Software Updates for ACSM Data Acquisition and Analysis

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2012 AMS Users Meeting

Outline

- Overview of most recent software versions
- Corrections which need to be made to ACSM data to calculate accurate aerosol mass loadings
- Corrections background
- Changes to ACSM DAQ to facilitate corrections
- Changes to ACSM Local to facilitate corrections

Latest software versions

- ACSM DAQ: v1.4.2.5
- ACSM Local: v.1.5.2.0
- Highly recommend using these versions – you need to use most recent ACSM local to use most recent ACSM DAQ

Acquisition

- ACSM DAQ 1.4.2.5
  - Fixed ‘Runaway OPC’ bug (there are still other connectivity issues).
  - Add optional ‘user defined scan modes’
  - Changed default data location – now C:\ACSM\ACSMData\ScanData
  - Added new reference state info on IE tab (stored in the data files…)

Analysis

- ACSM_Local_1520.ipf
  - Implemented new tools for corrections
    - Time Series
    - Relative Ion Transmission
  - Many incremental improvements and bug fixes.
  - Change default path for live loading data.

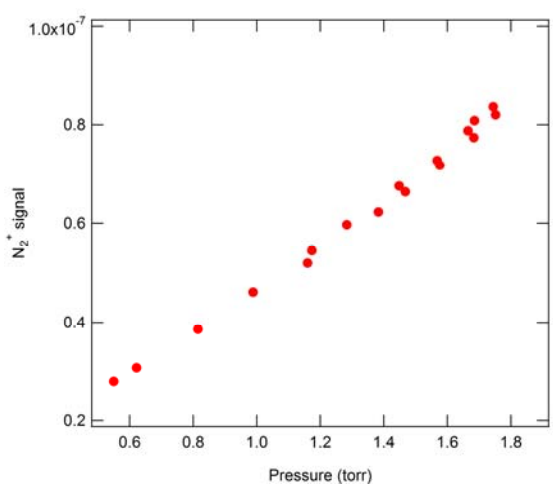
Software Updates

- Check for updates at ACSM users' google site: **https://sites.google.com/site/ariacsm**
  - Subscribe to changes and you'll get an email when new files are uploaded, etc.
- Provide feedback on users' site, too – let us know how the instruments are working, build a community where you can get feedback from other users.

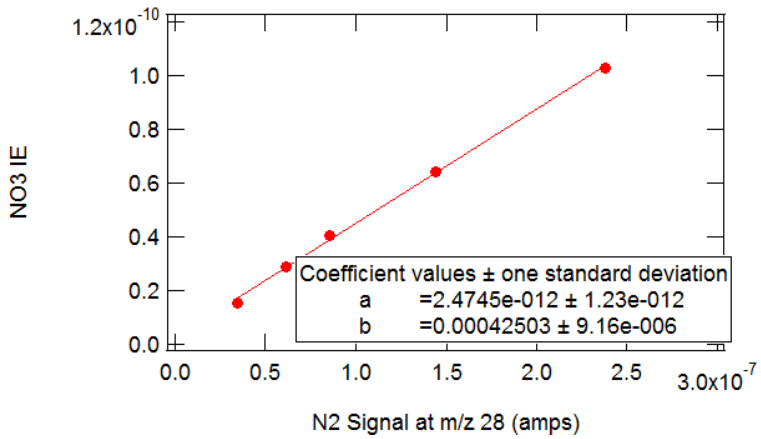
Corrections for ACSM Data

1. Time-series corrections
   1. Flow Rate/Pressure
   2. Instrument Response/Sensitivity
2. Relative Ion Transmission
   1. This is a mass-to-charge dependent correction to account for ions which are generated in the ion source but which do not make it to the detector

