Summary of Group Discussion on Absolute Quantification Issues with the AMS

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AMS Quantification Scheme

1. First we calculate the NO_3 equivalent mass for a given species, using all the peaks
2. Then we correct for:
   - Differences in ionization efficiency with respect to NO_3
   - Differences in particle collection efficiency (CE) with respect to 350 nm NH_4NO_3 particles (we estimate the CE of these is ~ 1.0)
   - Fragments that we do not meaure
3. The final mass concentration is:

$$C_{species} = \frac{C_{species}^{NO3\_equiv}}{REI_{species/NO3}\ CE_{species,particles}\ F_{measured}}$$

Example

- For example:
  - We measure 2.0 NO_3-equiv. μg m^{-3} of SO_4
  - REI_{SO4} is ~ 0.87
  - The collection efficiency is estimated ~ 0.5
  - The non-measured fragments are 20% of the total

$$C_{SO_4} = \frac{C_{SO_4}^{NO3\_equiv}}{REI_{SO_4/NO3}\ CE_{SO_4,particles}\ F_{SO_4}^{measured}} = \\ = \frac{2.0}{0.87 \times 0.5 \times 0.80} = 5.75\, mg\, m^{-3} \text{ of } SO_4$$

Values of REI

- REI_{NO3}=1.0 (by definition)
- REI_{SO4}=0.87
  - from Jimenez et al. paper
- $REI_{Organics}$=1.4
  - estimated from the same paper
  - At the users' meeting we said erroneously 0.7, which I think was just 1 / 1.4
- REI_{NH4}=4.5 (varies between 3-8)
  - This is always measured during calibration

Collection Efficiencies

- CE_{NH4NO3} = 1 (lab, or ambient externally mixed)
- CE_{SO4}
  - 2.34 in New York City (Frank Drewnick, comparison to PILS)
  - Houston (2000): 1.7
  - ACE-Asia (2001): 1.7
  - Vancouver: 1.8
  - Ron Brown (2002): To be determined
  - An important issue is that the calculation procedures to arrive at those numbers may not all be consistent

Collection Efficiencies II

- $CE_{NH4NO3} = CE_{SO4}$ (if internally mixed)
- $CE_{organics}$?

  = 1.0 if Pure, liquid (e.g oleic acid in lab)

  = C_{SO4} if on accumulation mode, and internally mixed with SO_4

  = 1.0 if not internally mixed with SO_4

  – Not sure what to do with small mode “traffic” organics
    - From other studies, they tend to be irregular, and thus should have CE < 1

Additional CE Issues

- CE
  - May be size dependent
  - May be time dependent if the morphology of ambient particles changes
    - Actually it is surprising how constant the correlations with the PILS have been in Houston, NYC. This seems to indicate that at these locations the shape of the aerosol (at least as the AMS focusing is concerned) does not change much.
    - But typically > 50% of the mass is in 2% of the particles (Jimenez et al., 2003), so really the critical shape is that of the few larger particles of the accumulation mode

Size Transmission Window

- The critical orifice limits the transmission of large particles
- The aerodynamic lens limits both small and large particles
  - The lens has been changing with time, so this effect may be different for different instruments
- These effects are not included in the CE terms above. CE only takes into account particles that exit the lens into vacuum, but do not reach the AMS vaporizer
- We agree that the AMS is best described as measuring something close to $PM_{1.0}$ (NOT $PM_{2.5}$ or PM_5)

Refractory Material

- AMS does not measure whatever does not evaporate quickly (< 5 sec) at the T of the oven
  - Crustal material (dust) & metals: ~5% urban
    - But we think we can measure the non-refractory species internally mixed with these particles
  - Black carbon: ~5% urban
    - But we do measure the organics and PAHs that are internally mixed with the soot
  - Refractory salts: NaCl, Sea Salt
    - We can measure e.g. NaCl by increasing the oven temperature to ~1000C, however this causes other problems (very large background, etc.)

Particle-Bound Water

- From Dan Imre's experiments and other scattered evidence, we estimate that ~60% of the H_2O evaporates in the lens, and 40% remains.

Issues when Comparing w/ Other Instruments

- Many instruments measure $PM_{2.5}$ instead of $PM_{1.0}$
  - A $PM_{2.5}$ cyclone has 50% transmission at 2.5 μm, but still some transmission up to 5 μm. Thus a $PM_{2.5}$ instrument can include significant mass above 1.0 μm. The AMS should measure a lower mass concentration, though this would depend on the location, i.e. on how much of the mass is above $PM_{1.0}$ in the ambient aerosol.
- PILS
  - Can have losses in lines
  - The cutpoint at large size is not clear, but is larger than 1 μm
- Filters, TEOM, MOUDIs
  - Artifacts: Losses or gains of volatiles & water; chemical reactions. Can be large especially for nitrate and organics.
  - Especially if not using denuders the errors can be very large