AMS/ACSM Calibration Protocols

The Aerodyne Team
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Outline

Primary calibrations to quantify aerosol mass loading and size*

• IE and RIE Calibrations (AMS and ACSM)
  • Anita will talk about SP-AMS calibration on Wednesday 1/20/2021.
• Velocity calibration – particle time-of-flight to size (AMS)
• Vaporizer temperature calibration (AMS)

*After your instrument is well-configured (lens aligned, MS tuned, gain measured, flow rate calibrated). CU Boulder group working on manuscript on detailed procedures. See Ben’s talk later today.
Ionization Efficiency for NO3 (IE_NO3)

• How to go from ions/s (what we measure) to mass loading (µg/m3).
• Mass-based method – compare MS signal to mass of particles sampled.
• Use NO3 from NH4NO3 for IE because
  • Vaporizes completely at 600 – 650 C
  • Doesn’t bounce, particles well-focused by aerodynamic lens
  • Creates only two main ions (NO⁺ at m/z 30 and NO2⁺ at m/z 46)
  • Readily soluble in water, not especially hazardous
• Requires equipment
  • Atomizer to generate particles + dryer to remove water
  • DMA to size-select
  • CPC to count particles
• New compact calibration module coming soon – see Phil’s talk Wednesday 1/20/2021!
Input Mass = Eff. Density x Volume(size) x Number

**Very Important!!**

- **Excess flow**
- **By-pass**
- **filter**
- **AMS/ACSM**
- **Instrument Response**
IE_NO3 Calculation with 300 nm NH4NO3, multiple concentrations

- Use mass loading similar to expected measurement, e.g., 0 – 20 µg/m3 NO3.

- IE Calibration units
  - Ions/molecule for AMS
  - Ions/pg for TOF-ACSM
  - Amps/(µg/m3) for Q-ACSM

- IE Analysis
  - Manual for AMS (in Squirrel or Pika)
  - Integrated in DAQ for ACSM

- Measure IE (and AB) at one point in time
  - Correct for variations in detector sensitivity (e.g., aging, temperature of instrument) with measured AB.
• NH4NO3 also gives RIE_NH4
• Acquire and analyze IE and RIE calibration data in the SAME way as your regular data acquisition
  • If you will do HR analysis on HR-AMS data, then analyze IE and RIE data in Pika.
• If NH4 vs NO3 is very noisy, you might have a high background of water interfering with NH4. Wait a few days and try again.
Note About Particle Size and Solution Concentration

- 300 nm / 5 mM.
- Want to avoid Q2 particles from DMA (~ twice the mass, but only count as 1 particle).
- In AMS, can remove Q2’s in analysis based on pToF.
  - Cannot remove Q2’s in ACSM data.
- Aim for maximum of 1,000 p/cc at 300 nm (with TSI 3076 atomizer).

![Graph showing normalized NO2 signal at 250 nm, 300 nm, and 350 nm with different solution concentrations.](image)
Use 300 nm NH4NO3 Particles!

Multiple charged diameters

- Dmob
  - 200 nm
  - 250 nm
  - 300 nm
  - 400 nm

Nitrate Signal

Calculated Mass

- intercept = 0.068 ± 0.041
- slope = 0.493 ± 0.003

Lens transmission limitation

ARI AMS Users Meeting, Virtual, January 19, 2021
Do Measure RIE_SO4 for Your Instrument!

- Use size-selected (NH4)2SO4 particles.
- NH4 is internal reference, so CE does not matter.
- But make sure you have a good RIE_NH4 from NH4NO3 cal!
- Use similar mass loading to ambient.
- Default RIE_SO4 = 1.2 is not correct for many instruments.
Can measure RIE_Cl with NH4Cl Particles

- Use size-selected NH4Cl particles.
- NH4 is internal reference, so CE does not matter.
- But make sure you have a good RIE_NH4 from NH4NO3 cal!
- Use similar mass loading to ambient.
- Default RIE_Cl = 1.3 is not correct for many instruments.
- NOTE: NaCl has a different RIE_Cl! See Hongyu Guo’s talk on Thursday 1/21/2021.

\[
\text{RIE}_\text{Cl} = 1.96 \pm 0.03
\]

Fit uncertainty only

\[
\text{RIE}_\text{Cl} = \text{slope} \times \frac{\text{RIE}_\text{NH4} \times 18}{35.45}
\]

Using \( \text{RIE}_\text{NH4} = 3.16 \)
Single Particle IE Calibration (AMS only)

• Single particle method (record data when signal crosses a threshold)
  • Brute Force Single Particle (BFSP) (AP240 – old data card)
  • Event Trigger (ET) (ADQ – new data card) – Ben will talk more about this later.

