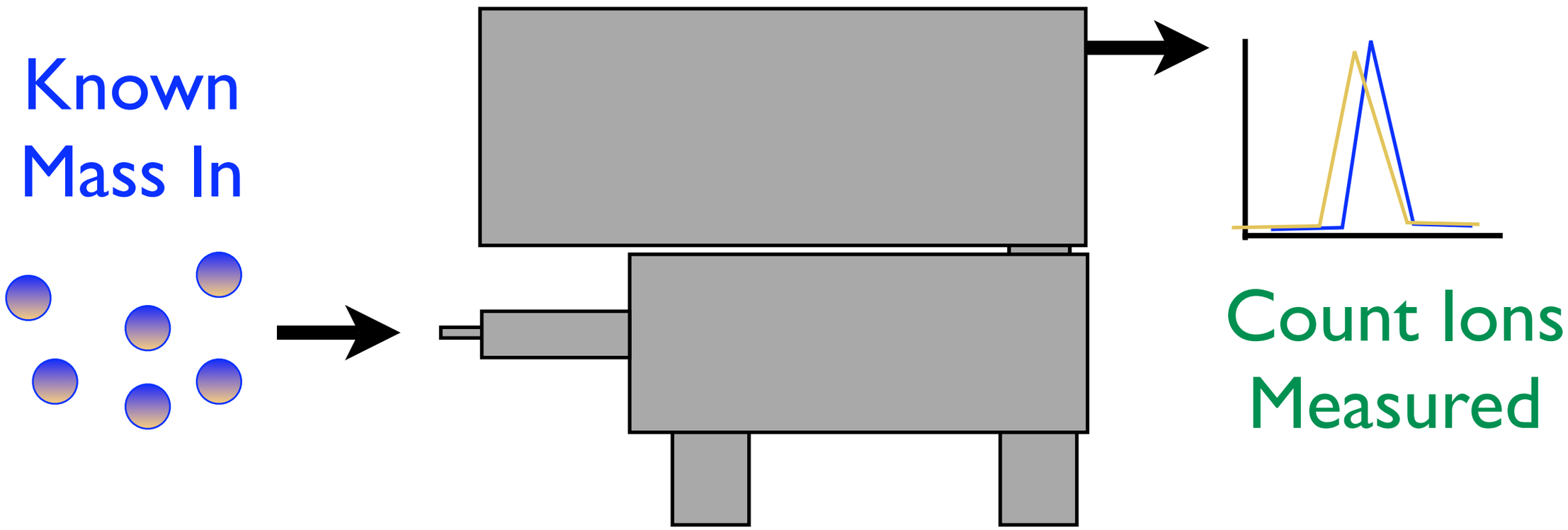
IE (and RIE) Calibration with the ToF-AMS

Pete

14-May-09

Principle to the calibration

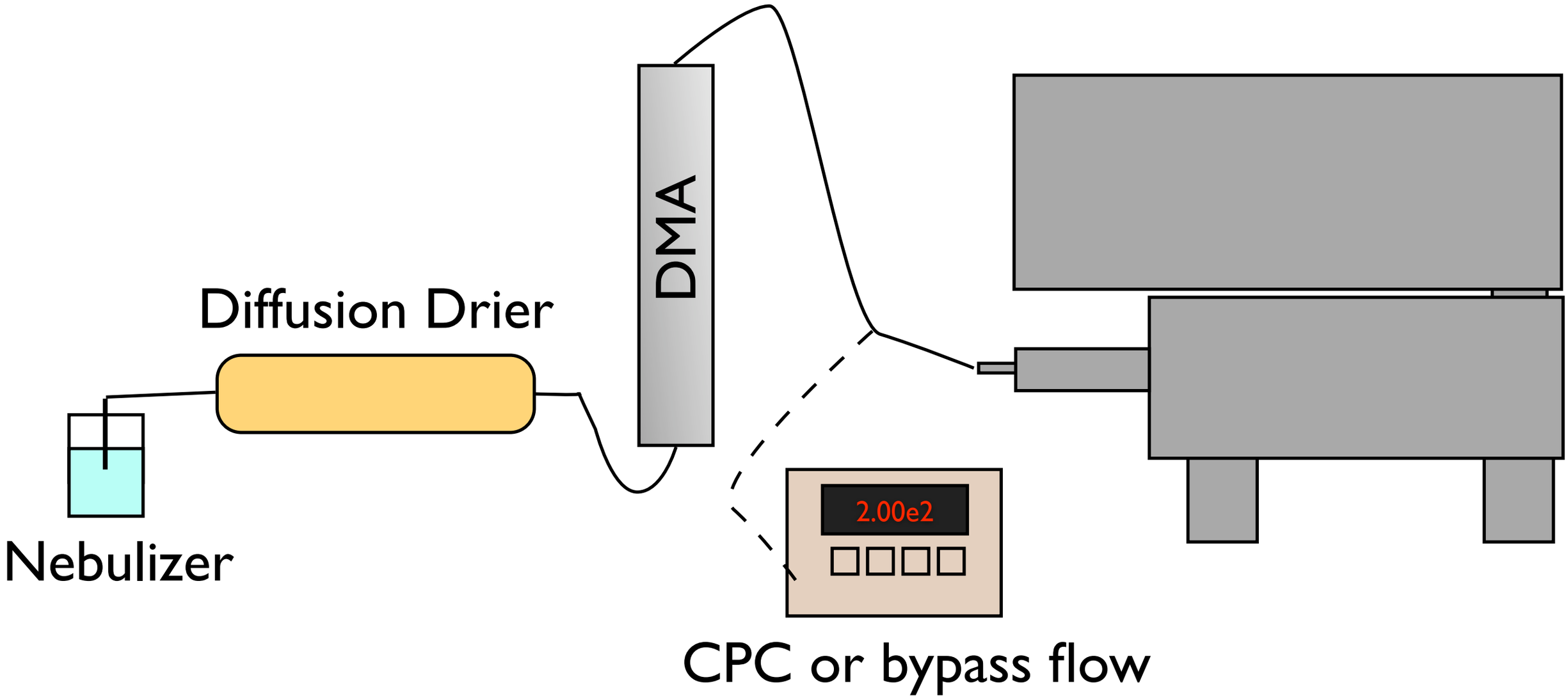


- The ionization (and transmission) efficiency (IE) is the number of ions measured from a “known” amount of mass.
- The Relative Ionization Efficiency (RIE) is the ratio of the IE of a species (e.g. NH_4) to IE_{NO3}

