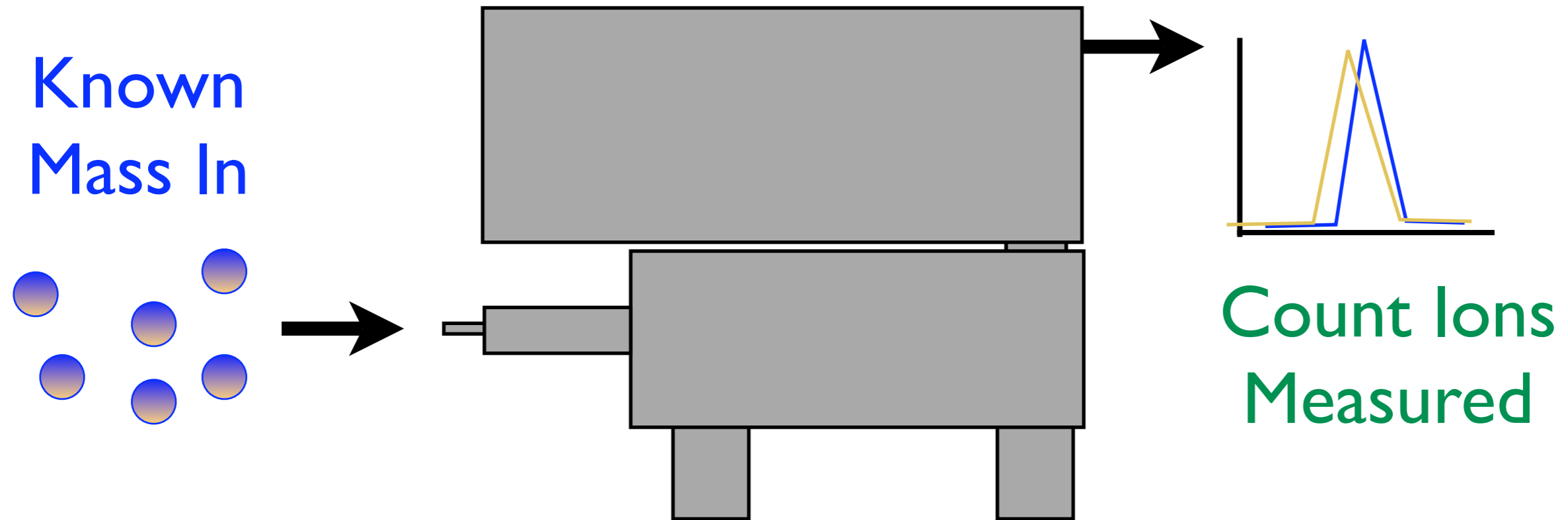


IE (and RIE) Calibration with the ToF-AMS

Pete
14-May-09

Principle to the calibration

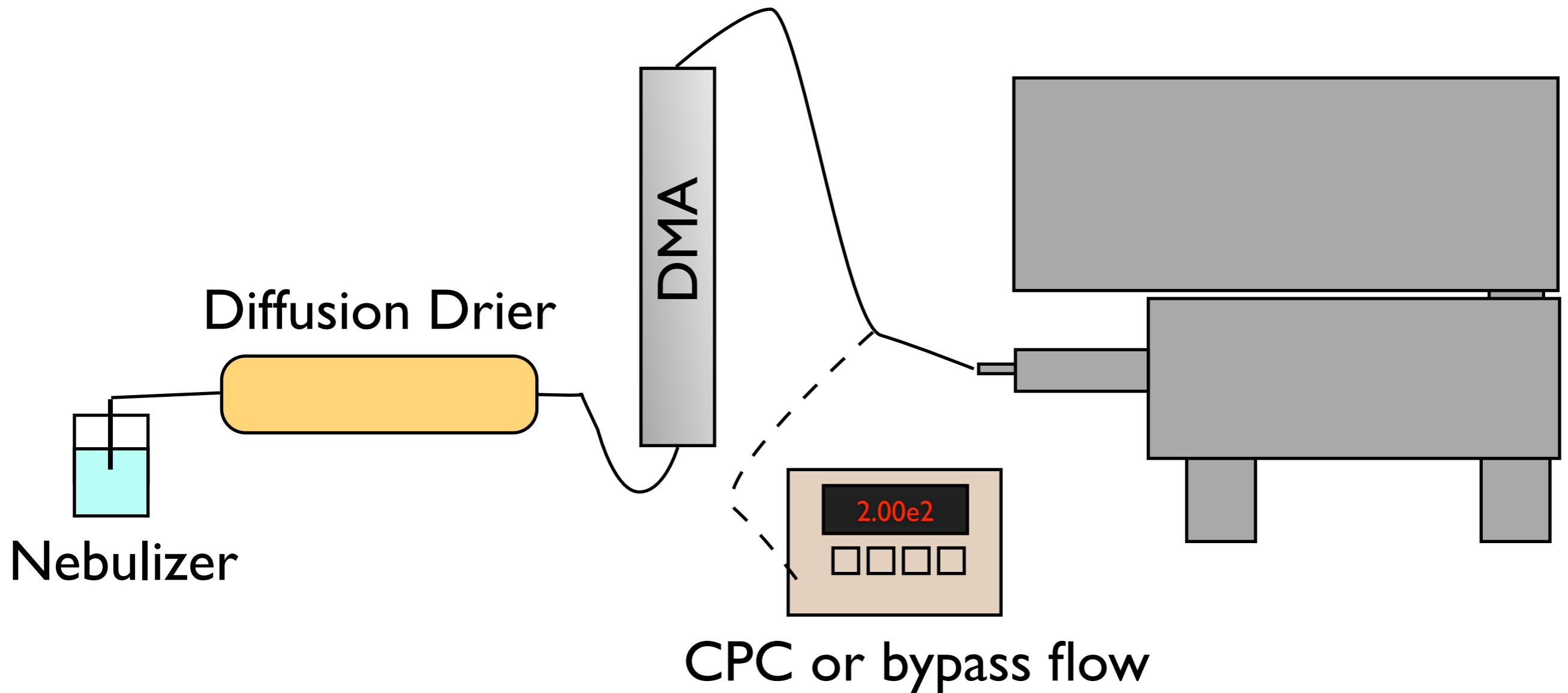


- The ionization (and transmission) efficiency (IE) is the number of ions measured from a “known” amount of mass.
- The Relative Ionization Efficiency (RIE) is the ratio of the IE of a species (e.g. NH_4) to IE_{NO_3}

“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

The screenshot shows the ToF-AMS DAQ software interface. At the top, it displays 'M1 : V-TOF : EI' and the date/time '5/13/2009 5:11:37 PM'. The main title is 'ToF-AMS DAQ' with the subtitle 'Data Acquisition and Instrument Control Software 3.0.3 (06-March-2009)'. Logos for 'af' and 'UNIVERSITY OF COLORADO' are visible, along with copyright information for P. DeCarlo, J. Kimmel, J. L. Jimenez, M. Canagaratna, J. Jayne, and D. Worsnop (2004-09).

Fields for 'Researcher(s)' (Pete) and 'Experiment' (Training) are present. A 'Menus' button and navigation arrows are shown. Below are buttons for 'Acquire', 'PTOF', 'MS', and 'BFSP', with blue and green arrows pointing to them. Further down are 'Calibrate', 'Servo', and 'BitWise' buttons.

A table of modes is displayed, with a checked 'TPS' checkbox above it. The table has columns for Nbr, Name, Ion, TOF, Modes, Save, and Switch. The first row is highlighted in blue. Blue and green arrows point to the 'BFSP' button and the first row of the table, respectively.

Nbr	Name	Ion	TOF	Modes	Save	Switch
1	V_EI_pos	EI	V	M.P.	150.0	Y
2	W_EI_po	EI	W	M.B.	375.0	Y
3	V_Drive	EI	V	M.P.	5.0	
4	V_pos_F	EI	V	M.P.	120.0	
5	W_pos_F	EI	W	M.	120.0	
6	V_MS_6s	EI	V	M.P.	60.0	
7	V_MST_	EI	V	M.P.	60.0	
8	W_1m	EI	W	M.	12.0	
9	IECal_V	EI	V	M.P.B.	100.0	
10	IE_W	EI	W	M.P.	60.0	

