



Using Event Trigger Panel for IE/AB and Transmission Curve Calibrations

Benjamin Nault + Jimenez Group
AMS User's Meeting, Portland
October 21st - 23rd, 2016

Take Away Points—ET is a Powerful Tool for AMS IE and Transmission Curve Calibrations

- ET **reduces the calibration time** for IE calibrations
 - This is especially important for IE calibrations out in the field
 - This also provides Lens Transmission checks with each calibration
- ET can be utilized for Lens Transmission Curve calibrations with **less uncertainty than mass transmission curves**

Typical Methods to Calibrate AMS IE with NH_4NO_3

Well covered by Ed Fortner and John Jayne in 11th¹ and 14th² Users Meeting

CPC Mass Calibration

- 1) Relies on mass measured by AMS with mass measured by CPC
- 2) Many errors can be introduced by uncertainties with CPC, DMA, lens alignment, doubles, etc.

Single Particle Calibration

- 1) Relies on detecting the number of ions from a single particle
- 2) Avoids errors introduced by CPC and CPC Mass Calibrations
- 3) Need low number conc. of NH_4NO_3 (150 – 250 particles/cc)
- 4) Typically use 400 nm, but can use anything between 300 – 450 nm

1. http://cires1.colorado.edu/jimenez-group/UsrMtg/UsersMtg11/Jayne_Calibrations.pdf
2. http://cires1.colorado.edu/jimenez-group/UsrMtg/UsersMtg14/ed_AMS_Calibrationsuser2013.pdf

The Way Single Particle (SP) is Measured Depends on the Data Acquisition Card Used for your System

AP240 (old data acquisition card) vs ADQ (new acquisition card)

- Old card is old; therefore, not as fast as the new ADQ
- For SP with old card, data had to be transferred from card to computer; then, card had to wait for next event
- For ADQ, the ADQ goes into SP mode to store all single particle events and then data is transferred (faster & more events)
- For ADQ, custom firmware from Tofwerk that makes SP faster
- **ADQ needs less signal to run, so the SI is lower **Important for comparisons****

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ADQ IS BETTER FOR SP

then data is transferred (faster & more events)

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- **ADQ needs less signal to run, so the SI is lower **Important for comparisons****

Using Old Data Card for Single Particle IE Cals

Pros:

- Do not need to use CPC to measure IE
- Can use CPC to compare CPC and BFSP counts
- Ability to spot check 1 point on lens transmission curve

Cons:

- Take 45-60 minutes to get enough statistics (e.g., > 300 events)
- Ability to only spot check 1 point on lens transmission curve
- One data file per event

Using Old Data Card for Single Particle IE Cals

Pros:

Do not need to use CPC to

Cons:

Take 45-60 minutes to get enough

**Older Card = Slower Acquisition =
Slower Cal & Less Points**

transmission curve

Using New Data Card for Single Particle IE Cals → Event Trigger!!

Pros:

- Do not need to use CPC to measure IE
- Can use CPC to compare CPC and ET counts
- Ability to spot check 1 point on lens transmission curve

Con:

- Cannot be used to calibrate capture vaporizers
- Similar to prior SP cals, can't use ET to calculate NH₄ RIE

Advantages compared to Old Card:

- Take ~15 minutes to get enough statistics (e.g., > 1000 counts)
- Can do multiple lens transmission curve points in same amount of time as old card
- One data file for entire run

Using New Data Card for Single Particle IE Cals → Event Trigger!!

Pros:

Do not need to use CPC to

Advantages compared to Old Card:

Take ~15 minutes to get enough

**Newer Card = Faster Acquisition =
Faster Cal & More Points**

transmission curve

One data file for entire run

Con:

Cannot be used to calibrate capture vaporizers

Similar to prior SP cals, can't use ET to calculate NH₄ RIE

Comparison of Old Card vs New Card IE Calibration on Same Day

Old Card SP Calibration Values

**NOTE: After correcting for different SI values between old and new card

- $IE = 2.07 \times 10^{-7}$
- **$IE/AB = 7.25 \times 10^{-13}$**

New Card SP Calibration Values

- $IE = 2.22 \times 10^{-7}$
- **$IE/AB = 7.42 \times 10^{-13}$**

Comparison of Old Card vs New Card IE Calibration on Same Day

Old Card SP Calibration Values

**NOTE: After correcting for

New Card SP Calibration Values

The two methods typically agree to within 5% when comparing IE/AB and correcting for the difference in the SI values between the two cards.

- $IE/AB = 7.25 \times 10^{-13}$

- $IE/AB = 7.42 \times 10^{-13}$

Setting the Pulsing Period for the Maximum Signal

The screenshot displays the 'ToF-AMS Menu' software interface. The main window is titled 'ToF-AMS Menu' and shows various configuration panels. The 'Timing' tab is active, displaying parameters for ToFMS and PTOF.

ToFMS Parameters:

- Pulsar Period (us): 15.45 (64.7 kHz)
- Trigger Delay (ns): 7496
- Sampling Interval (ns): 0.625
- Nbr of Samples: 12544 (Max m/z)
- + Pulse Width (ns): 2000
- Pulse Width (ns): 2000

PTOF Parameters:

- Chopper Frequency (Hz): 106.0 (105.9 Hz)
- Data Delay (us): 0.00
- ToF Spectra / Chopper: 610 (Max Ova)
- Nbr Co-Adds: 1

ePToF Parameters:

- Enable:
- Sequence Length: 127
- Oversample: 6 (Configure)

Mass Cal: $Sample\ m/z = m \cdot \sqrt{mass} + b$
Slope: 2767.98 Intercept: -6728.6

ToFMS Timing Diagram:

- Mass Spectrum Window: 12544 ToFMS samples
- Trigger Delay: 7496ns
- Data Acq.: 7840ns
- Wait For Trigger: 114 ns
- Mass Range: Minimum: 7, Maximum: 48
- Chopper Cycle Timing: 610 ToF Extractions, 106 Hz (9.4 ms)
- Particle Size Range: 0 to 16042 nm
- Data Delay: 0.0ms
- Data Acq.: 9.4ms
- Wait For Chopper: 0.0ms

Co-Adding is OFF. There will be 610 extractions, adjacent spectra will NOT be summed, yielding 610 time bins. Each time bin is 15 us wide.