“Known” amount of mass

- The known amount of mass is based off of size selected dry particles from an DMA system.
- Typical sizes used in the calibration are 350 -450 nm. (I prefer 400 nm particles)
- Short sampling lines are better in this calibration
- Dry particles are important
- Temperature of environment can also have an impact on the measurement)

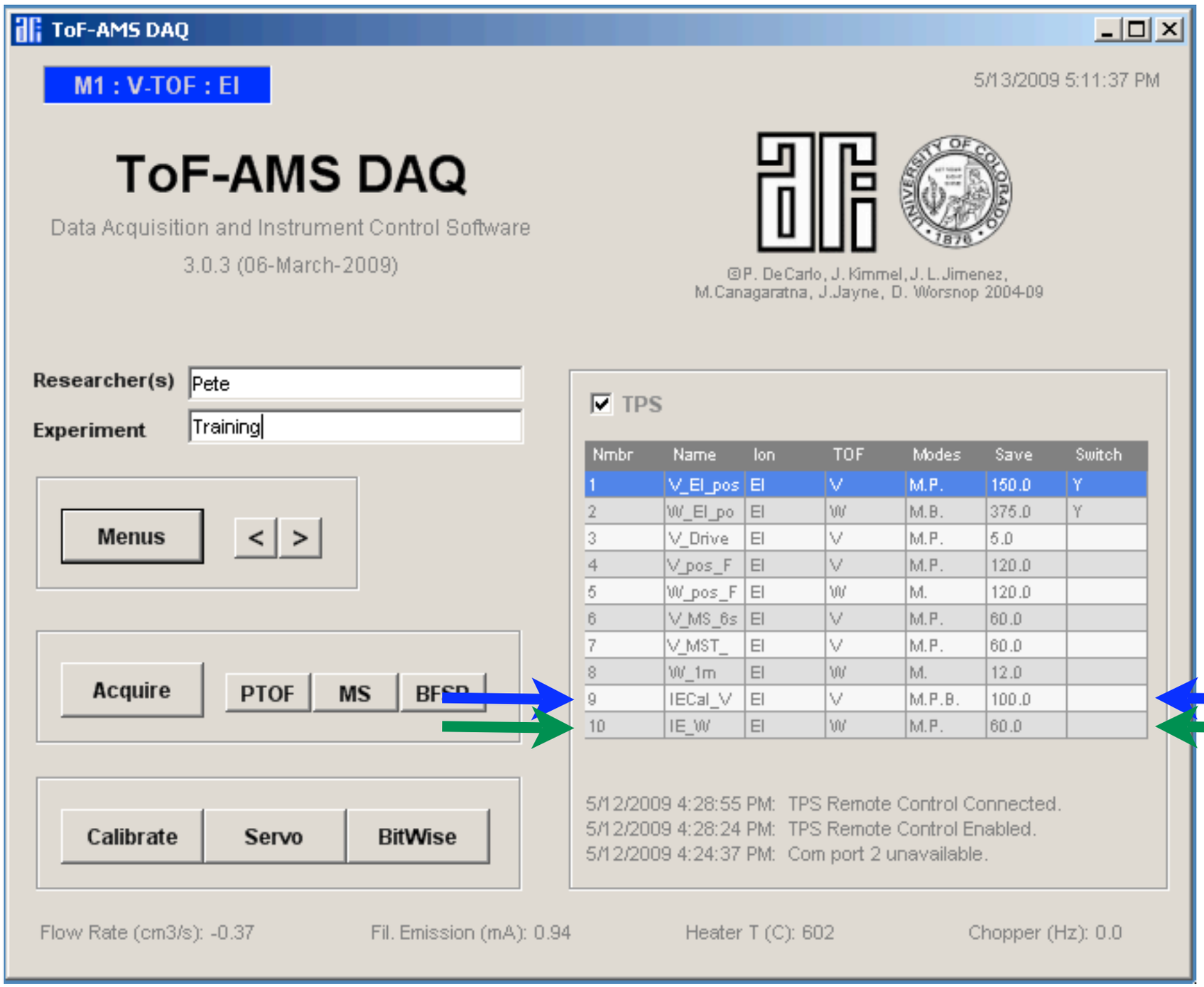
General Set-up



- CPC is not strictly necessary for BFSP calibrations
- Keep sampling lines short if possible

Setting up AMS for measurement

- Use specific V and W mode Calibration menus



Example V Timing

ToF AMS Menu - ToF-AMS Version: 3.0.3 (06-March-2009)

Save and Close (Q) | Close and Undo All Changes (X) | 5/13/2009 5:12:45 PM | Help

Menu Summary | Timing | ToF-AMS | Averaging and Saving | AP240 | Analog / Digital | Defaults

Recalculate

Chopper Parameters

Chopper Frequency (Hz)	145.0	*(0.0 Hz)*
Data Delay (us)	100	
ToF Spectra / Chopper	200	Max Dva
Nbr Co-Adds	1	

ToF-MS Parameters

Pulser Period (us)	25	40.0 (kHz)
Trigger Delay (ns)	3000	
Nbr of Samples	18976	Max m/z
+ Pulse Width (ns)	2000	
- Pulse Width (ns)	2000	
Timing Offset	◉ 50	○ 100 ns