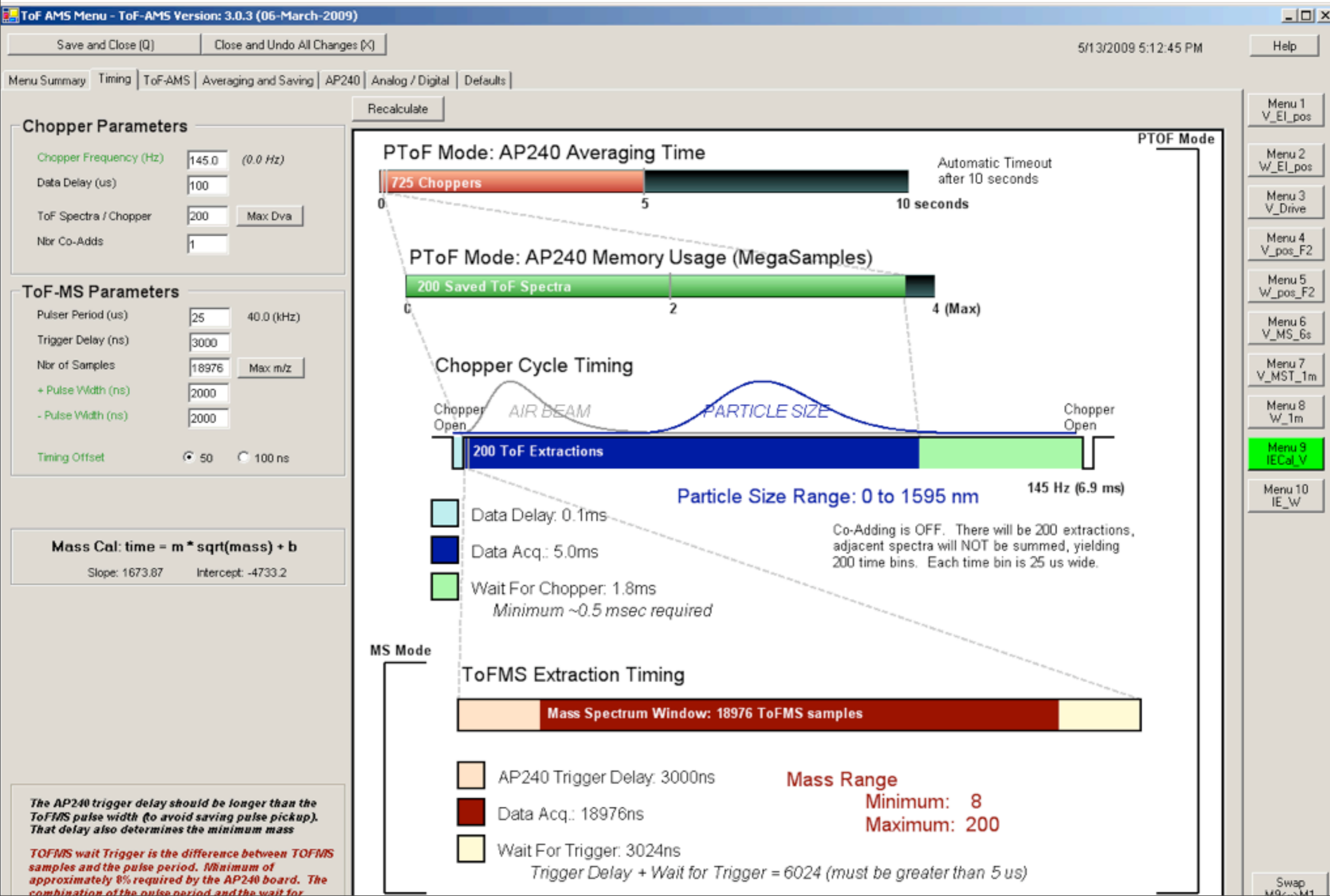
Log messages at the bottom of the table area:

- 5/12/2009 4:28:55 PM: TPS Remote Control Connected.
- 5/12/2009 4:28:24 PM: TPS Remote Control Enabled.
- 5/12/2009 4:24:37 PM: Com port 2 unavailable.

System parameters at the bottom:

- Flow Rate (cm³/s): -0.37
- Fil. Emission (mA): 0.94
- Heater T (C): 602
- Chopper (Hz): 0.0

Example V Timing



Example V Timing

ToF AMS Menu - ToF-AMS Version: 3.0.3 (06-March-2009) 5/13/2009 5:12:45 PM

Save and Close (Q) Close and Undo All Changes (X) Help

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

Recalculate

No Co-Adds

Chopper Parameters

Chopper Frequency (Hz) (0.0 Hz)

Data Delay (us)

ToF Spectra / Chopper Max Div

Nbr Co-Adds

ToF-MS Parameters

Pulser Period (us) 40.0 (kHz)

Trigger Delay (ns)

Nbr of Samples Max m/z

+ Pulse Width (ns)

- Pulse Width (ns)

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 0 5 10 seconds Automatic Timeout after 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

Particle Size Range: 0 to 1595 nm 145 Hz (6.9 ms)

- 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_EI_pos

Menu 2 W_EI_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 M9 <=> M1

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

No Co-Adds

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: 1671.87 Intercept: -4733.2

Faster Pulsing

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 0 5 10 seconds Automatic Timeout after 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

Particle Size Range: 0 to 1595 nm 145 Hz (6.9 ms)