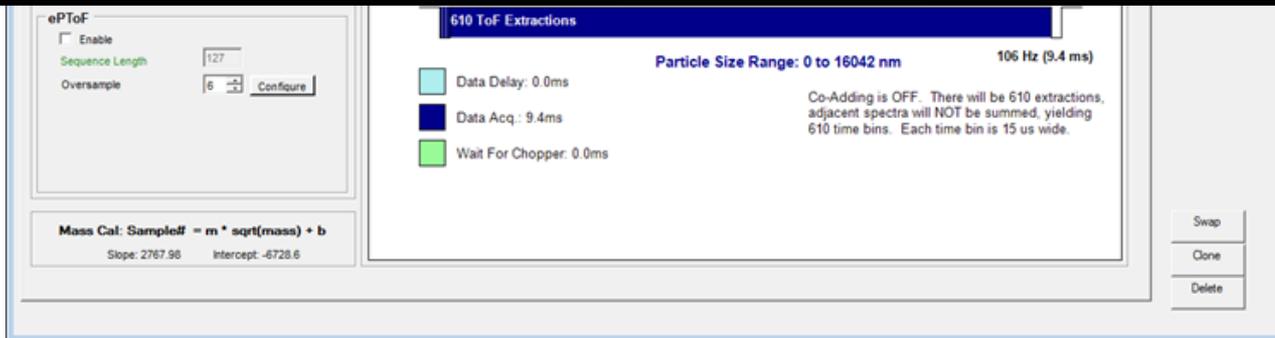
The pulser period (~14 – 16 μ s) for ET needs to be squeezed (max $m/z=48$) in order to measure full single event profile profile of NH_4NO_3 while minimizing evaporation loss during the measurement.

Setting the Pulsing Period for the Maximum Signal



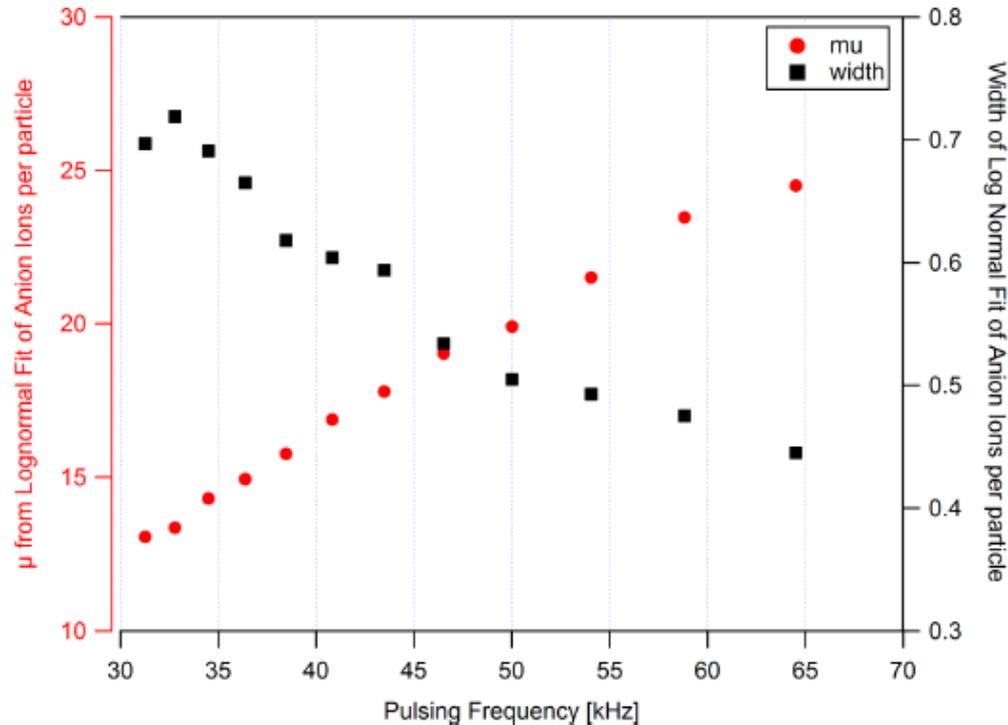
The pulser period (~14 – 16 μ s) for ET needs to be

**Pulsing Period ~ 14 – 16 μ s
(NEED TO CONFIRM!!!)**



loss during the measurement.

Pulsing Frequency Impacts the Width and Ions Per Particle



Increasing the pulsing frequency leads to more ions per particle and decrease in the distributions.

Setting Up ET for Calibrations (IE or Lens Transmission Curve)

The screenshot displays the ToF-AMS software interface. The 'Event Trigger' panel is highlighted with a red box. It contains the following settings:

- Enable Region 1:** Start m: 30, End m: 30, Minimum time: 7.00
- Enable Region 2:** Start m: 46, End m: 46, Minimum time: 5.00
- Enable Region 3:** Start m: 104, End m: 47, Minimum time: 1.50
- Region Combination Logic:** OR
- Pre Segments:** 10
- Post Segments:** 15
- Waveforms/Segment:** 1
- Bursts:** 100
- Writes:** 100

Other panels visible include 'GenAlt Run Profile' (Dwell Time: 120.0 s/Run), 'Data Files' (Auto Save Data checked), and 'Acquisition Clock' (None selected).

This is where you set-up the ion thresholds for your ET Cal prior to running the cals.

BOTTOM LINE: Find settings the minimize false counts (ideally, < 30 counts during blank run) while maximizing number of events measured.