Mass Cal: time = m * sqrt(mass) + b

Slope: 1673.87 Intercept: -4733.2

The AP240 trigger delay should be longer than the ToFMS pulse width (to avoid saving pulse pickup). That delay also determines the minimum mass

TOFMS wait Trigger is the difference between TOFMS samples and the pulse period. Minimum of approximately 8% required by the AP240 board. The combination of the pulse period and the wait for

PTOF Mode

PToF Mode: AP240 Averaging Time

725 Choppers

Automatic Timeout after 10 seconds

0 5 10 seconds

PToF Mode: AP240 Memory Usage (MegaSamples)

200 Saved ToF Spectra

0 2 4 (Max)

Chopper Cycle Timing

Chopper Open — AIR BEAM — PARTICLE SIZE — Chopper Open

200 ToF Extractions

145 Hz (6.9 ms)

Particle Size Range: 0 to 1595 nm

Data Delay: 0.1ms

Data Acq.: 5.0ms

Wait For Chopper: 1.8ms

Minimum ~0.5 msec required

Co-Adding is OFF. There will be 200 extractions, adjacent spectra will NOT be summed, yielding 200 time bins. Each time bin is 25 us wide.

MS Mode

ToFMS Extraction Timing

Mass Spectrum Window: 18976 ToFMS samples

AP240 Trigger Delay: 3000ns

Data Acq.: 18976ns

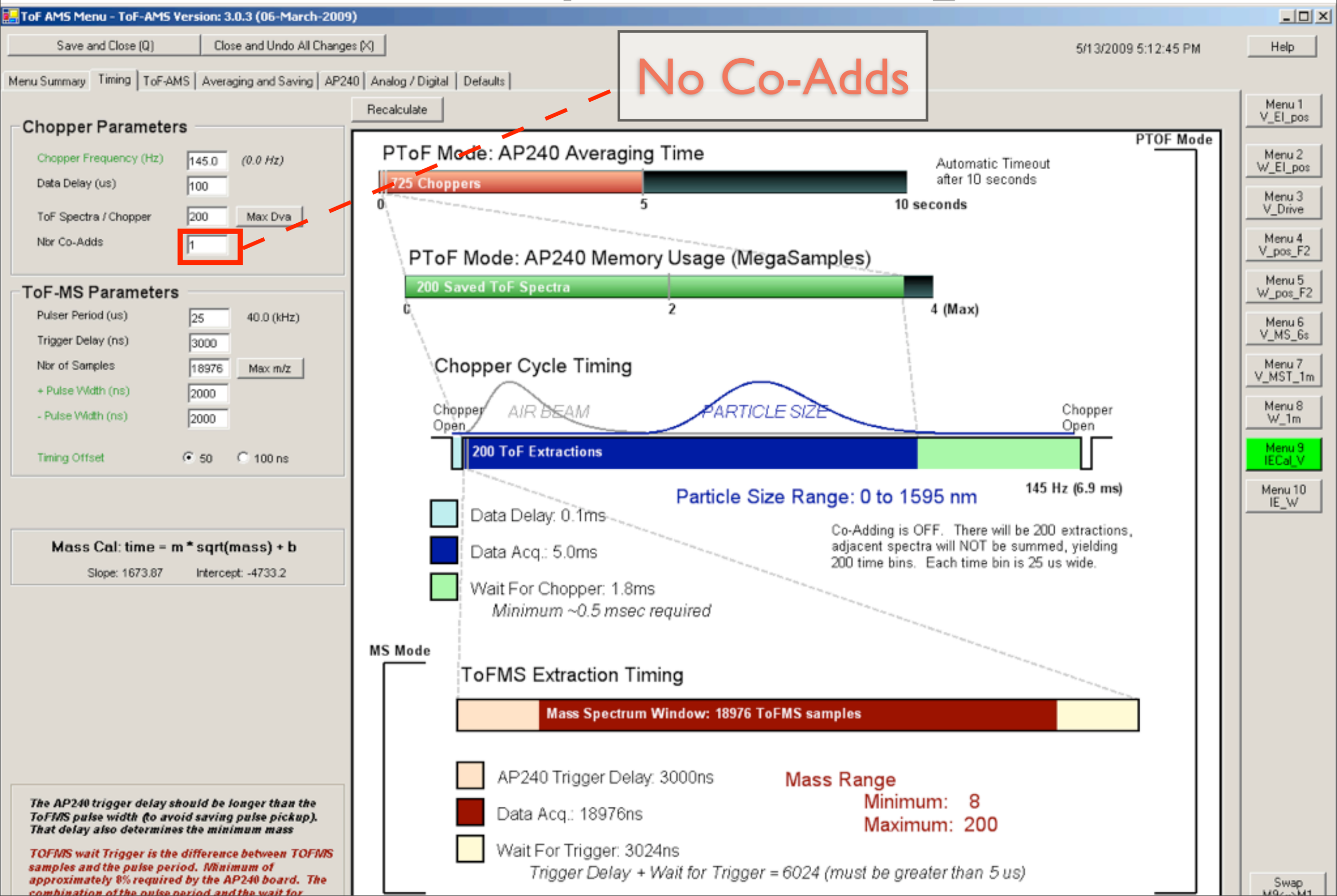
Wait For Trigger: 3024ns

Trigger Delay + Wait for Trigger = 6024 (must be greater than 5 us)

Mass Range
Minimum: 8
Maximum: 200

Menu 1 V_El_pos
Menu 2 W_El_pos
Menu 3 V_Drive
Menu 4 V_pos_F2
Menu 5 W_pos_F2
Menu 6 V_MS_6s
Menu 7 V_MST_1m
Menu 8 W_1m
Menu 9 IECal_V
Menu 10 IE_W
Swap

Example V Timing



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Faster Pulsing

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0 — 2 — 4 (Max)

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Menu 5 W_pos_F2
Menu 6 V_MS_6s
Menu 7 V_MST_1m
Menu 8 W_1m
Menu 9 IECal_V
Menu 10 IE_W
Swap