- 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_EI_pos

Menu 2 W_EI_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 M9 <-> M1

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

GenAlt Fast MS Light Scatter

1.) Save BFSP, MS, PTOF

2.) Save itx and HDF files

3.) Filter BFSP data for Am Nitrate

GenAlt Run Profile

Active Dwell Time (sec)

MS 5.0

PTOF 5.0

BFSP 15.0

% Open 50 Closed: 2.5 Open: 2.5

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

Auto Save Data

Save ITX Files

Save HDF Files

Max HDF File Size (MB) 600.0

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

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

Menu 1 V_EI_pos

Menu 2 W_EI_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 IECa_V

Menu 10 IE_W

Swap M9<->M1

M1 : V-TOF : EI

Group 1
1 2 3 4 5
6 7 8 9 10

Note Capture

Baseline Check Output

Baseline & Peaks MS: Ratios

Electronic Baseline

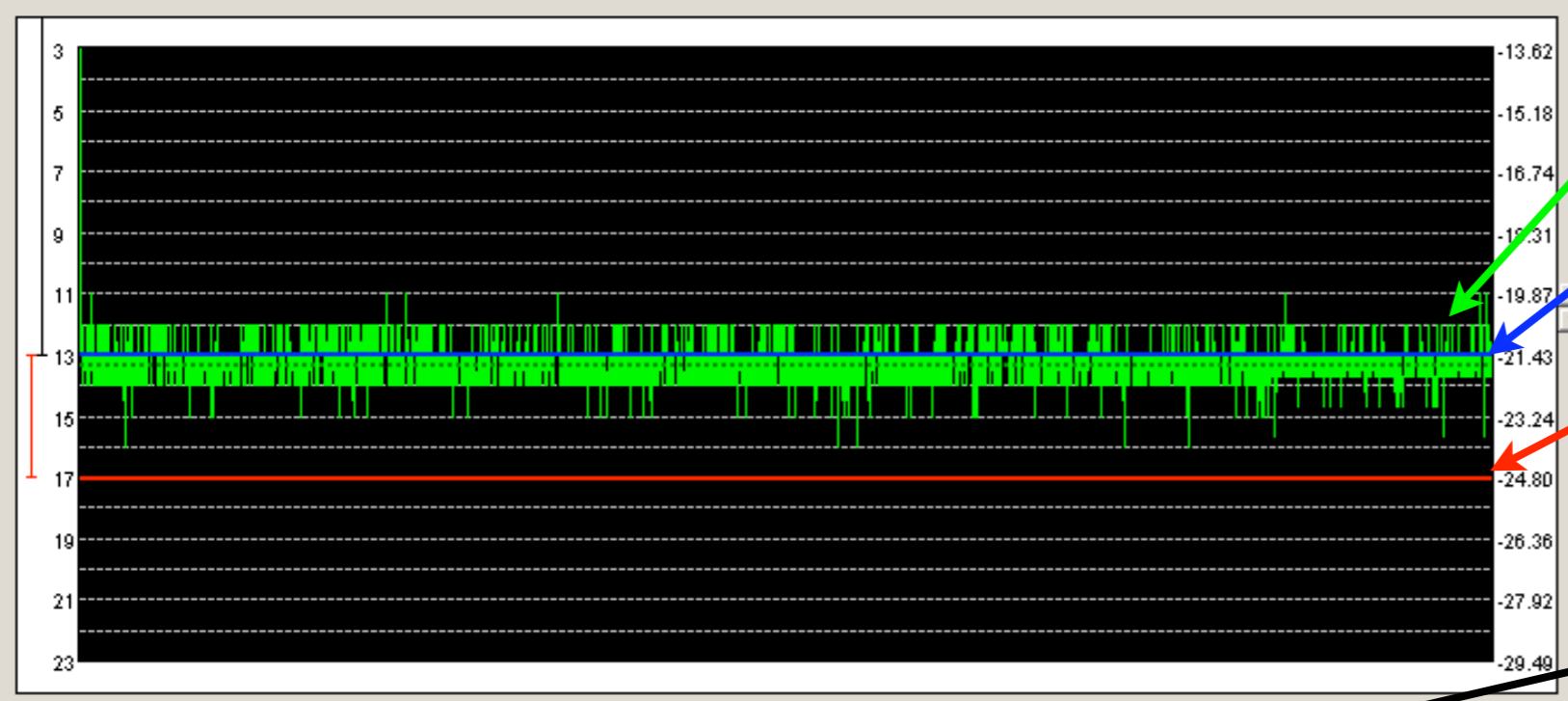
Start
Stop
Set Baseline

	PASS	TOTAL
Passes Completed: 54	13.31 bits (0.72)	13.31 bits (0.03)
	-21.67 mV (0.57)	-21.67 mV (0.03)