Exact details covered in appendix slides for later.

Setting Up ET for Calibrations (IE or Lens Transmission Curve)

Set-up for the calibration has been explained in numerous other presentation^{1,2,3,4}.

Bottom line:

1. Make sure to have an initially low concentration (< 250 particles/cc without dilution)
 - This ensures that you are measuring 1 particle at a time
 - This minimizes doubles
2. Make sure particles are dried
3. Make sure you have the shortest line possible to minimize evaporative loss

1. http://cires1.colorado.edu/jimenez-group/UsrMtgs/UsersMtg11/Jayne_Calibrations.pdf
2. http://cires1.colorado.edu/jimenez-group/UsrMtgs/UsersMtg14/ed_AMS_Calibrationsuser2013.pdf
3. <http://cires1.colorado.edu/jimenez-group/UsrMtgs/EUCAARIClinic2010/PSI-IECalibration.pdf>
4. http://cires1.colorado.edu/jimenez-group/UsrMtgs/UsersMtg7/ie_cal_tutorial.pdf

Analyzing ET for Calibration (IE or Lens Transmission Curve)

NOTE: The background for our ET (IPP < 50) is extremely low because we use a cryogenic pump.

Typically, the background for IPP < 50 will be much higher.

ToF AMS Ionization Efficiency Calibration Panel for ET v1.0.5F

Instructions

Load ET Data

Single file

Folder **Step 1. Select ET folder** Num. files 4

ET file folder E:\ET_and_Doug_Expts\ET:2016.10.06\Normal_ET:

Data folder root:\Normal_ET:

Alt. Step 1. Set panel to prev. data

ET settings:

mz30<7 OR mz46<5 Single ion (mv*ns) 2.51

Start AMU 7 Stop AMU 47 Start AMU 7 Stop AMU 47

Num. segments 26 Pulser period, us 15.45

Trigger segment num. 10 Sample interval (ns) 0.625

Num. events in file 3034 File time 10/6/2016 9:51:09 PM

User Inputs

Compound **NH4NO3**

m/z List 30,46,15,16,17 Selected Dm (nm) **400**

Anion MW 62 Cation MW 18 (Opt.) MS AB Hz 3.875e+05

Density (g cm⁻³) 1.72 (Opt.) CPC NaN +/- NaN

Jayne shape factor 0.8

Step 2. Accept inputs, perform calculations

Outputs

IE Average 3.65e-07 +/- 2.55e-09

RIE Average 4.74 +/- 0.07

Ions Per Particle

Anion 126.55 +/- 0.89

Cation 144.68 +/- 1.53

Other IPP

Final IE event count 2921

% events in CER 96.3

IE / AB 9.409e-13

Flow (cm³ s⁻¹) 0.577

Chopper duty cycle, % 2.0

CER # events/cc nan

CER # events/sec nan

Individual Particle Time of Flight

Step 3. Adjust Cal Event Region (CER), baseline (BL), etc

CER begin 203 min IPP 1 min IPP 1

CER end 227 max IPP 200 max IPP 200

Baseline Seg. 9 max BL 0.5 max BL 0.5

Graph Tweaks

Show PTof histogram

Show error bars on Seg Avg

Show only events in CER

CER zoom CER autoscale

Pop Examine event num. -1 Blacklist

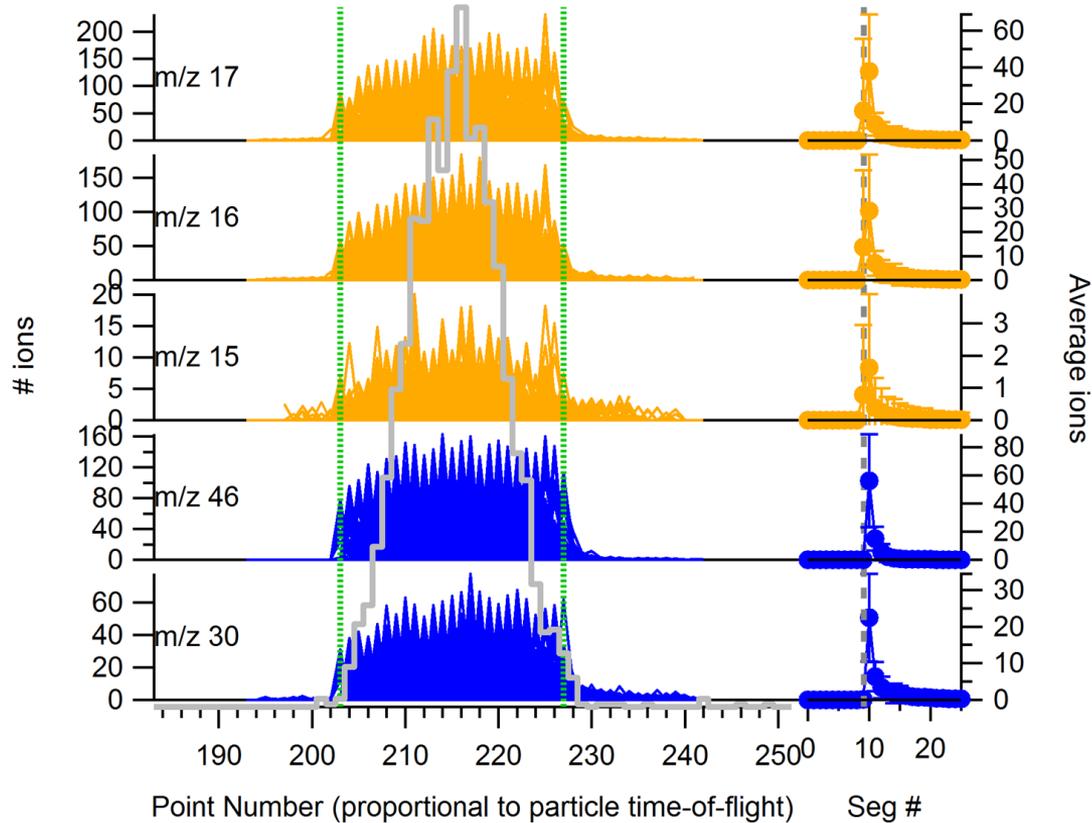
Average IE and RIE

anion RIE cation

anion Ions

Histograms of IPP for Cal Event Region (CER)

After Removing Doubles, Finding the Proper CER, Etc., Your Final Results Should Look Something Like This



NOTE: Green line is near the edges of the PToF (grey) line, which indicates the events that are being used for the IE Calibration.