Airbeam variation with pressure



Airbeam variation with response factor



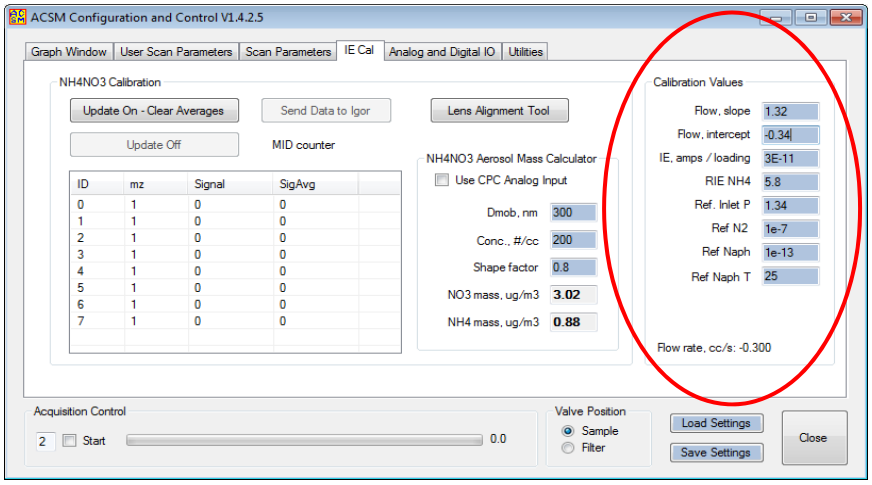
Relative Ion Transmission: You get what you pay for

- The small, inexpensive quadrupole that the ACSM uses has some performance limitations.
- Less than 100% of ions generated in the ion source reach the detector
- This percentage decreases with m/z – a smaller fraction of heavier ions are detected.
- But, we can correct for this using naphthalene.

Naphthalene as Ion Transmission Reference

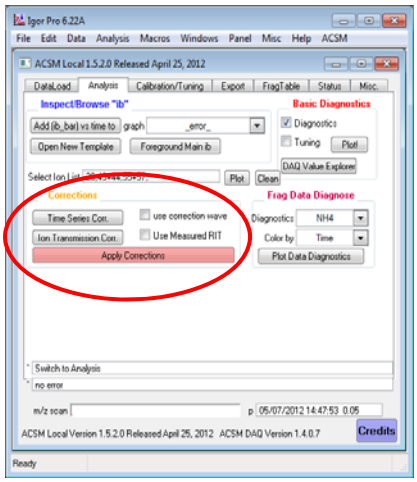
- Fragmentation from Electron Impact Ionization is quantifiable – i.e. a given molecule will always generate the same ratios of ion fragments
- Naphthalene has ion has fragments throughout the m/z range the ACSM uses.
- If we know the fragmentation pattern of naphthalene (as measured with an instrument which does not suffer from this ion transmission issue) we can compare measured naphthalene fragmentation pattern to the known fragmentation pattern to determine how much of what m/z's we're missing at the detector.

DAQ Changes to facilitate corrections

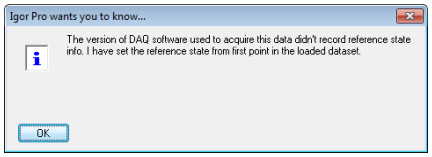


- When you do IE calibration don't forget to set up your reference state in DAQ software

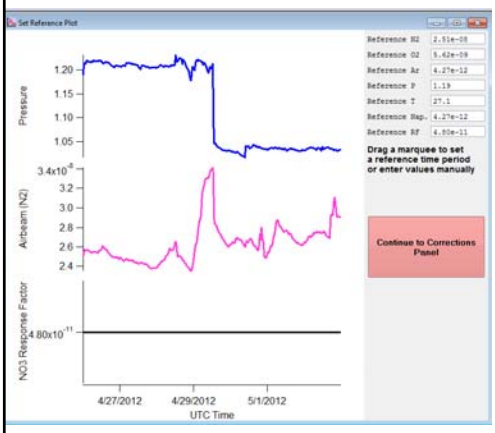
Find corrections tools on ‘Analysis’ Tab



- If your DAQ version is old, you get a notification that it couldn’t find your reference state

