Particle beam/laser beam Alignment Procedure and other SP-AMS details

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SP-AMS Orthogonal Detection Axes

- Characterization of particle-laser interaction region:
  - Vertical Particle Beam Walk
  - Horizontal/Vertical Beam Width Probe
  - Horizontal/Vertical Laser Beam Walk

Ion Extraction and MS detection

Sampled Particles

Laser Desorption
Particle Beam Width Comparisons

Overlap mismatch is in one dimension

SP-AMS Laser Width
What you need to do the alignment

- The vaporizer needs to be in
- Ammonium Nitrate particles
- Black carbon particles (Regal black as ambient surrogate)
- Atomizer, DMA (Need monodisperse particles when doing the alignment)
- CPC so that you can normalize signal to # concentration
Step 1

Do lens alignment with Ammonium Nitrate. Center the lens both vertically and horizontally with respect to the Ammonium Nitrate particle beam.

If unsure of your lens freedom of movement turn TPS off and make sure you can move lens vertically and horizontally before turning TPS back on.

Do an Ammonium Nitrate IE also.
Step 2

Get a nice TEM00 towards the middle of the screen

You can use the HENE laser to do this if necessary but that will require venting the instrument.

Note: this is a nice TEM00 but not to close to the middle so my range of motion if I need to move the beam won't be that large.
Step 3

Get your black carbon calibrant flowing and do a vertical lens walk

On this graph 0 height on the x axis is the center of the AN particle beam. WHEN DONE MOVE PB BACK TO CENTERED POSITION ON AN
Step 4

Calculate difference between center of ammonium nitrate beam and center of black carbon beam

Use the equation \((348 \text{ mm}/140 \text{ mm}) \times (\text{center AN on the lens vertical} - \text{center BC on the lens vertical})\) to determine how many millimeters off of center the BC peak is at the vaporizer. Vaporizer diameter is 3.8 mm.

This diagram shows that if you move the lens down .1 mm or 100 um you raise the particle beam at the point of the vaporizer by \((348/140) \times .1 \text{ mm} = .248 \text{ mm}\) rise at vaporizer.
Step 5

BEFORE YOU MOVE THE KNOBS AT ALL TAKE A SCREEN SHOT WHICH SHOWS WHERE THE CAMERA IS SO YOU CAN GO BACK TO THAT POSITION LATER. DO THIS FOR ALL OF THE TEM00 POSITIONS YOU GO TO.

If you have to move the laser vertically walk the laser by moving the top adjuster screw on both sides of the ToF by roughly the same amount but opposite directions. If the screw is pushing further out on one side it should be moving closer in on the other side. Get a new TEM00 at this new position and repeat the particle beam walk see if you are closer to the center of the ammonium nitrate and figure out how much more you need to move the laser beam to achieve this situation where the peak for the black carbon is within .5 millimeter of the center of the vaporizer at the vaporizer.
Moving the image down as shown with the arrow moves the laser beam up in reality inside the ionization chamber because the camera is inverted.
Step 6

Horizontal movement of the laser beam; do this after all vertical centering.

Walk the TEM00 horizontally by some combination of moving the screws on both sides of the TOF. Check sensitivity at these different horizontal positions. The optimum sensitivity will probably be near the center but it is good to check it and verify. Make sure whatever adjustment you make you can undo.
Moving the beam to the right in camera space moves the laser beam forward in the ionization chamber because the image is inverted.
After Optimizing the beam horizontally and vertically and tuning the system and maybe a heater bias walk its time to do AN and BC calibrations
This is not mandatory for lens alignment but is a good check, do a heater bias walk.

Our SPAMS #2

Ga Tech HR-ToF_AMS
Do the AN Cal

- I usually do 300nm the key is to keep Q2s low
- I prefer the 4 point cal with CPC but you could also do BFSP
- Calculate Ion Efficiency and picograms/ion for AN

\[
an\_picosec = \text{numconc} \times \frac{\pi}{6} \times (300 \times 10^{-7})^3 \times 1.72 \times 0.8 \times 1 \times 10^{12} \times 1.28 \times \frac{62}{80}
\]

\[
an\_molec = \text{numconc} \times \frac{\pi}{6} \times (300 \times 10^{-7})^3 \times 1.72 \times 0.8 \times 1.28 \times 6.022 \times 10^{23} \frac{1}{80}
\]

This gives you IE.
Coefficient values ± one standard deviation

\[ a = -4645.6 \pm 1.7e+004 \]
\[ b = 1.0921e-007 \pm 2.99e-008 \]
Do the Regal Black cal

- Atomize with water between cals
- I use a TSI atomizer with at least 25 psi pressure on input to atomizer otherwise you can get sluggish response.
- Get a picograms/ion value for Regal Black
- Use a size that limits Q2s but also makes it through the lens 250, 300,
- Do a 4 point CPC cal
- Get RB ions per picogram
- \( cx\_picosec = \text{numconc2} \times \frac{\pi}{6} \times (300e^{-7})^3 \times 0.9 \times 1e12 \times 1.28 \)
So $\text{RIE} = \frac{190.61}{1060.8} = .18$ as calculated for this instrument.
Now you should do a Laser Power Drop. These experiments are VERY hard to do correctly!