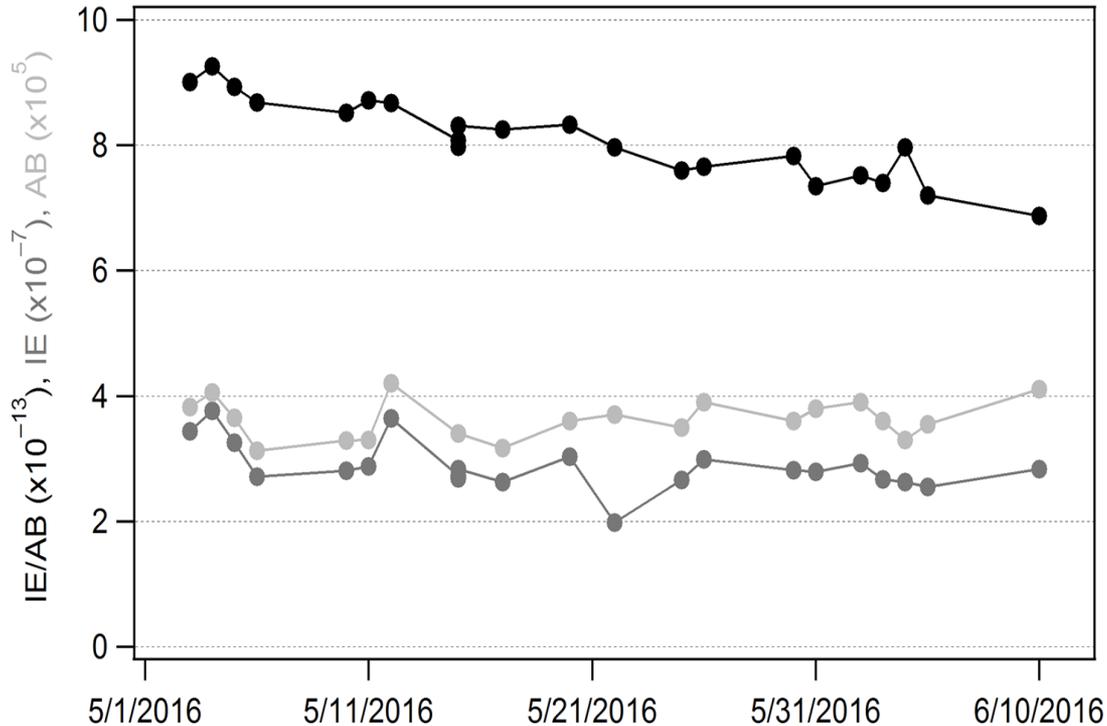
Also, note that doubles (see prior slide) are removed.

ET Provided the Ability to Measure the IE/AB after Each Flight during KORUS-AQ (2016) and ATom (2016)

Added the calibration system to our flight rack in order to have the ability to calibrate IE/AB after each flight during our last two campaigns.



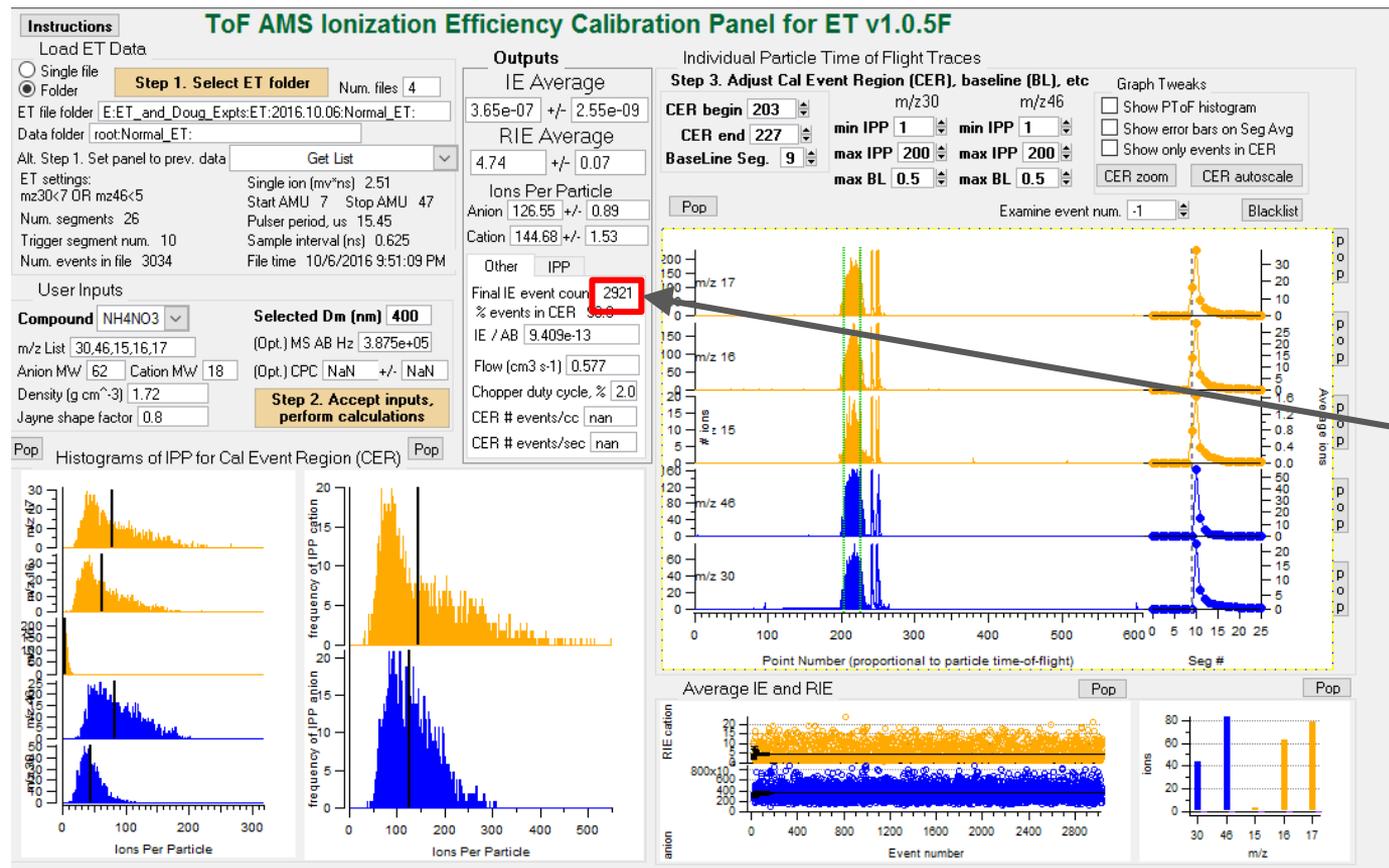
ET Provided the Ability to Measure the IE/AB after Each Flight during KORUS-AQ (2016)