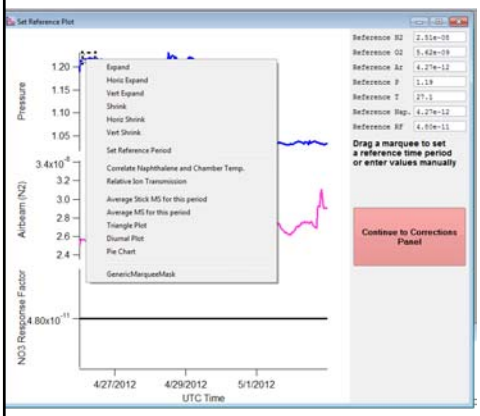


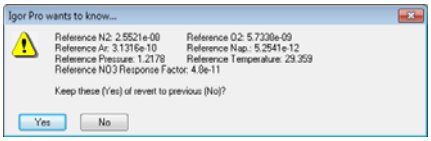
Set Reference Plot



- Text boxes on the right should be automatically populated with earliest recorded reference state.

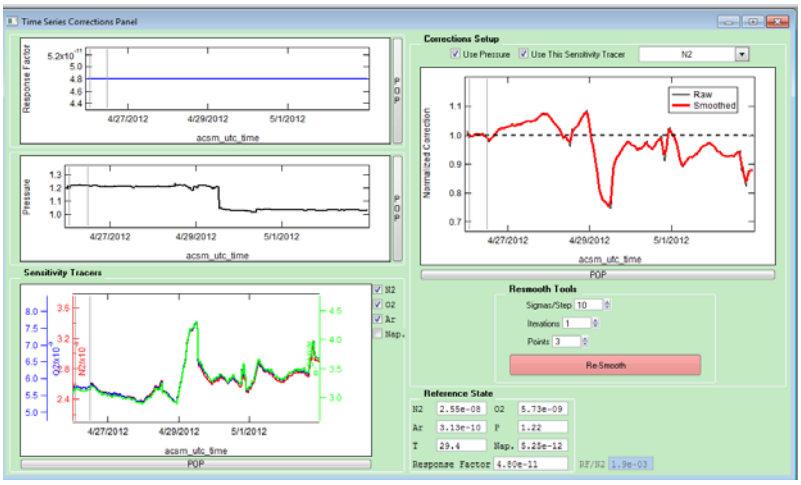
You can also set reference time period instead



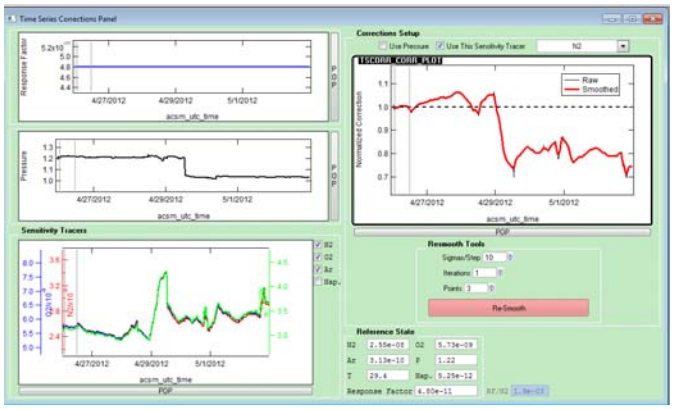


- Drag a marquee and right-click then select 'Set Reference Period'
- You can then manually edit if you want something different for any of the reference point values
- Click 'Continue to Corrections Panel'

Time series corrections panel

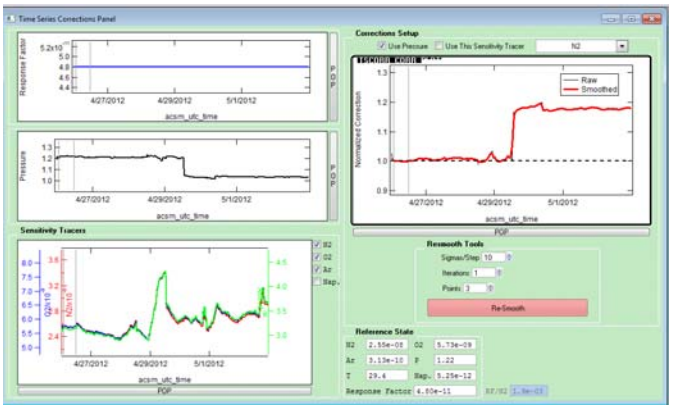


Uncheck ‘Use Pressure’