- Laser changes modes
- Cannot saturate camera if using as power monitor
Now if you want to remove the conventional vaporizer

• After removing the vaporizer pump back down the system and retune with no heater bias.

• Do RB cal again and see if you can get the same sensitivity in picograms/sec
Before Vap Removal

After Vap Removal

Coefficient values ± one standard deviation

Before Vap Removal:
\[ a = -152.79 \pm 65 \]
\[ b = 196.91 \pm 4.34 \]

After Vap Removal:
\[ a = -174.59 \pm 60.1 \]
\[ b = 188.32 \pm 3.35 \]
1. RIE = 0.2 a reasonable value
2. Individual instruments show differences, likely due to differences in alignments of laser, particle beam, filament
3. Need to work on calibrating with coated BC particles (simultaneous RIE)
Possible reasons for RIEs that are significantly different from .2

- Particle Beam/Laser Beam/Ion Extraction Hole Overlap
- Tune with respect to optimum HB for AN
- Filament Position
Ionizer Configurations

Standard AMS
- Filaments on sides of ion chamber
- Filament position is mechanically set
- Filament wire is typically well positioned with respect to well formed slits in ion chamber walls

SP-AMS
- Filament is on bottom of ion chamber
- Filament position is moveable (vert & horz)
- Filament slit width and breadth may vary due to custom procedure
- Large holes in sides to accommodate laser beam
What About This HENE Laser Alignment Tool

• There is a step by step procedure detailed in the SP-AMS manual which we don’t have time to examine now
• It requires venting the instrument so you don’t want to do this very often
• It is primarily useful if you think you may have drifted substantially away from the center
• It works great for giving you a centered beam usually do need slight adjustment to one knob
End
$$mIE_{rBC} = 150 - 300 \text{ ions/pg}$$

Nascent Flame Soot CE ~ 0.75
Denuded Flame Soot CE ~ 0.5
BC3 results

Diffusion flame soot, ER = 0.7

- 350 nm nascent soot
- 350 nm nascent-denuded + coated-denuded

int = 0.20451 ± 0.081
slope = 0.50858 ± 0.017
V_r2 = 0.93

Nascent/Denuded Flame Soot CE ~ 0.5
• NOTE – appears that BC2 and BC3 have nascent flame soot at ~0.5 CE, using RB as calibration. At least for larger size particles (200-300 mobility diameters). Need same CE as fxn of size or mass – how about CE ratio vs BC mass (nascent or denuded core from CPMA).
Ionizer Configurations

Standard AMS
- Filaments on sides of ion chamber
- Filament position is mechanically set
- Filament wire is typically well positioned with respect to well formed slits in ion chamber walls

SP-AMS
- Filament is on bottom of ion chamber
- Filament position is moveable (vert & horz)
- Filament slit width and breadth may vary due to custom procedure
- Large holes in sides to accommodate laser beam
The $3\sigma$ detection limits for refractory black carbon:
0.26 $\mu$g·m$^{-3}$ for 1 second sampling and
0.03 $\mu$g·m$^{-3}$ for 1 minute collection.
Calibration: $mI{E}_{rBC}$

$mI{E}_{rBC} \sim 150 \text{ ions/pg}$

Nascent Flame Soot CE $\sim 0.7$
Denuded Flame Soot CE $\sim 0.4$

Calibrate versus CPMA/APM (lab), SMPS using effective densities, SP2
SP-AMS vs. SP2 Mass Loadings

CalNex2010

The CE is low when size is small.

Massoli et al., 2012
HR Batch and Frag adjustments

(a) High Resolution ‘Batch’ Table

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<thead>
<tr>
<th>HR_specname_list</th>
<th>HR_spec_list</th>
<th>HR_specFrag_list</th>
<th>HR_specIEFac_list</th>
<th>HR_specCEfac_list</th>
<th>HR_specFamilyBase</th>
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<tr>
<td>HRblackcarbon</td>
<td>HRBC</td>
<td>HR_frag_blackcarbon</td>
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<td>1</td>
<td>familyCx</td>
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(b) High Resolution ‘Frag’ Table

<table>
<thead>
<tr>
<th>HR_specMassAlgebra</th>
<th>HR_frag_organic</th>
<th>HR_frag_blackcarbon</th>
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</thead>
<tbody>
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<td>{C},-HR_frag_blackcarbon[{C}]</td>
<td>0.625*HR_frag_blackcarbon[{C3}]</td>
</tr>
<tr>
<td>j13C</td>
<td>0.0108157*HR_frag_organic[{C}]</td>
<td>0.0108157*HR_frag_blackcarbon[{C}]</td>
</tr>
</tbody>
</table>

C1/C3 Ratio
- Regal Black
- Traffic Measurements
- Ethylene flame soot
Regal Black Effective Density
(CPMA vs SMPS)

![Graph showing effective density vs mobility](image-url)
Measuring Laser Beam Movement in Ion Formation Chamber