During KORUS-AQ, we had a total of ~20 IE/AB calibrations.

~17 of these calibrations occurred after one of the research flights, during the 2 hours provided after landing.

Analyzing ET for Calibration (IE or Lens Transmission Curve)

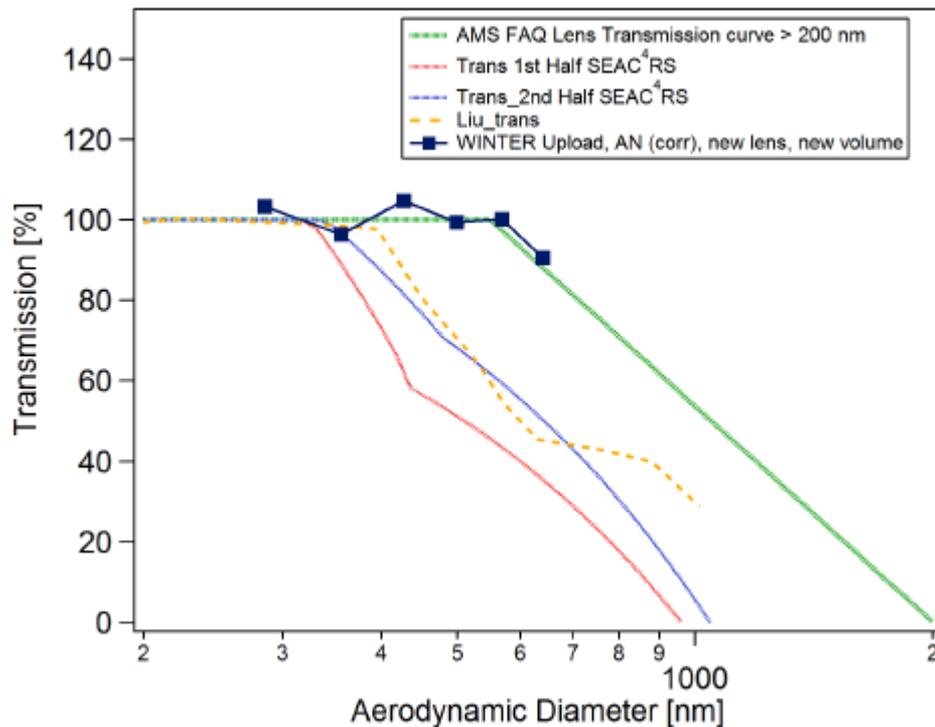


Finally, you can use the Final IE event count with the flow rate (make sure to document down the flow rate during the calibration) along with sampling time (how long you ran ET) and duty cycle (2%) to calculate the particles/cc sampled.

This value should be used as a spot check on the transmission of particles or to create a transmission curve.

The Need to Do Lens Transmission Curves

The transmission curve should constantly be checked and verified.



Even during a campaign, as shown to the left, the transmission curve can change.

Also, the transmission curve of a specific instrument may not be close to the theoretical transmission curve (green); therefore, the actual curve needs to be known.

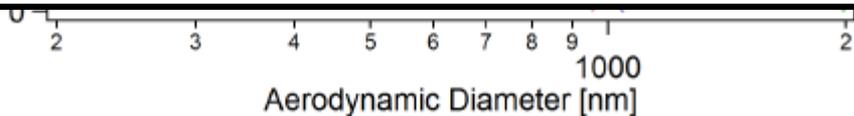
ET provides opportunities for spot checking the transmission during each calibration and a total check, **with the only uncertainties stemming from counts and flow rate** (vs. uncertainties in flow rate, counts, “Jayne factor”, particle size, etc.)²²

The Need to Do Lens Transmission Curves

The transmission curve should constantly be checked and verified.