Example V Menu - Saving

ToF AMS Menu - ToF-AMS Version: 3.0.3 (06-March-2009)

Save and Close (Q) | Close and Undo All Changes (X) | 5/13/2009 5:14:41 PM | Help

Menu Summary | Timing | ToF-AMS | Averaging and Saving | AP240 | Analog / Digital | Defaults

1.) Save BFSP, MS, PTOF
2.) Save itx and HDF files
3.) Filter BFSP data for Am Nitrate

Menu 1 V_El_pos | Menu 2 W_El_pos | Menu 3 V_Drive | Menu 4 V_pos_F2 | Menu 5 W_pos_F2 | Menu 6 V_MS_6s | Menu 7 V_MST_1m | Menu 8 W_1m | Menu 9 IECal_V | Menu 10 IE_W

( ) GenAlt ( ) Fast MS ( ) Light Scatter

GenAlt Run Profile

1.)

Active		Dwell Time (sec)	
☑	MS	5.0	% Open 50 — Closed: 2.5, Open: 2.5
☑	PToF	5.0	
☑	BFSP	15.0	

Cycle Time (s): 25.0

Number GenAlt Cycles: 4

Save Time (s): 100.0 Calculate

25.0 s/cycle x 4 cycles = 100.0 s/save

C | O | P | B

☐ Save on Fixed Time Grid Wait Time After Save (s): 0

Data Files

Run Number: 11302

2.)

☑ Auto Save Data
☑ Save ITX Files
☑ Save HDF Files

Max HDF File Size (MB): 600.0

GZIP Compression

☑ Apply

MS Deflate Level: 4 PToF Deflate Level: 4

PToF

Nbr of Choppers: 725 = 5.0 sec.

☐ Save Raw CH1 Data (*.bin , *_p.hdf)

Channel 2

( ) Stick data ( ) Raw data ( ) Both

3.)

BFSP

Data Filtering

With filtering, run data are processed in order to determine the existence of particles. Empty data is not saved. This may bias your BFSP data. It will, however, significantly reduce the amount of data saved to your hard drive

( ) No Filtering Signal Threshold (Bits): 10

(•) CH1: Filter for All Particles

( ) CH1: Filter for Particles in Size Range Min Dva (nm): 100 Max Dva (nm): 1000

( ) CH2: Filter for Events Row Sum (bits): 0

Single Species Chem Filter

☑ Enable Am Nitrate (30, 46)

User (m1, m2, m3): 0.5000,400

User Thresholds: 1 1 1

☐ Save CH1 Binary BFSP Data

Save Channel 2:

Fast MS

Avg Time (s): 0.5 s Closed Blocks (s): 5.0

Cycles: 1 Open Block (s): 30.0

Ligh Scattering

Run Duration (s): 15.0 Particle Number: 1

☐ 2-Channel Recording (6024E)