MCP

Low Menu Val -10V
+10V

Set (V): 1000
Read (V): 1007



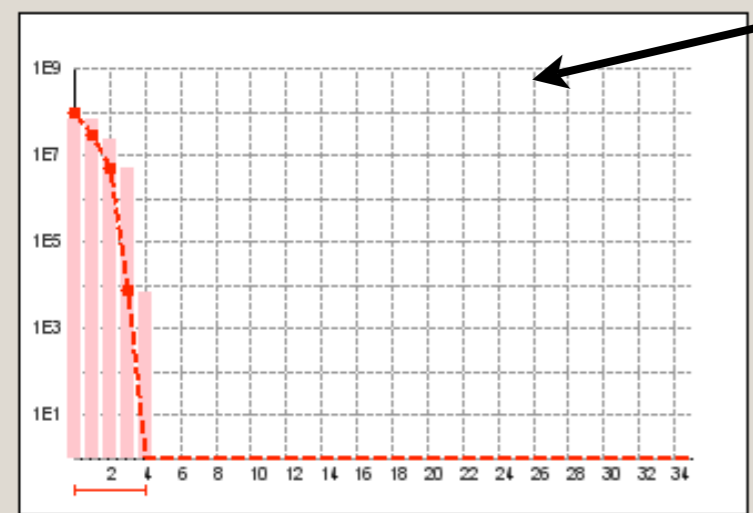
Menu Baseline: -21.7 mV Menu Thresh: 4 Bits / 3.1 mV 0 V

raw electronic baseline

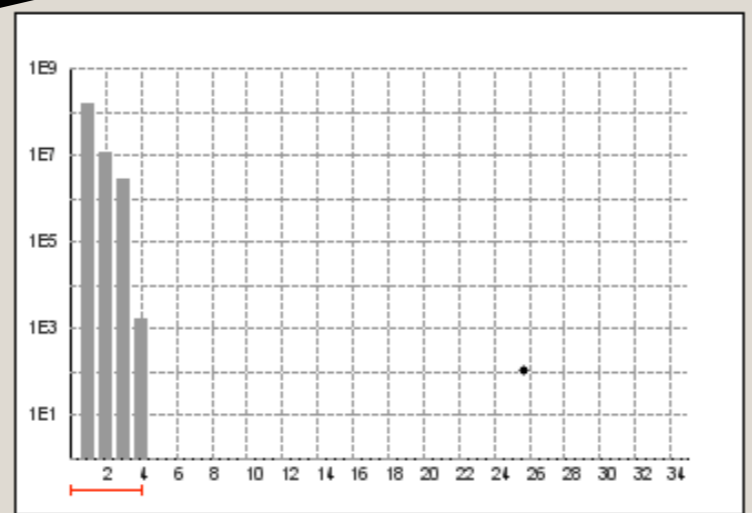
Set electronic baseline in ADC

Set Threshold value in ADC

Threshold Breaker Frequency (Hz)



Scattered Ion Height Distribution (Hz)