1. Vertical Laser & Particle Beam movements at two different horizontal positions
2. Same IE sensitivity at a given horizontal position, independent of vertical position
3. Calibration of Laser movement (using camera) inside ion formation cage (~0.35 mm ion chamber / mm camera)
• Method for tracking Laser Beam with respect to Ion Extraction region (defines range of adjustability)

• Defines correlation between TOF position and Laser Camera Position (assuming non-measured horizontal = measured vertical)
- BC IE variability due to Laser – Ion Extraction Interaction Region Overlap
- NOTE that the colored points were done for configuration with a misaligned filament wire, whereas the black points were done with a correctly aligned filament wire
- Ion extraction axis is close to center of camera (machined to be true)
- Horizontal positioning of laser can have significant effect on mIE_rBC
Laser – Ion Extraction Interaction Region

- BC IE variability due to previously undefined Laser – Ion Extraction Interaction Region Overlap
**Laser Beam Width Calculations**

**Fig. B1**

- **Output Coupler Mirror Surface**
  - 1.08 mm (1/e² diameter)

- **CCD Camera Surface**
  - 1.1 mm (1/e² diameter)

- **Particle Beam Location**
  - 0.957 mm (1/e² diameter)

- **Nd:YAG flat mirror surface**
  - 0.818 mm (1/e² diameter)

**Measurements**
- **Output Coupler Power** = ~0.3 Watts
- **Output Coupler Transmission (measured)** = 3e-4
- **Cavity Laser Power** = 1000 Watts
- **Peak Laser Power Intensity** = 2.78e+05 Watts/cm²

*Barry McManus, ARI*
Fig. B2

Particle Beam Width Measurements

Coefficient values ± one standard deviation

\[ Y_0 = 2.5215 \pm 0.0296 \]
\[ \sigma = 0.43524 \pm 0.0208 \]
\[ X_0 = 0.05157 \pm 0.0237 \]
\[ R_w = 0.25 \pm 0 \] (Wire Radius)

FWHM = \( 2.35482 \times \sigma = 2.35482 \times 0.43524 = 1.02435 \text{ mm} \)
Other issues affecting SP-AMS IE calibrations

- Filament wire alignment along particle beam axis with respect to slit in ion formation cage and distance from ion formation cage can affect sensitivity curve significantly (order 100% sensitivity)
- Filament wire orientation between HR-AMS and SP-AMS cause differences in true emission currents (i.e., electrons generated) and holes for laser in SP-AMS ion formation cage may effect ion generation/extraction (order 40% in sensitivity)
- Slope in TOF position along axis due to ToF flange position – minor issue (order 1% in sensitivity)
- Mirror refracts laser position on Camera image – based on mirror position – suggest marking mirror and leaving in same position (axial) every time (order 10% in position)
- Laser strikes the ion formation cage, heating it when laser on. This can cause an increase in the filament emission current (hotter wire – more electrons) as well as an increase in the background signals in the SP-AMS. As this increase in background is changing with time, but slower than close/open, this can cause apparent different MS signals. Issue for when operating with both vaporizers in and turning laser on/off. (order 200% for m/z44 background closed signal)
- Tune on m/z 28 airbeam rather than 36 BC signal, but stay to low side of HB maximum signal (highlighted in figure below) (order 20% in sensitivity)
Laser Beam Width Determination (1D Gauss Fit)

IF, the convolution of two Gaussian functions (i.e. laser beam and particle beam) generates a gaussian function with $c = \sigma$ of $c = \sqrt{c_1^2 + c_2^2}$,

Then in the case of the laser beam $= c_1$ (unknown) and particle beam $= c_2$ (0.34 mm from horizontal - i.e. along laser axis - BWP measurements) and the convolution of the two $= \text{particle beam walk experiment, } c$ (0.72 mm from particle).

Thus, laser beam width, $c_1 = \sqrt{c^2 - c_2^2} = \sqrt{0.72^2 - 0.34^2} = 0.634665$ mm (FWHM $= 1.49452$ mm)

300 nm Regal Black Particles
Laser Beam Width Determination (ERF Function Fit)

IF, the convolution of two Gaussian functions (i.e. laser beam and particle beam) generates a gaussian function with $c = \sigma$ of $c = \sqrt{c_1^2 + c_2^2}$,

Then in the case of the laser beam = $c_1$ (unknown) and particle beam = $c_2$ (0.34 mm from horizontal - i.e. along laser axis - BWP measurements) and the convolution of the two = particle beam walk experiment, $c$ (0.72 mm from particle).

Thus, laser beam width, $c_1 = \sqrt{c^2 - c_2^2} = \sqrt{0.72^2 - 0.435^2} = 0.574$ mm (FWHM = 1.35 mm)

300 nm Regal Black Particles
Overlap mismatch is in one dimension.
Laser Vaporizer
Detection Scheme

\[ R \cdot BC(s) \xrightarrow{\text{laser absorption}} R'_{(g)} + C_m(g) \xrightarrow{\text{e}^- \text{ ionization}} R''^+ + C_n^+ \]

Optical Detection

Coating Evaporating

Core Evaporating

Laser Beam

Mass Spectrometric Detection

Gao et al., 2007