Recall:

- (1) Since ET requires low particle conc. (< 250 particles/cc), **doubles are minimized** (lens transmission curve worst enemy!!!!)!!!
- (2) ET Panel provides the ability **to remove any doubles**.
- (3) **Doubles are typically <5% of the particle counts**; therefore, the comparison of counts (ET) to counts (CPC) is not impacted the same way doubles impact CPC mass lens transmission curves.



calibration and a total check, **with the only uncertainties stemming from counts and flow rate** (vs. uncertainties in flow rate, counts, “Jayne factor”, particle size, etc.)²³

The Power of ET for Lens Transmission Curve Calibrations

- (1) Since ET requires low particle conc. (< 250 particles/cc), doubles are minimized (lens transmission curve worst enemy!!!!)!!!
- (2) ET Panel provides the ability to remove doubles.
- (3) Doubles are typically $< 5\%$ of the particle counts; therefore, the comparison of counts (ET) to counts (CPC) is not impacted the same way doubles impact CPC mass lens transmission curves.

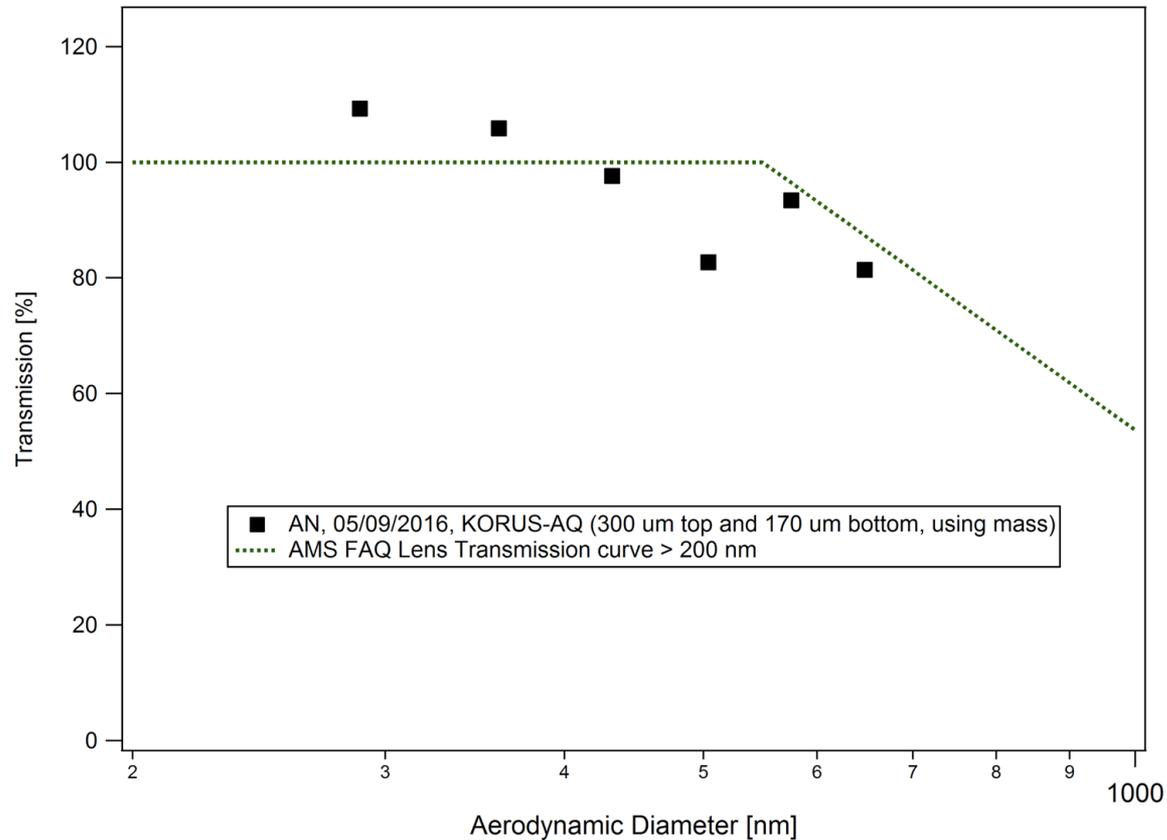
The Power of ET for Lens Transmission Curve Calibrations

(1) Since ET requires low particle conc. (< 250 particles/cc), doubles are

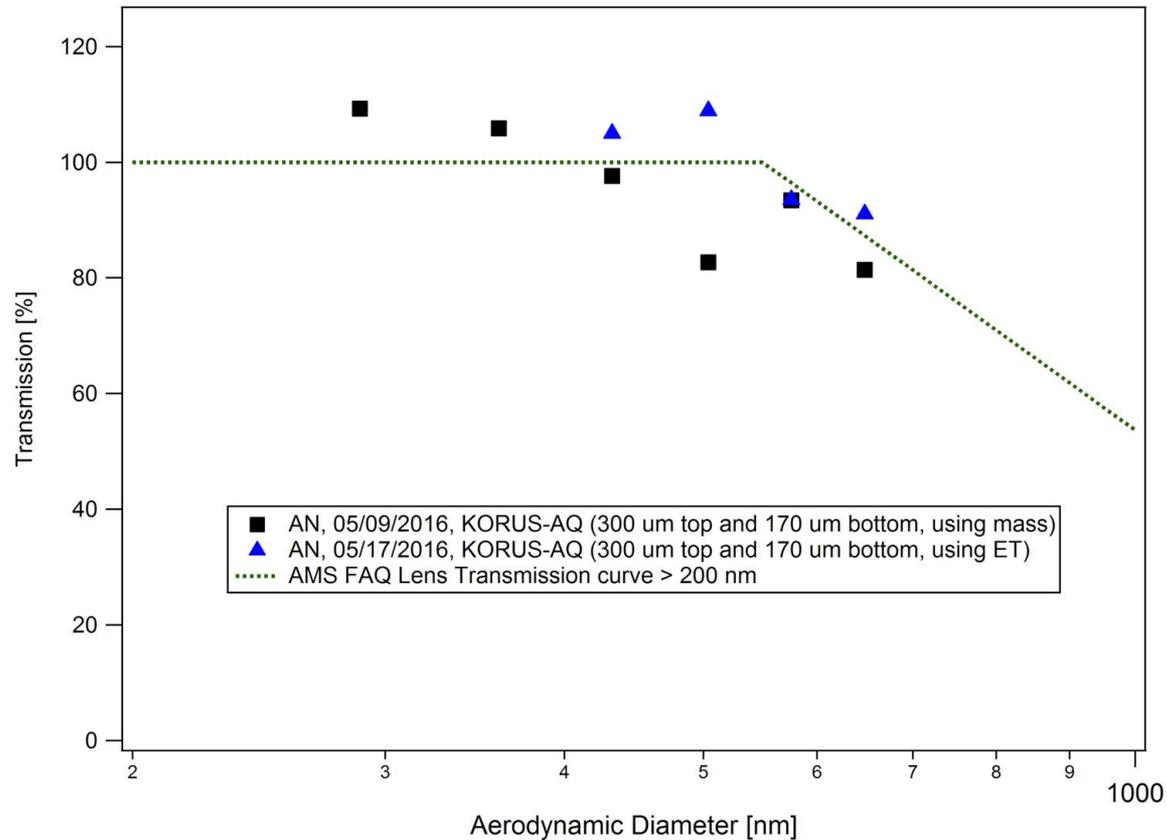
**ET Makes Lens Transmission
Curves Easy!!**