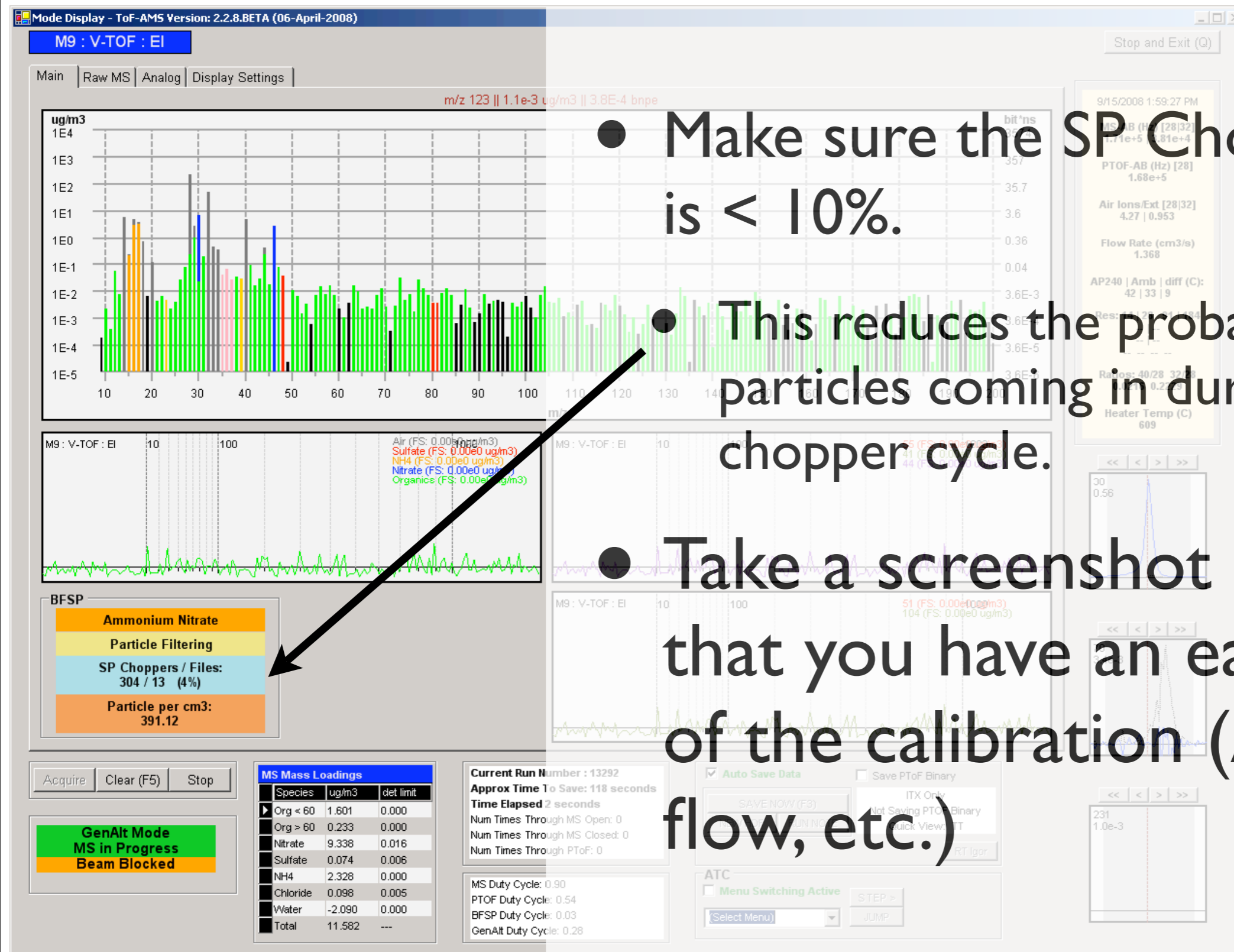
This graph shows the electronic noise around the baseline. In general one does not want vertical bars exceeding your threshold value red line at bottom. One should *not* adjust the baseline to prevent this, as that can reduce the linearity of the ion measurement and compromise data quality. The next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

Instructions 1.) To 2.) **S Ionization Efficiency Calibration Panel v 3.1.3** Analysis Date & Time 5/13/09 18:35:07

Load BESP

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:2009-0]

Compound [NH4NO3] BFSP Run #'s [41813-41823] Data Folder [bfsp_41813_41823] Starting AMU (set automatically) [] Clear All On Load Save Raw

m/z List [30;46;15;16;17;] MW of Anion [62] MW of Cation [18] Jayne Shape Factor [0.8] Density (g cm⁻³) [1.72]

loading 41823raw particle cnt 221 Cal Date & Time [3/22/2009 6:45:01]

Load Data 3.)

Inputs

Particle Dva Range: Low [0] High [0] Single Ion (bit*ns) [20] Selected Dm (nm) [0] Co-Adds [1] Minimum IPP for Anion [-99] Min IPP for All Traces [-99] **Do It!**

Baseline #1 Range: Low [0] High [0]

Baseline #2 Range: Low [0] High [0]

Outputs

IE Average [0.00e+00] +/- [0.00e+00] RIE Average [0.00] +/- [0.00] Ions Per Particle [0.00] +/- [0.00] Other Outputs: % particles used in calc [0] IE / AB [0.0000e+00] 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**

Individual Particle Time of Flight Traces

Update pToF traces Graph in New Window particle # [-1] **Add to Blacklist**

1. Find your “BFSPData” folder
2. Find your “AutoSaveData” folder
3. Load your Data

Processing cont.

ToF AMS Ionization Efficiency Calibration Panel v 3.4.0 Analysis Date & Time 5/13/09 18:35:07

Instructions

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...

BFSP Run #'s 41813-41823

Outputs

IE Average 0.00e+00 +/- 0.00e+00
RIE Average 0.00 +/- 0.00

Individual Particle Time-of-Flight Traces

Update pToF traces Graph in New Window particle # -1 Add to Blacklist

Particle Time of Flight

particle # -1 Add to Blacklist

Particle Summation Range
Particle Arrival Range
Baseline Range #1

m/z 17
m/z 16
m/z 15
m/z 46
m/z 30

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

Expand
Horiz Expand
Vert Expand
Shrink
Horiz Shrink
Vert Shrink
ToF IE Calibration - Set Dva Range

Graph in New Window

4. Graph Data in New Window

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

Processing Cont.

