Ionization Efficiency Introduction

Sunday 13:45

Particle Mass Loadings Reported by the AMS require an Ionization Efficiency

From Mass Spectrometer
Ionization Efficiency calibration

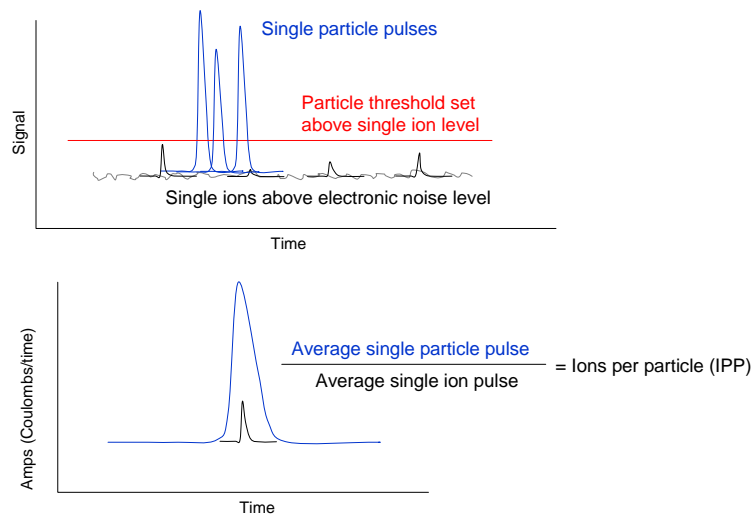$$\frac{mass}{volume} \implies \frac{\mu g}{m^3}$$

From volumetric flow rate

Ionization Efficiency Calibration
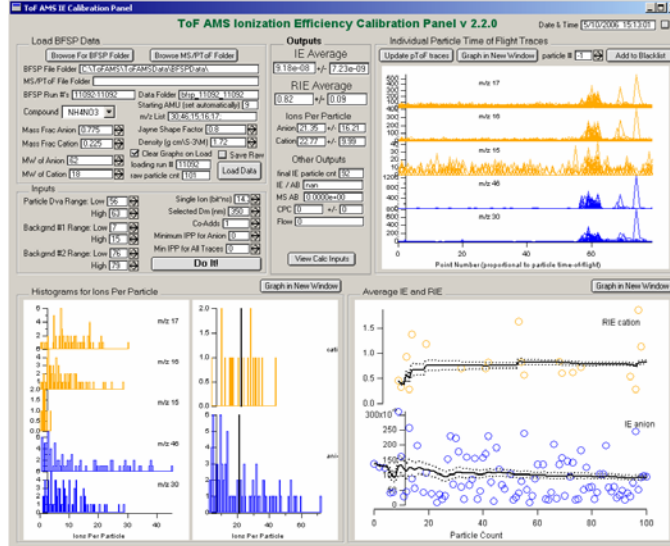
Currently there are two methods being used