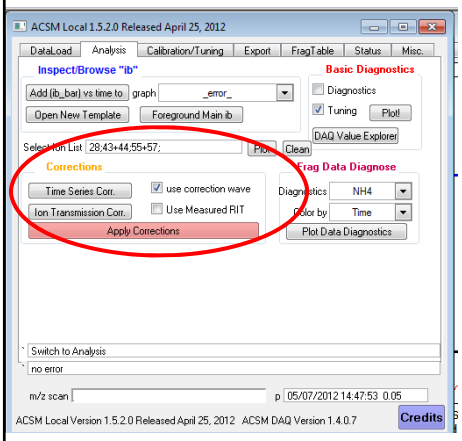
- To not consider the pressure in our correction, we remove the pressure influence from the measured airbeam signal.

Uncheck ‘Use This Sensitivity Tracer’



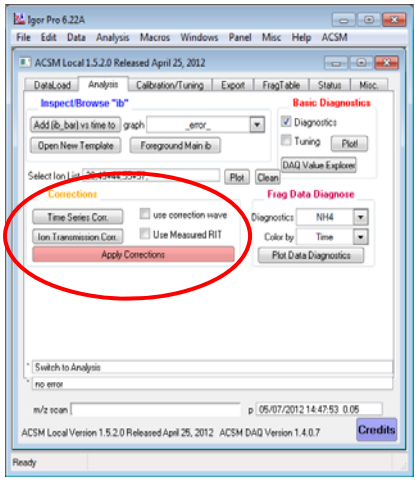
- Now the correction factor is just the inverse of the measured pressure.

OK, I’ve got my correction calculated how do I apply it?



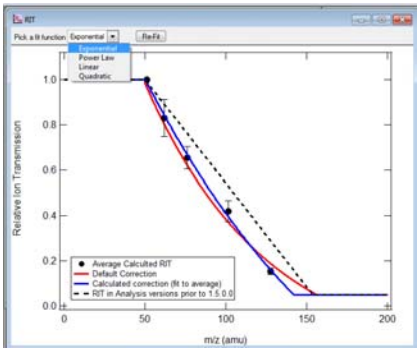
- Back to the analysis tab.
- Check ‘use correction wave’
- Click ‘Apply Corrections’

Find corrections tools on ‘Analysis’ Tab



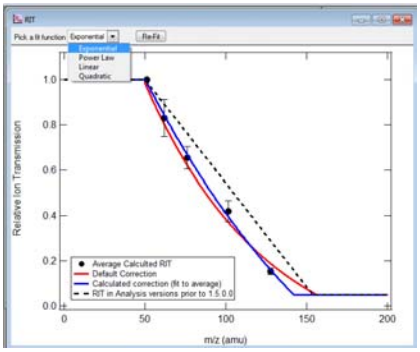
- Click on the ion transmission correction button to measure the relative ion trasmission.

Relative Ion Transmission Correction



- This plots the ratio of measured naphthalene fragments across the m/z range relative to the NIST fragmentation pattern, then normalized to the lowest m/z fragments (~m/z 50).
- This makes the assumption that for m/zs less than 50, we have 100% transmission (such an induction range is expected and confirmed by measurements comparing the same mixture of gases in a big quad and the Prisma quad…)

Relative Ion Transmission Correction – How the plot works

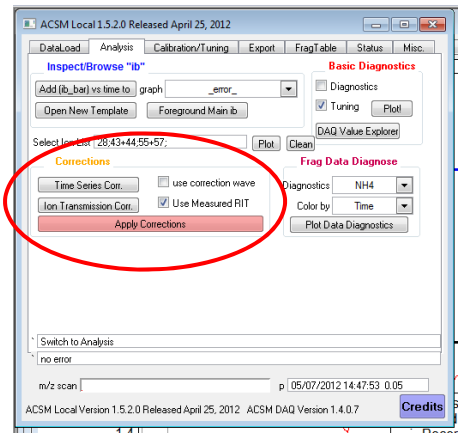


- The red line is a default correction (typical of recently delivered instruments)
- The black dashed line is based on ARI's prototype instrument
- The blue line is a fit to the average data from the currently loaded time series.
- In all cases, we truncate the correction at 0.05 (a factor of 20)
- The default blue fit is an exponential – if that looks bad (and sometimes it does), you can select a different fit from the dropdown menu and click "Re-Fit" to find something that looks okay.

