these complex physicochemical properties and how they evolve for aerosols in the atmosphere. I thinks for so many important types of particles SOA, sea spray aerosol, mineral dust, these properties can end up influencing their climate and health effects and I want to make detailed measurements to understand how this happens.

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5.) Are there new aerosol research areas/directions that you see as particularly interesting or important?

I think we are at a really exciting time in aerosol science, where we are able to gain insight into how aerosols are look and behave at the single particle level under ambient conditions. For so long, imaging was limited to large particles like asbestos or under the high vacuum of an electron microscope. However, today with so many methods being developed and applied to aerosols, such as atomic force microscopy, environmental electron microscopy, optical tweezing, and surface enhanced Raman spectroscopy (SERS) we are able to look at these particles one-by-one and really appreciate their complexity. Using these new tools to determine how complex physicochemical properties determine impacts on climate and health, is a fascinating direction for future research. With the amazing analytical advances in materials science and the life sciences, I am very interested in seeing how those can help us address key questions related to optical properties, cloud formation, and health effects. •

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In Case You Missed It

By Jason D. Surratt

Toxic Metal Concentrations in e-Cigarette Liquid and Aerosol Samples.

Researchers at the John Hopkins Bloomberg School of Public Health and colleagues investigated the transfer of metals from the heating coil to the e-liquid in the e-cigarette tank and the generated aerosol from daily e-cigarette users. They find that e-cigarettes are a potential source of exposure to toxic metals and that higher concentrations of these metals were in the aerosol and tank samples, demonstrating that the coil contact induced e-liquid contamination. This article was published in the latest issue of Environmental Health Perspectives:

Olmedo et al. (2018), Metal Concentrations in e-Cigarette Liquid and Aerosol Samples: The Contribution of Metallic Coils, *Environmental Health Perspectives*

https://doi.org/10.1289/EHP2175

Automotive Emissions of Volatile Organic Compounds (VOCs) on the Decline: VOCs from Pesticides, Coating, Printing Inks, Adhesives, Cleaning Agents, and Personal Care Products Now Contribute Equally to Urban Secondary Organic Aerosol.

Researchers at the National Oceanic and Atmospheric Administration (NOAA) show that success in controlling air pollution has changed the amounts of sources of anthropogenic VOC emissions in the United States, lowering the relative contribution from volatile chemical products (e.g., cleaning agents and personal care products). This article was recently published in Science:

McDonald, B.C. et al. (2018), Volatile Chemical Products Emerging as Largest Petrochemical Source of Urban Organic Emissions, *Science* 359, pp. 760-764

DOI:10.1126/science.aaq0524

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China Tests Giant Air Cleaner to Combat Smog.

Nature recently published a news article that describes how a 60-meter high chimney was built in Xian, China in order to purity the air. This outdoor air-cleaning system is powered by sunlight and is designed to filter out adverse particles and gases. The results from the prototype have not been published yet and already have its skeptics. For more information on this technology and the discussion around it, visit the following article:

Cyranoski, D. (2018), China Tests Giant Air Cleaner to Combat Smog, *Nature*, 555, pp.152-153

DOI: 10.1038/d41586-018-02704-9

High Levels of Stratospheric Smoke Particles Observed Above Southern France.

Researchers found that severe boreal forest wildfires in North America resulted in pyrocumulonumbus firestorms that injected large amounts of smoke particles into the stratosphere. By using ground-based and space-borne lidars, these researchers found that the stratospheric aerosol mass loading from the wildfires was similar to that of moderate volcanic eruptions. The impact of these smoke-derive particles is currently unclear on stratospheric processes, such as ozone layer chemistry. This article was published in Geophysical Research Letters:

Khaykin, S.M. (2018), Stratospheric Smoke with Unprecedentedly High Backscatter Observed by Lidars Above Southern France, *Geophysical Research Letters*, 45(3), pp. 1649-1646

DOI: 10.1002/2017GL076763 •

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