counts (ET) to counts (CPC) is not impacted the same way doubles impact CPC mass lens transmission curves.

Lens Transmission Curve: Comparing Mass to ET



Lens Transmission Curve: Comparing Mass to ET



ET is a Powerful Tool for AMS IE and Transmission Curve Calibrations

- ET **reduces the calibration time** for IE calibrations
 - This is especially important for IE calibrations out in the field
 - This also provides Lens Transmission checks with each calibration
- ET can be utilized for Lens Transmission Curve calibrations with **less uncertainty than mass transmission curves**

Thank you! Questions?

Extra Slides for Discussion/Upload

Setting Up ET for Calibrations (IE or Lens Transmission Curve)

This is where you set your baseline for events.

If you set the minimum ions low, you start counting false events, which can be seen when you are doing a blank (and comparing values vs. CPC).

If you set the minimum ions too high, you start missing events (again, can be seen in comparison vs. CPC).

Ideally, the minimum ions should be set so that you have < 10 particles/cc (< 30 events in a run) during a blank.

The screenshot displays the 'ToF-AMS Menu' software interface. The 'Event Trigger' panel is highlighted with a red box, showing the following settings:

- Enable Region 1
 - Start m: 30, End m: 30
 - Minimum ions: 7.00
- Enable Region 2
 - Start m: 46, End m: 46
 - Minimum ions: 5.00
- Enable Region 3
 - Start m: 104, End m: 47
 - Minimum ions: 1.50

The 'Region Combination Logic' is set to 'OR'. Other settings include 'Pre Segments: 10', 'Post Segments: 15', 'Waveforms/Segment: 1', 'Bursts: 100', and 'Writes: 100'. An arrow points from the text on the right to the 'Minimum ions' field in the 'Enable Region 2' section.

Setting Up ET for Calibrations (IE or Lens Transmission Curve)

This is where you set logical restrictions for the minimum ion count.

Selecting AND can lead to a too strict minimum ions and missing events.

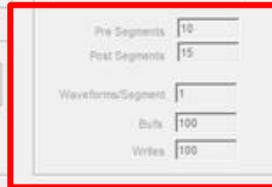
With OR and the right minimum ion threshold (prior slide), we can get a false event count of ~10 particles/cc in 120 sec (< 30 events in that time).

The screenshot shows the 'ToF-AMS Menu' software interface. The 'Event Trigger' panel is highlighted, showing the 'Region Combination Logic' section where the 'OR' radio button is selected. The 'Event Trigger' panel also shows 'Duration (s)' set to 120.0, 'Enable Region 1' (Start m: 30, End m: 30, Minimum ions: 7.00), 'Enable Region 2' (Start m: 48, End m: 48, Minimum ions: 5.00), and 'Enable Region 3' (Start m: 104, End m: 47, Minimum ions: 1.50). The 'Data Files' panel shows 'Auto Save Data' checked, 'Save HDF Files' checked, and 'Apply GZIP to HDF' checked. The 'Acquisition Clock' panel shows 'Time Grid' set to 'None'. The 'GenAlt Run Profile' panel shows 'MS' set to 20.0, 'PToE' set to 10.0, and 'Cycles / Run' set to 4. The 'Fast MS' panel shows 'Avg Time (s)' set to 1 s, 'Closed Block #1 (s)' set to 6.0, and 'Open Block (s)' set to 54.0.

Setting Up ET for Calibrations (IE or Lens Transmission Curve)

Still under development.

Currently, to calibrate with ET, the settings should be Pre Segments = 10, Post Segments = 15, and Waveforms/Segment = 1.



Analyzing ET for Calibration (IE or Lens Transmission Curve)

ToF AMS Ionization Efficiency Calibration Panel for ET v1.0.5F

Instructions

Load ET Data
 Single file
 Folder **Step 1. Select ET folder** Num. files 4

ET file folder E:ET_and_Doug_Expts:ET:2016.10.06:Normal_ET:
 Data folder root:Normal_ET:
 Alt. Step 1. Set panel to prev. data Get List

ET settings:
 m/z30(7 DR m/z46<5 Single ion (mv²/ns) 2.51
 Num. segments 26 Start AMU 7 Stop AMU 47
 Trigger segment num. 10 Pulser period, us 15.45
 Num. events in file 3034 File time 10/6/2016 9:51:09 PM

User Inputs
Compound NH4NO3 **Selected Dm (nm)** 400
 m/z List 30,46,15,16,17 (Opt.) MS AB Hz 3.875e+05
 Anion MW 62 Cation MW 18 (Opt.) CPC NaN +/- NaN
 Density (g cm⁻³) 1.72 (Opt.) Chopper duty cycle, % 2.0
 Jayne shape factor 0.8 **Step 2. Accept inputs, perform calculations**

Outputs

IE Average
 3.65e-07 +/- 2.55e-09

RIE Average
 4.74 +/- 0.07

Ions Per Particle
 Anion 126.55 +/- 0.89
 Cation 144.68 +/- 1.53

Other IPP
 Final IE event count 2921
 % events in CER 96.3
 IE / AB 9.409e-13
 Flow (cm³ s⁻¹) 0.577
 Chopper duty cycle, % 2.0
 CER # events/cc nan
 CER # events/sec nan

Individual Particle Time of Flight Traces

Step 3. Adjust Cal Event Region (CER), baseline (BL), etc.