Additional Notes on RIT Correction

- If it looks like you've got really big error bars, have a look at your naphthalene time series.
- You can make a plot of the RIT for any time period by dragging a marquee on any time-series graph.
  - There's not yet an easy way to apply this but plan to include one soon.
- The correction has a noticeable effect on SO4 and Org
- While this seems like a big correction (and it is) it is only very big for high m/zs which is not where most of the aerosol mass is.
- Using the measured RIT also will correct for any m/z dependence of the SEM detector's response.

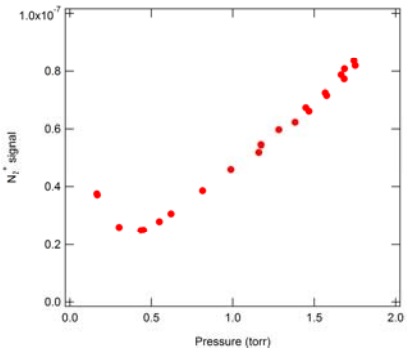
Applying the RIT Correction



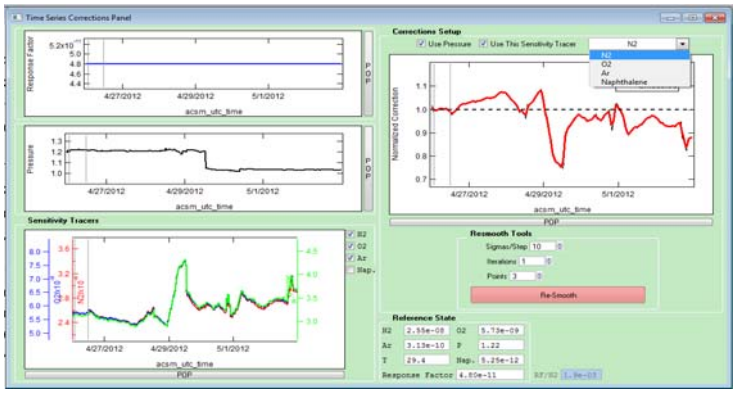
- Check the 'Use Measured RIT' Correction
- Click 'Apply Corrections'
- The red-line default correction is applied by default – you can control the default by editing the fit coefficients at the top of acsm_local (defaultRITk0-2) these are the coefficients of an exponential.

END

Below a certain pressure, this is no longer valid, But…



- The turnaround isn't too important since at a higher pressure (closer to 1 Torr than 0.5) the performance of the aerodynamic focusing lens changes and you're no longer sampling same aerosol size range…



Time-series correction theory

- When we perform a calibration, we are measuring 'Response Factor' (RF) for NO_3
  - We often refer to it as an 'ionization efficiency' which is inaccurate language
- The RF we measure depends on the gain and the tuning state of the instrument
- By measuring quantities which vary proportionally with the RF and knowing their states when the calibration was performed, we can correct for variations in RF.

Time series correction theory – cont.

- In addition to the RF, the measured aerosol signal depends upon the instrument flow rate – this governs the amount of sample which is sampled per unit time
- So, when we calibrate, the result is dependent upon the sample flow rate (inlet pressure)
- We can use changes in the measured inlet pressure to correct for variations in the flow rate (the pressure is directly proportional to the flow rate)

Time series corrections theory – cont.

- The most abundant signal in our mass spectrum is the N_2^+ ion at m/z 28 – we refer to this as the 'airbeam' signal.
- Its variations depend upon the variations in both instrument response (gain, etc.) and flow rate (pressure – at a lower pressure a proportionally smaller amount of air enters the system)
- Because it has high signal-to-noise and folds in both RF and flow rate changes, the airbeam signal is the most likely candidate to use to define a correction factor.

Time series corrections panel