RealTime Data

☑ Write RealTime (RT) Files Clear Existing

16
28
30
41
46
48
55
60
64
184

Add to List

Remove Selected

Reset To Default Values

☐ Output Real Time Data to Serial Port

☑ Output TimeTrace.txt (Redundant to RT) New TT

Serial Port

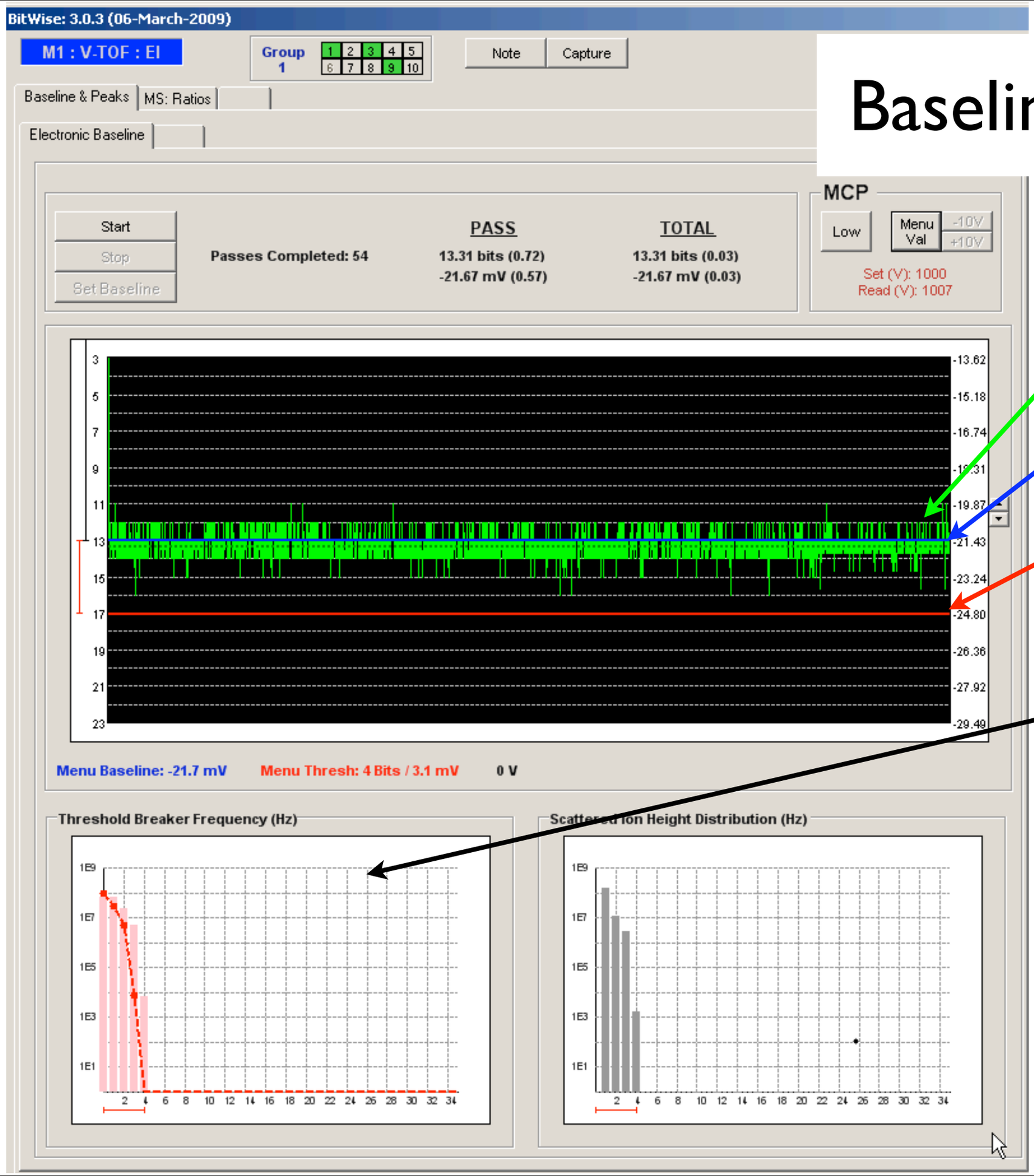
Com Port: 2

Parity=None Baud Rate: 9600

Data Bits: 8 Stop Bit: 1

Swap M9<->M1

Baseline Check Output



raw electronic baseline

Set electronic baseline in ADC

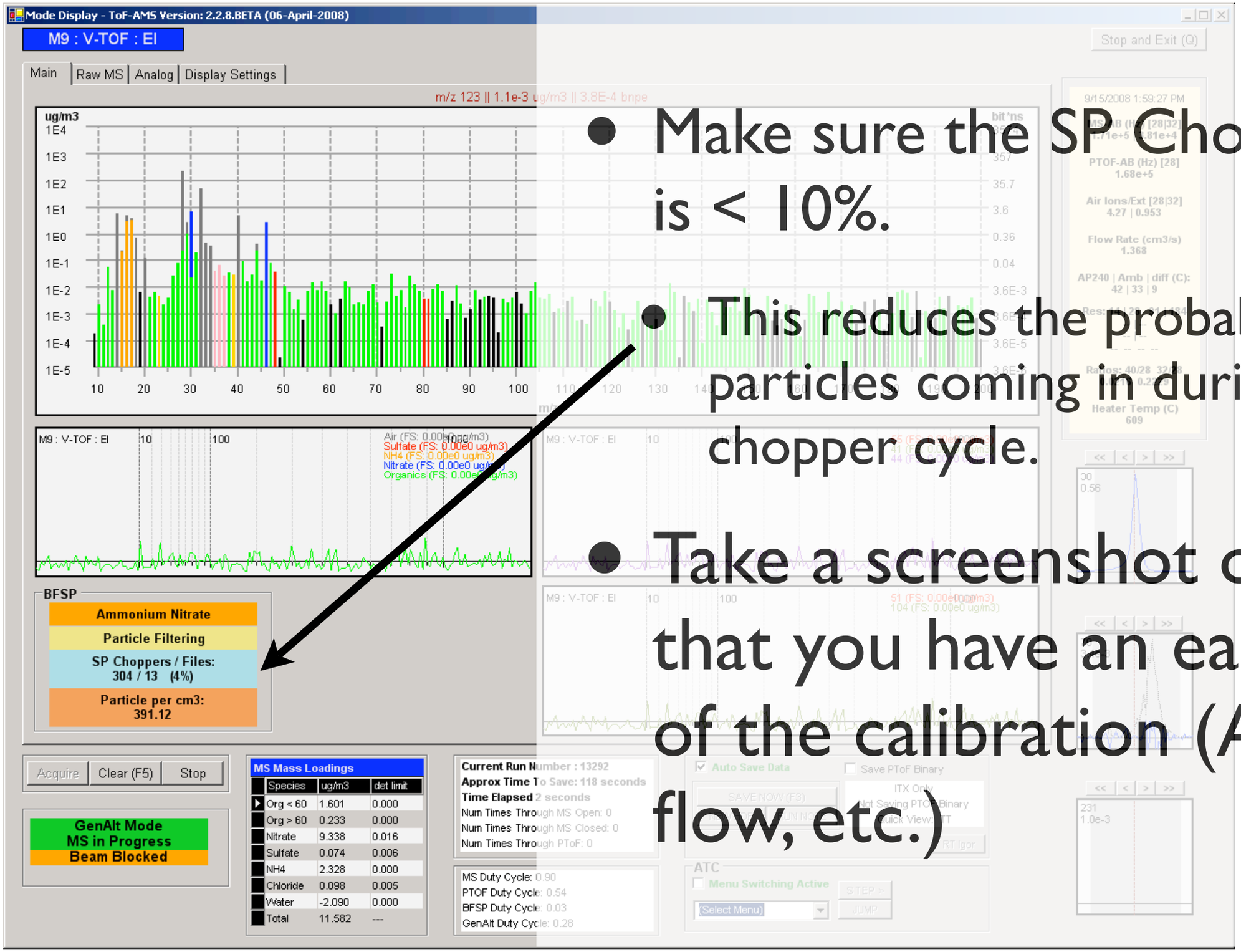
Set Threshold value in ADC

This graph shows the electronic noise around the baseline. In general one does not want vertical bars exceeding your threshold value red line at bottom. One should *not* adjust the baseline to prevent this, as that can reduce the linearity of the ion measurement and compromise data quality. The next tests guide ones decision on the threshold value

