

A case for developing particle standards having
known size, shape and composition to improve
atmospheric measurements and model
performance

Jim Smith and Nicole Riemer

Background: “The aerosol standards white paper”

- **At a breakout session at a Joint ARM User Facility and ASR PI Meeting, we wanted to discuss ...**
 1. How can we integrate different experimental techniques to characterize mixing state as fully as possible?
 2. How can we use this information to compare to mixing-state-aware models.
- **Outcome of the discussion:**
 - Aerosol calibration procedures are a key issue for several “routine” measurement techniques, including techniques for measuring, for example, size distributions and cloud condensation nuclei (CCN) concentrations.
- **Key need:**
 - Capability to produce “aerosol standards,” or aerosol particles of atmospheric relevance that are well-characterized in terms of composition and size.
- **Benefits:**
 - Having such aerosol standards would directly help with calibration procedures for routine measurements and enable the development of quantitative comparison methods between mixing-state-aware measurements and models.
- **This led to “the aerosol standards white paper”:** <https://tinyurl.com/particlestandards>



We asked aerosol measurement experts the following questions:

1. What do modelers want from your measurements?
2. What calibration methods are currently used?
3. What are the measurement errors or inconsistencies that are not being addressed by existing calibration techniques?
4. What intercomparisons, standards, best practices, etc., promise to reduce uncertainties?

The following measurements were discussed:

Aerosol Particle Physico-Chemical Properties

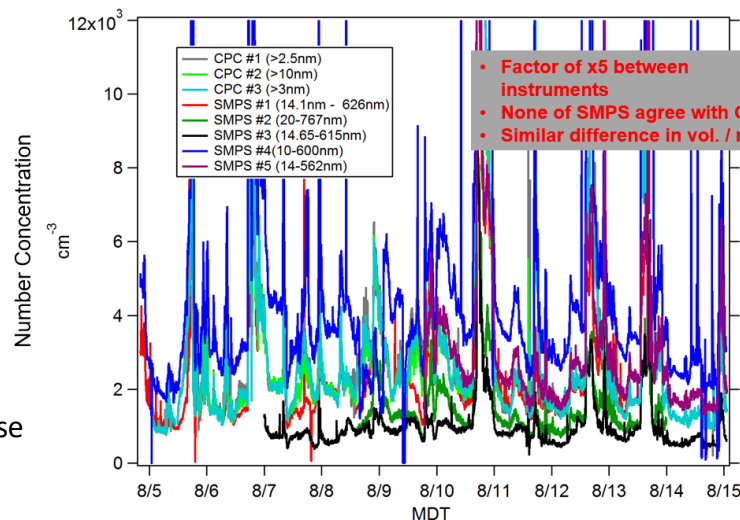
- Size Distributions and Number Concentrations
- Submicron Particle Species-Resolved Mass Concentration
- Nanoparticle Species-Resolved Mass Concentration

Aerosol Particle Climate-Relevant Properties

- Soot Particles and Aerosol Optical Properties
- Particle Hygroscopicity: Water Uptake and CCN
- Ice Nucleating Particles

Common themes for different types of measurements

- Cost of instruments and facilities needed for instrument calibration.
 - This points towards the need for centralized facilities.
- Every multi-instrument measurement campaign should take a few days to perform calibrations using a common standard.
 - Currently this is not often a priority but calibration activities such as these are essential to the production of good science.
- Users of the same techniques across multiple groups should hold meetings to discuss the details of instrument operation including calibration and best practices as these techniques tend to evolve rapidly and are not always well documented in the literature.



J. Jimenez

Extra slides

Submicron Particle Species-Resolved Mass Concentration

Manjula Canagaratna, Philip Croteau, Cassandra Gaston, and Jose Jimenez

Q1: What do modelers want from your measurements?

- Overall, instruments like the AMS are providing useful data with sufficient accuracy for models
- The biggest challenges are associated with instrument response to changes in ambient humidity, temperature, aerosol size, composition, liquid water content, and mixing state.
- **Inorganics** (important because thermodynamic models such as ISORROPIA-II used this for predicting aerosol liquid water and pH)
 - Ammonium sulfate is one of the easiest species to quantify due to its low volatility.
 - Ammonium nitrate is challenging due to its semi-volatile nature and because different forms of nitrate have different detection efficiencies
- **Organics** (account for 20-90% of ambient sub-micron mass)
 - There are hundreds of thousands of different organic compounds in particles, and each has a different detection efficiency
 - SOA has different volatilities and phase states:
 - Volatilities important for modeling absorptive partitioning
 - Phase state also important for partitioning as well as detection efficiency

Submicron Particle Species-Resolved Mass Concentration

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Q2: What calibration methods are currently used?