Instructions **ToF AMS Ionization Efficiency Calibration Panel v 3.1.3** Analysis Date & Time 5/13/09 18:35:07

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:2009-0

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 Save Raw
Jayne Shape Factor 0.8 Save Raw
Density (g cm⁻³) 1.72 Save Raw

Load Data

loading 41823 e cnt 221
Cal Date & Time 6:45:01

Inputs

Particle Dva Range: Low 118 High 136
Single Ion (bit*ns) 20
Selected Dm (nm) 40
Co-Adds 1
Minimum IPP for Anion 2
Min IPP for All Traces -999

Do It!

Outputs

IE Average 0.00e+00 +/- 0.00e+00
RIE Average 0.00 +/- 0.00
Ions Per Particle
Anion 0.00 +/- 0.00
Cation 0.00 +/- 0.00
Other Outputs
final IE particle count 0
% particles used in calc 0
IE / AB 0.0000e+00
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

Individual Particle Time of Flight Traces

Update pToF traces **Graph in New Window** particle # -1 **Add to Blacklist**

Particle Summation Range
Baseline Range #1
Particle Arrival Range
Baseline Range

m/z 17
m/z 16
m/z 15
m/z 46
m/z 30

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

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

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 4182: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

Single Ion (bit*ns) 20

High 136

Selected Dm (nm) 40

Baseline #1 Range: Low 20

Co-Adds 1

High 59

Baseline #2 Range: Low 189

Minimum IPP for Anion 2

High 204

Min IPP for All Traces -99

Do It!

Outputs

IE Average

6.99e-08 +/- 1.73e-09

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

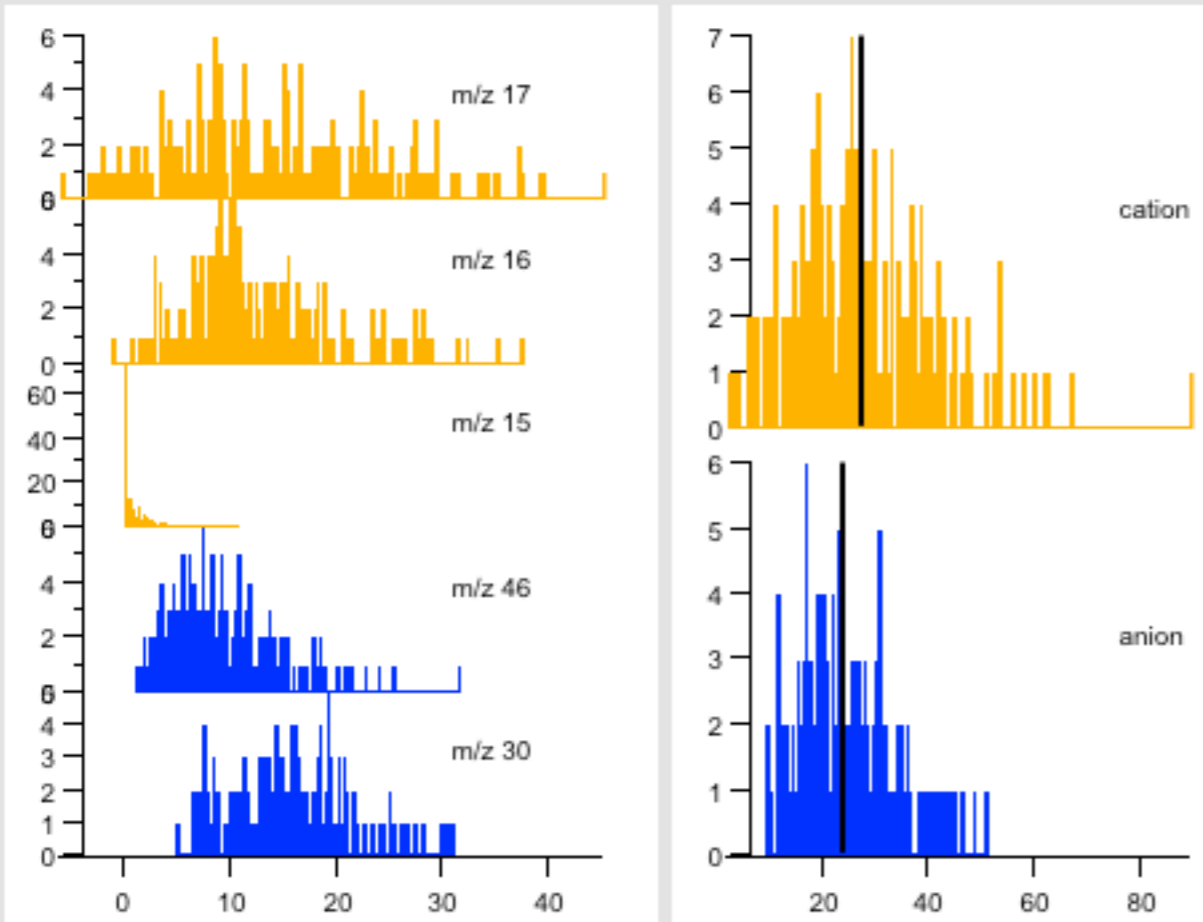
View Calc Inputs

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.