Why to do those things

- No Co-Adds - This gives better size resolution by a factor of 2.
- Faster Pulsing - This increases the number of ions measured and should improve the IPP measurement
  - The measured IE value will need to be scaled by the ratio of the Pulsing Period during calibration to the Pulsing Period during measurement
- Save all Modes (with a focus on BFSP).
  - The other modes are important for looking at doubly charged particle corrections (PTOF) and RIE (MS) since signal to noise is higher in these modes
- HDF and itx saving... itx files are needed for the IE calibration procedure, and HDF files are needed for use in Sqrl. Save both
- Filter for Ammonium Nitrate Particles so you don't save too much data. This tells the DAQ software to only save BFSP data if an AmmNit particle is detected

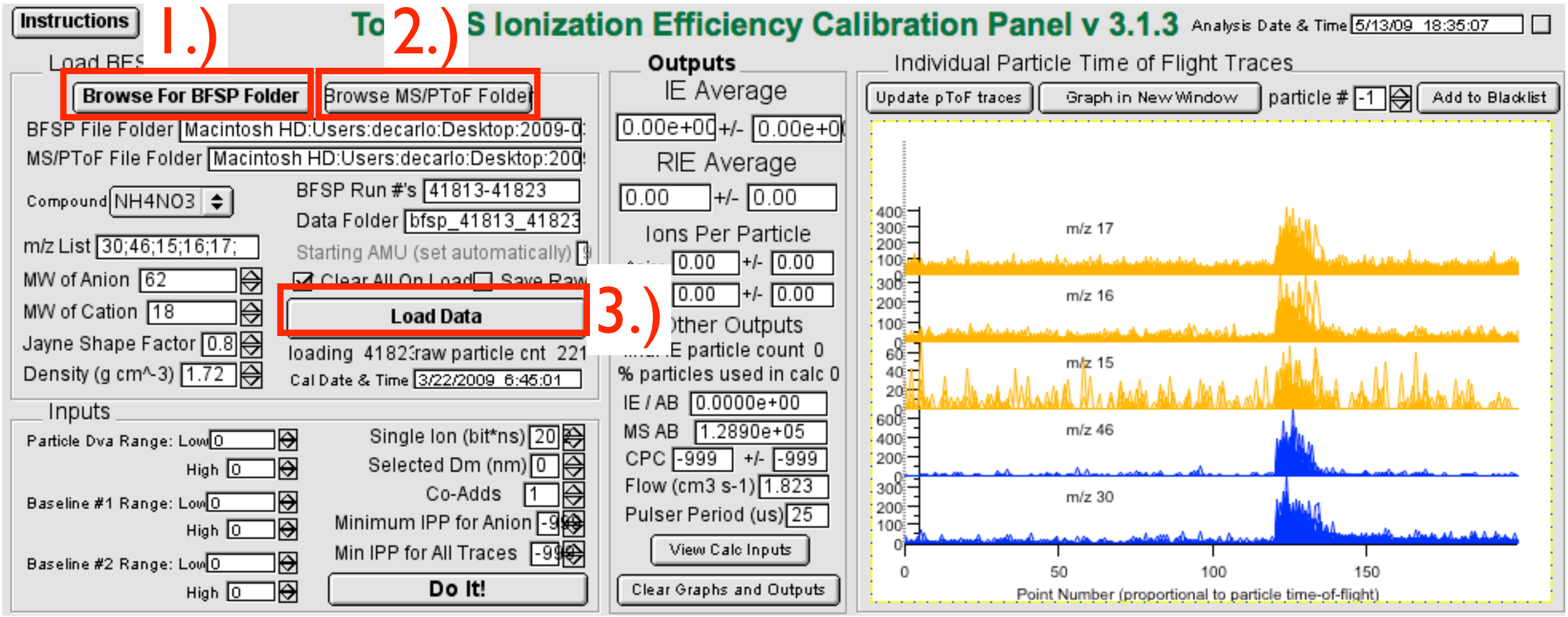
When Taking Data:



- Make sure the SP Choppers / Files is < 10%.
- This reduces the probability of 2 particles coming in during the same chopper cycle.
- Take a screenshot or 2 so that you have an easy record of the calibration (Airbeam, flow, etc.)

Processing Data

Loading the Data



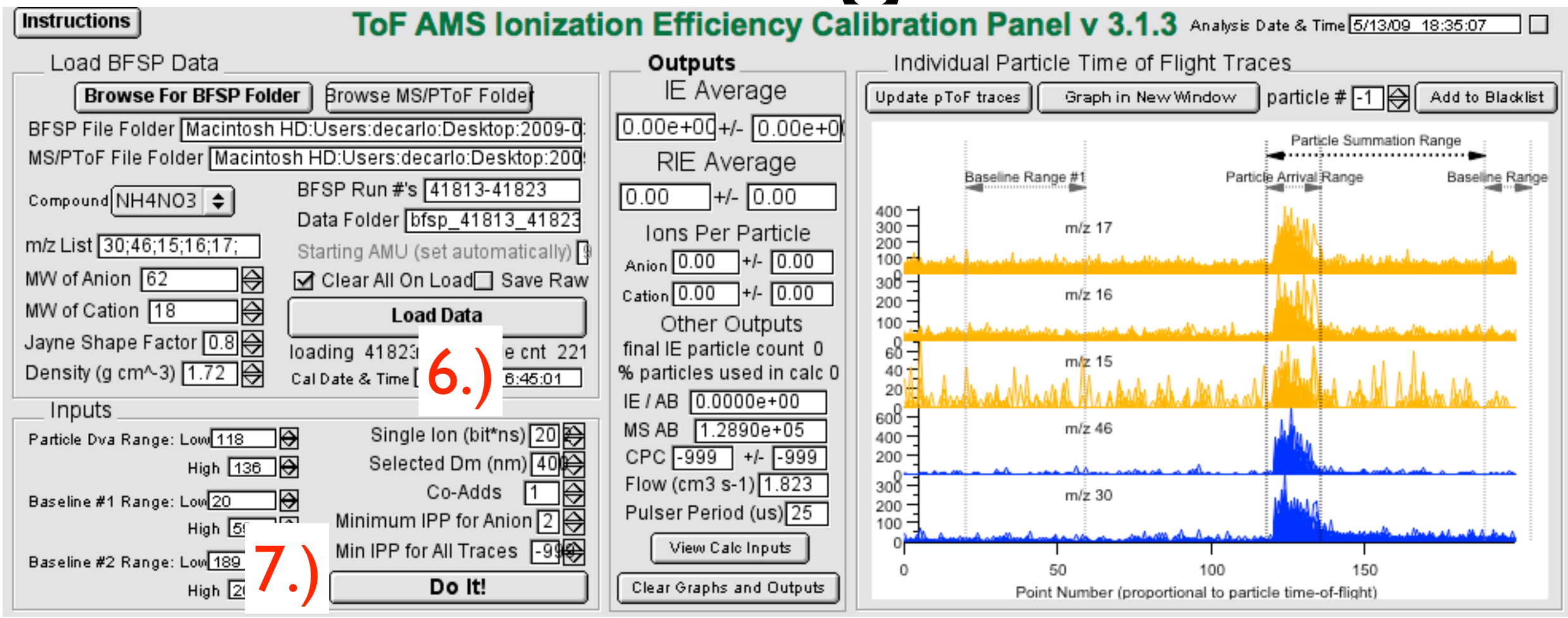
1. Find your "BFSPData" folder
2. Find your "AutoSaveData" folder
3. Load your Data