- For the **AMS and ACSM**, typically calibrated directly with aerosol particles
- NH_4NO_3 particles are generated with an atomizer and dried with a diffusion dryer.
- The polydisperse aerosol is then size-selected with a DMA and split between the instrument and a CPC.
- Input particle mass loading is calculated from the mobility diameter, number concentration, material density, and shape factor and compared to signal to determine the ionization efficiency (IE, mass detected vs. mass sampled).
- The IEs of species other than NO_3 are calculated as the product between a species-dependent relative ionization efficiency (RIE) and the calibrated NO_3 IE.
- The RIE of NH_4 can be measured directly from NH_4NO_3 .
- For SO_4 or Cl, the RIE can be measured using NH_4Cl or $(\text{NH}_4)_2\text{SO}_4$ solutions.
- Since OA consists of many different types of individual species, an average value of RIE based on laboratory calibrations is utilized for measurements of ambient OA.

Submicron Particle Species-Resolved Mass Concentration

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Q3: What are the measurement errors or inconsistencies that are not being addressed by existing calibration techniques?

- These calibration schemes are not simple or rugged enough for routine-use with aerosol instruments that are utilized in the field and are often expensive.
- Mass concentrations calculated from the selected size of the calibrant particles can have significant errors due to uncertainties in particle shape and density.
- A key weakness of current laboratory mass calibration methods is that they utilize single component aerosol particles.
- Organic laboratory standards also do not accurately capture the complex chemical properties of ambient OA. There is a lack of commercially available species that can be used as laboratory surrogates of the highly oxidized organics

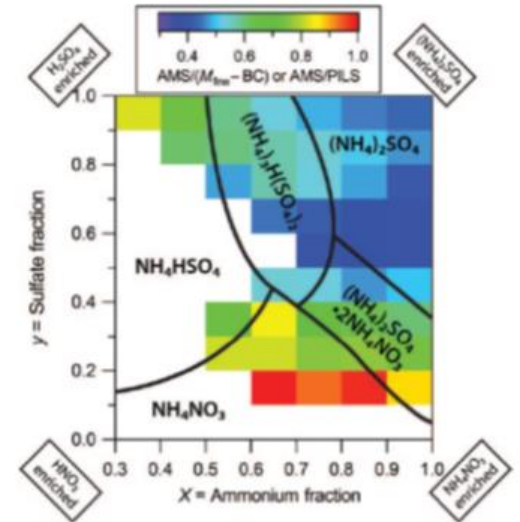


Figure 3.2: AMS collection efficiencies estimated as ratios between the mass measurements from the AMS and other carefully operated instruments from 3 different field studies. The composition-dependent variation in the estimated collection efficiencies is shown on the phase diagram for mixtures of various mole fractions of ammonium, sulfate, and nitrate.

Submicron Particle Species-Resolved Mass Concentration

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Q4: What intercomparisons, standards, best practices, etc., promise to reduce uncertainties?

- Calibrations should also be performed as much as possible under the conditions that will be utilized for the measurement of interest.
- For lab studies, the equipment used to generate a known mass of aerosol should be well-calibrated.
- Intercomparisons are important. They suggest re-aerosolizing particles collected on filters or by chemical processing of realistic precursors in an oxidative flow reactor or a smog chamber.
- Important to consider volatility:
 - low volatility of SO_4^{2-} makes it a strong candidate for cross-comparison between off-line and on-line techniques
 - NO_3^- , because of its higher volatility, is more difficult to compare across different techniques because of potential losses

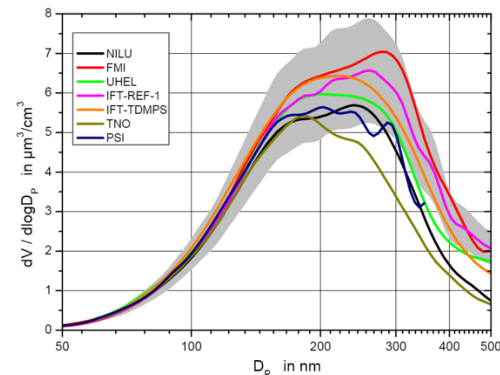


Fig. 8. Intercomparison of the ambient volume particle size distribution of the mobility particle size spectrometers. The shaded area marks the $\pm 10\%$ range around the reference mobility particle size spectrometer (IFT-REF-1).