• Always measure mass-based IE, too!
  • If they don’t agree, trust the mass-based IE.
  • Pitfalls with getting enough signal per particle.
  • Only need ET IE measurement if taking ET data.

• Mass-based method only as good as your DMA and CPC
  • Spot check DMA sizing with PSLs.
  • Compare CPC to others.
Velocity Calibration (AMS only)

• How to go from particle time of flight (what we measure) to size (what we care about)

• Semi-empirical equation (somewhat meaningful parameters)

\[ Vel(D_{va}) = V_{gas, lens} + \frac{V_{gas, exit} - V_{gas, lens}}{1 + \left(\frac{D_{va}}{D^*}\right)^b} \]

Velocity = \frac{Distance}{pToF}

215-series:
Distance = 0.295 m

255-series:
Distance = 0.395 m
Velocity Calibration with Size-selected NH4NO3 Particles at Many Dmob

\[ \text{pToF} = 0.00178 \text{ s} \]

\[ \text{Vel} = \frac{\text{Chamber Length}}{\text{pToF}} = \frac{0.295 \text{ m}}{0.00178 \text{ s}} = 166 \text{ m/s} \]

\[ D_{va} = D_{mob} \times \text{Density} \times \text{Shape Factor} = 70 \text{ nm} \times 1.72 \times 0.8 = 96 \text{ nm} \]
Velocity Calibration

\[ \text{Vel}(D_{va}) = V_{\text{gas, lens}} + \frac{V_{\text{gas, exit}} - V_{\text{gas, lens}}}{1 + \left(\frac{D_{va}}{D^*}\right)^b} \]

- Remember to enter parameters in DAQ!
- Or Squirrel if you need to correct sizing after data is collected.

\[ \begin{align*}
V_{\text{gas, lens}} &= 32.371 \pm 0.561 \\
V_{\text{gas, exit}} &= 499.51 \pm 11.9 \\
D^* &= 21.106 \pm 1.34 \\
b &= 0.6015
\end{align*} \]
Velocity Calibration Tips

• Velocity calibration only changes if lens P changes!
  • Different elevation, aircraft campaign, new lens

• Or you change your chopper servo and aren’t careful about rotational alignment of chopper flange.

• Every time you do an IE calibration, double check your velocity calibration. 300 nm NH4NO3 should be Dva = 413 nm!

• Use the widest possible range of particle sizes
  • Curve does not extrapolate well.
  • Be careful on the small particle side that you actually see Q1’s.
  • Be careful on the large particle side that you have a clean pToF signal (NH4NO3 tends to break up at sizes > 450 nm).
  • Can use PSLs (at Vaporizer T = 800 C) or NaNO3 (at Vaporizer T = 750 C) for larger sizes. Use half height on rising edge for pToF. Remember to use correct density and shape factor to calculate Dva.

• Fit is underdetermined, so don’t worry about exact values of parameters.
Measuring Vaporizer Temperature with pToF for 300 nm NaNO₃ particles (AMS only)

- Want 600 to 650 °C for complete vaporization of non-refractory and long life for vaporizer.
- pToF traces for NaNO₃ (m/z 30) get narrower as vaporizer T increases.
Determine amp setting where pToF gets narrow.

- Fit falling edge of PToF with single exponential.
- Plot tau vs amps.
- pToF are narrow at 700 to 750 C, usually ~ 1.1A.
- Vaporizer is glowing dull orange from back (front is cooler than back).
- Subtract 0.1 A to get operating T of 600 to 650 C.
Vaporizer Temperature Tips

• Warning: For older AMS instruments, T readout can be off by 100’s of degrees due to thermocouple detachment.

• If your measured vaporizer T is dropping with time, don’t just turn up the current/power.

• If vaporizer current is NOT about 1 to 1.1 A, need to check true vaporizer temperature! Probably should check it anyway.

• Look at NaNO3 mz30 pToF. Sharpens up at 700 to 750 C. Subtract 0.1 from amps to get operating current.

• Look at back of vaporizer. If glowing dull orange, 700 to 750 C. Too hot for normal operation.

• ACSM: We calibrate temperature vs power. If T is unexpectedly low, trust the calibration curve.

• Working on chemical vaporizer T calibration for ACSM – ideas welcome!