Processing cont.

4. Graph Data in New Window

5. Use Marquee function and right click to select the 3 areas for the IE calibration

Processing Cont.



6. Check the SI value, enter the mobility diameter used in the IE calibration, adjust other parameters as desired
7. Click "Do It!"

Setting the min IPP to e.g. 2 is fine. Play with these numbers and see how things change. Avoid setting too high of a min IPP...

Instructions

ToF AMS Ionization Efficiency Calibration Panel v 3.1.3

Analysis Date & Time 5/13/09 18:57:41

Load BFSP Data

Browse For BFSP Folder | Browse MS/PToF Folder

BFSP File Folder: Macintosh HD:Users:decarlo:Desktop:2009-0

MS/PToF File Folder: Macintosh HD:Users:decarlo:Desktop:200

Compound: NH4NO3

BFSP Run #'s: 41813-41823

Data Folder: bfsp_41813_41823

m/z List: 30;46;15;16;17;

Starting AMU (set automatically)

MW of Anion: 62

Clear All On Load | Save Raw

MW of Cation: 18

Load Data

Jayne Shape Factor: 0.8

loading 41823 raw particle cnt 221

Density (g cm^-3): 1.72

Cal Date & Time: 3/22/2009 6:45:01

Inputs

Particle Dva Range: Low 118 High 136

Baseline #1 Range: Low 20 High 59

Baseline #2 Range: Low 189 High 204

Single Ion (bit*ns): 20

Selected Dm (nm): 40

Co-Adds: 1

Minimum IPP for Anion: 2

Min IPP for All Traces: -99

Do It!