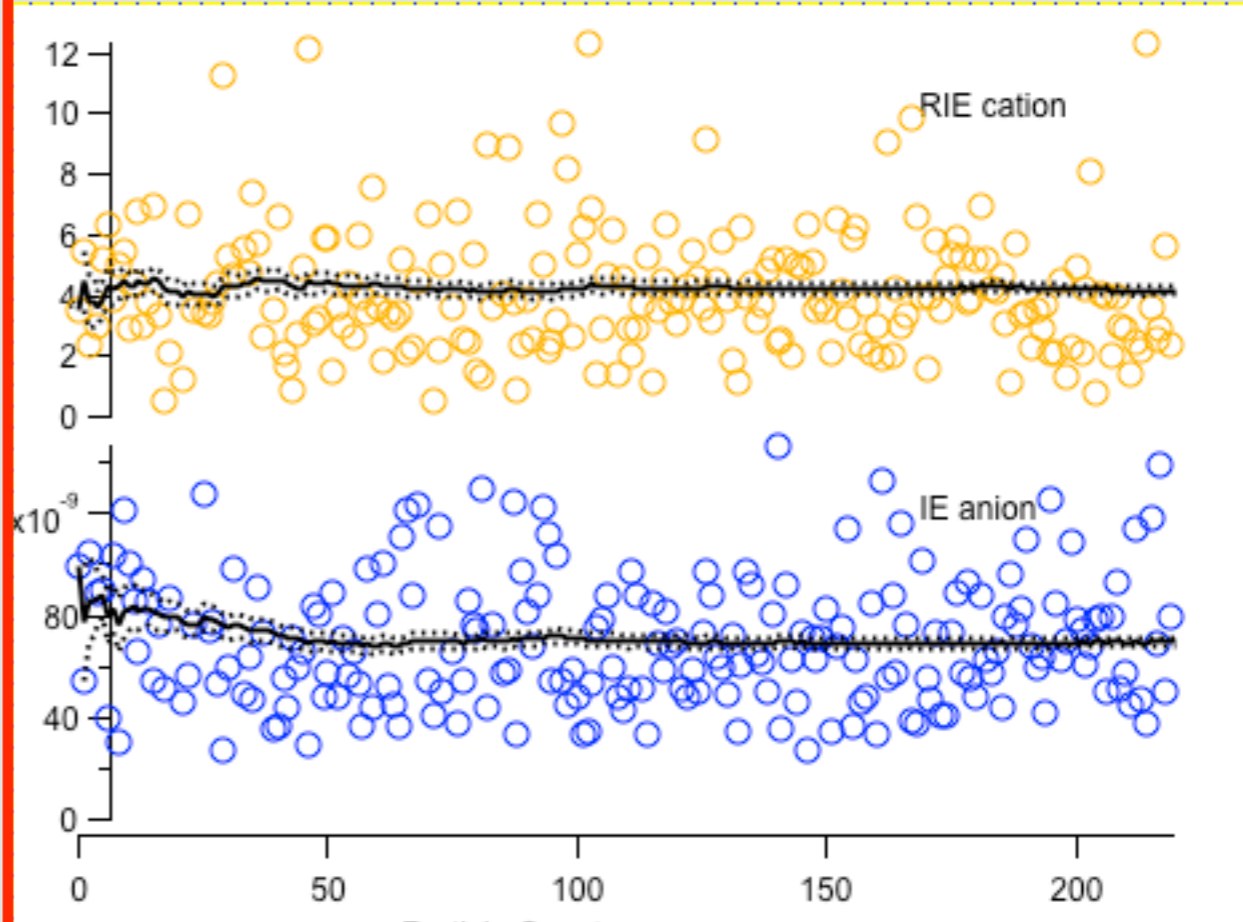
Histograms for Ions Per Particle

Graph in New Window



Average IE and RIE

Graph in New Window



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!
- $IE_{DAQ} = IE_{Meas} * \text{PulserPeriod}_{IE} / \text{PulserPeriod}_{Acq}$
- 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](#)