CER begin 203 m/z30 min IPP 1 min IPP 1
 CER end 227 m/z46 max IPP 200 max IPP 200
 BaseLine Seg. 9 max BL 0.5 max BL 0.5

Graph Tweaks

- Show PTof histogram
- Show error bars on Seg Avg
- Show only events in CER

CER zoom CER autoscale

Pop Examine event num. -1 blacklist

Average Ions

Point Number (proportional to particle time-of-flight)

Seg #

Average IE and RIE

Pop

RIE cation

Event number

Ions

Pop

Ions

m/z

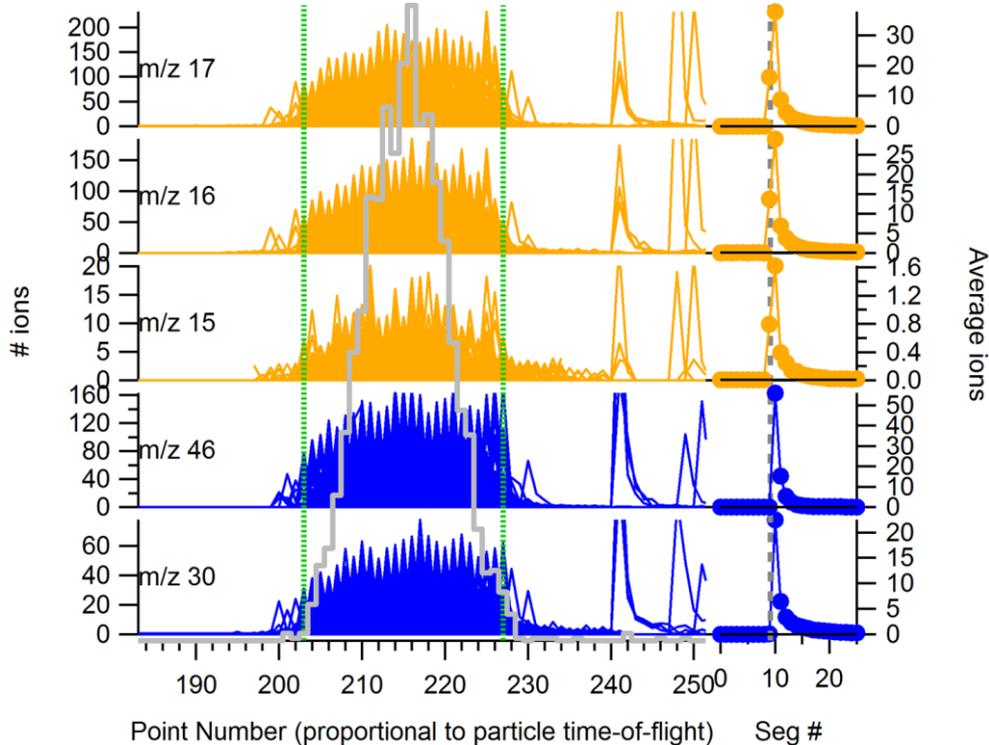
Pop Histograms of IPP for Cal Event Region (CER)

frequency of IPP anion

Ions Per Particle

The other new feature, compared to BFSP, are the Graph Tweaks.

Showing PToF Histogram Box



By selecting the show PToF histogram, a histogram of the PToF during the ET calibration is shown, in grey.

This is provide validation of a normal distribution, without doubles, in your final CER and IPP selection to calculate your IE, IE/AB, Ions Per Particles, and Final IE Event Count.

Analyzing ET for Calibration (IE or Lens Transmission Curve)

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ET settings:

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Num. segments 26 Start AMU 7 Stop AMU 47

Trigger segment num. 10 Pulser period, us 15.45

Num. events in file 3034 File time 10/6/2016 9:51:09 PM

Sample interval (ns) 0.625

User Inputs

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Flow (cm³ s⁻¹) 0.577

Chopper duty cycle, % 2.0

CER # events/cc nan

CER # events/sec nan

Individual Particle Time of Flight Traces

Step 3. Adjust Cal Event Region (CER), baseline (BL), etc

CER begin 203 m/z30 m/z46

CER end 227 min IPP 1 min IPP 1

BaseLine Seg. 9 max IPP 200 max IPP 200

max BL 0.5 max BL 0.5

Graph Tweaks

Show PTof histogram

Show error bars on Seg Avg

Show only events in CER

CER zoom CER autoscale

Pop Examine event num. -1 blacklist

The other new feature, compared to BFSP, are the Graph Tweaks.

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- Show error bars on Seg Avg
- Show only events in CER

CER zoom CER autoscale

Pop Examine event num. -1 blacklist

Average Ions

Average IE and RIE

Ions

The other new feature, compared to BFSP, are the Graph Tweaks.

Extra Slides: How to Convert ET Final Counts to Particles/cc

$$\frac{\textit{Particles}}{\textit{cc}} = \frac{\textit{Final ET Counts}}{\textit{ET Acquisition Time} * \textit{Flow Rate}} * \left(\frac{1}{\textit{Duty Cycle}} \right)$$