Outputs

IE Average: 6.99e-08 +/- 1.73e-0

RIE Average: 4.15 +/- 0.15

Ions Per Particle

Anion 24.27 +/- 8.74

Cation 27.56 +/- 13.42

Other Outputs

final IE particle count 21

% particles used in calc 9

IE / AB: 5.4257e-13

MS AB: 1.2890e+05

CPC: -999 +/- -999

Flow (cm3 s-1): 1.823

Pulser Period (us): 25

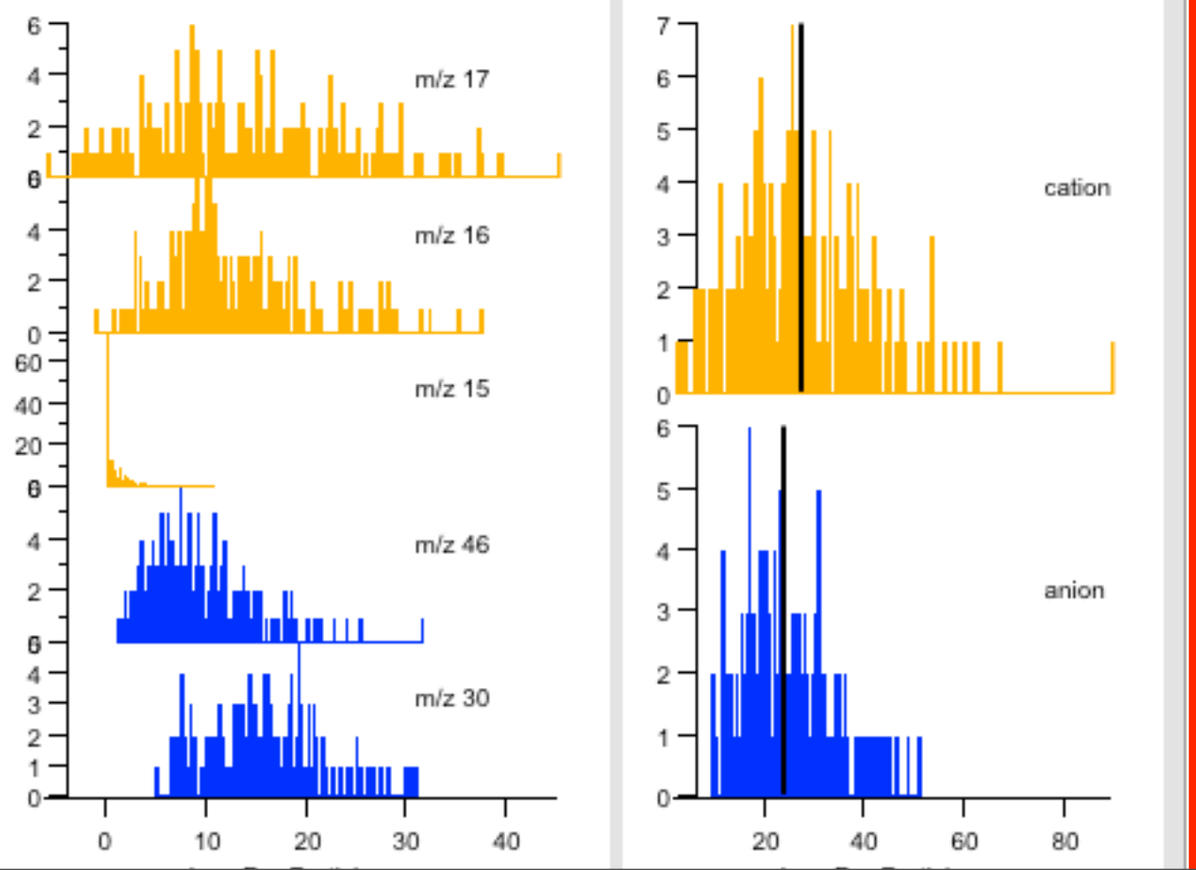
View Calc Inputs

Clear Graphs and Outputs

- Output is the IE, RIE (better to use MS mode), Ions per particle, IE/AB, Flow and Pulser Period
- Diagnostic graphs are very useful for interpretation
- The IE/AB is the number that should be used for input into the DAQ.

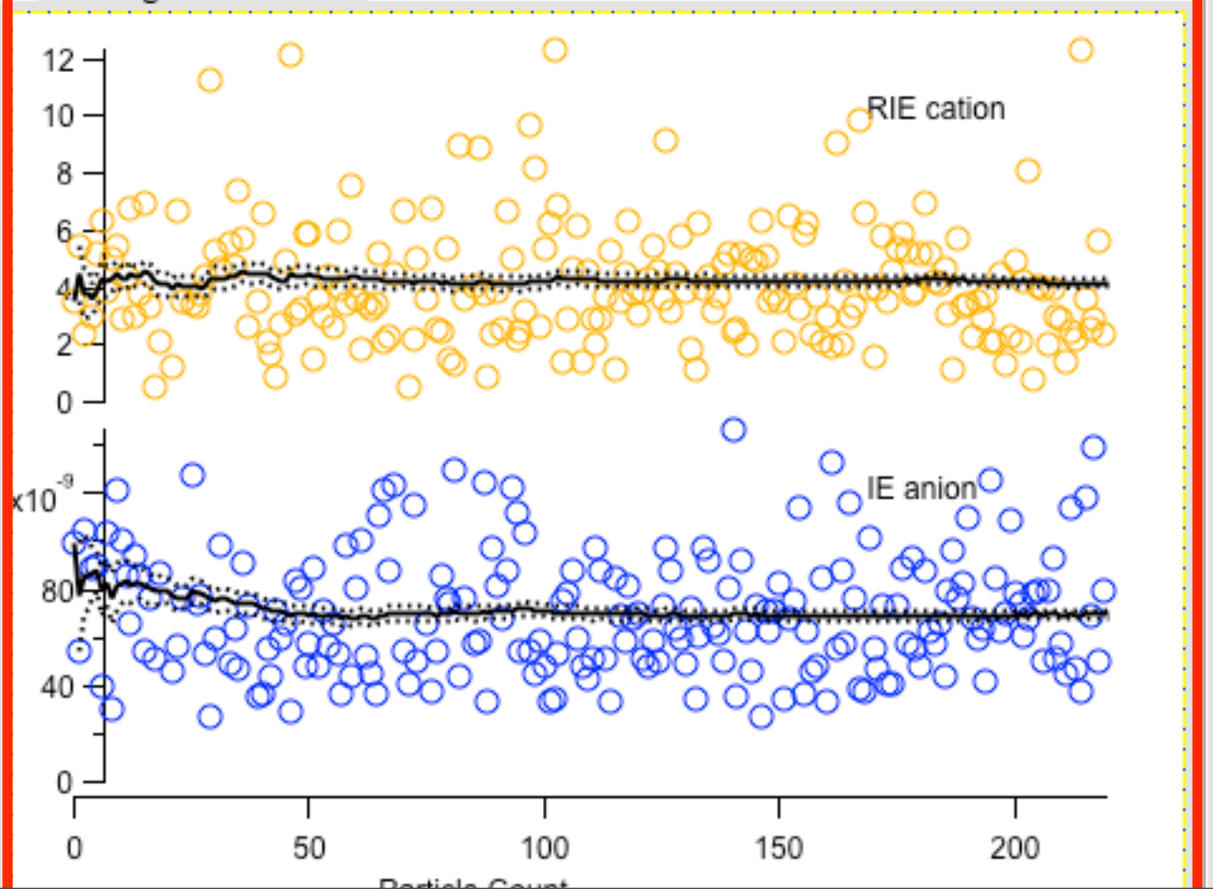
Graph in New Window

Histograms for Ions Per Particle



Graph in New Window

Average IE and RIE



Input into DAQ: IE/AB number

- If your pulser period is different for your Calibration menu, then the IE you input will be different than the IE you measured, but your IE/AB will be the same!
- $IE_{DAQ} = IE_{Meas} * PulserPeriod_{IE}/PulserPeriod_{Acq}$
- Or alternatively:
- $IE_{DAQ} = IE/AB_{Meas} * AB_{Acq}$
- Where IE_{DAQ} is the value to input into the Menu in the DAQ software

More information

- Theoretical explanation of Mass Quantification with AMS see section 5 of:
  - Jimenez et al. Ambient Sampling using the Aerodyne Aerosol Mass Spectrometer JGR, 2003
- See Edward Dunlea's presentation from AMS User's Meeting:
- http://cires.colorado.edu/jimenez-group/UsrMtgs/UsersMtg7/ie_cal_tutorial.pdf
- ipf for IE processing:
  - http://cires.colorado.edu/jimenez-group/ToFAMSResources/ToFSoftware/index.html#ToF_IE_Cal