1. DMA/CPC mass based method.
2. Single particle based method (BFSP).

Single Particle Based Mass Calibration
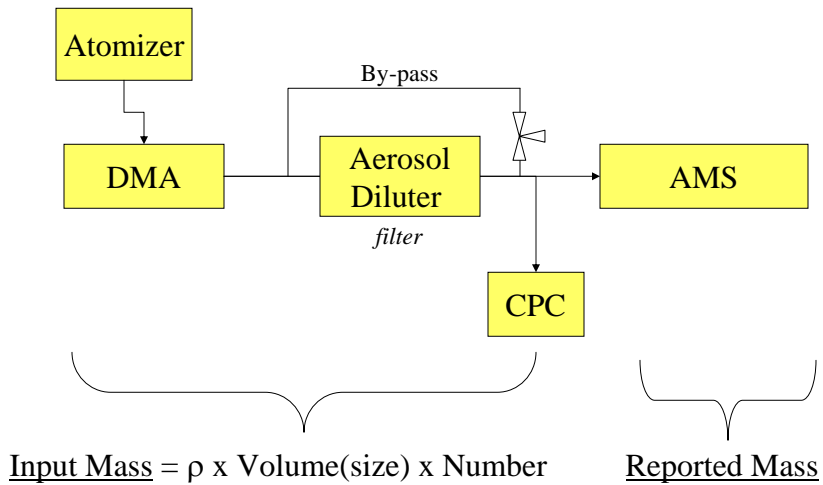

Ionization Efficiency = IPP/Molecules per Particle

BFSP Analysis Panel for IE Determination

Edward Dunlea

Setup for Mass Based IE Determination

Input Mass = ρ x Volume(size) x Number   Reported Mass

Plot Measured Mass vs Input Mass

Mass Based IE Determination

Mass Based IE Determination

Multiple charged diameters
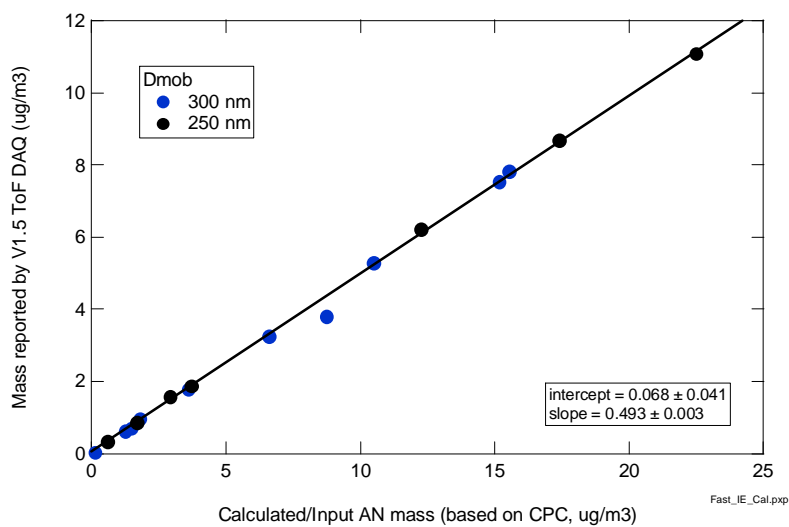
Lens transmission limitation
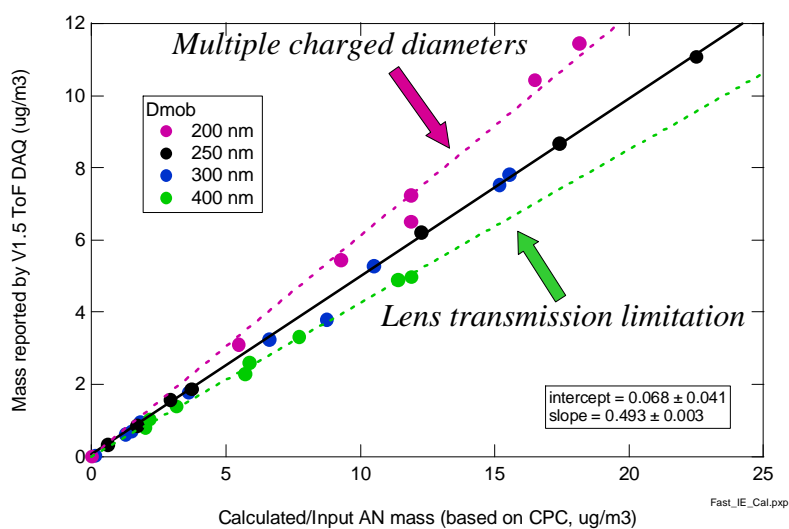
Need to consider fragmentation pattern for NH$_4$NO$_3$

Comparison of Mass and CPC Based Ionization Efficiency Determination

Method	Advantages	Disadvantages
CPC/Mass	Multiple point calibration	Requires a CPC and a DMA
	Better precision	Lens transmission consideration
		Multiple charged DMA diameters
Single Particle	Does not require a CPC	Single point calibration
	Not dependent on lens transmission properties	Breaks down in the limit of low IPP
	Not dependent of multiple charged diameters exiting DMA	
	Could be performed without a DMA	
	Velocity selector?	

Ionization Efficiency Calibration Tutorial for the ToF-AMS

Roya Bahreini
AMS Users Meeting- 2007

Thanks to: Ed, Pete, James, Ken, Ingrid, Dara, Qi, Shane, Ann, John, Jose, Tim, Doug…

The purpose → Quantification!!!
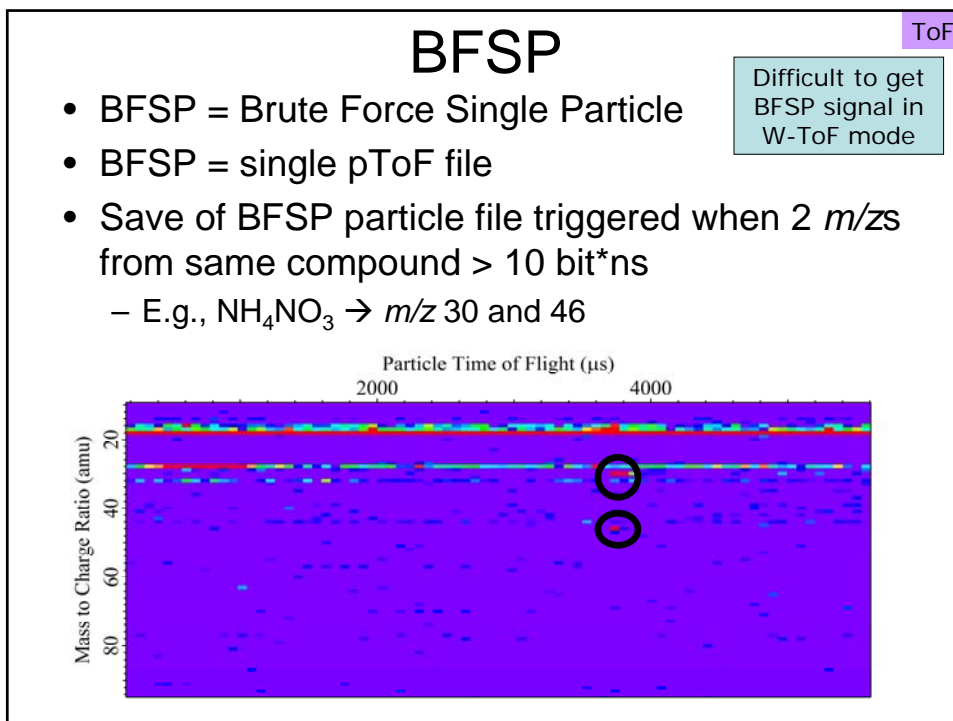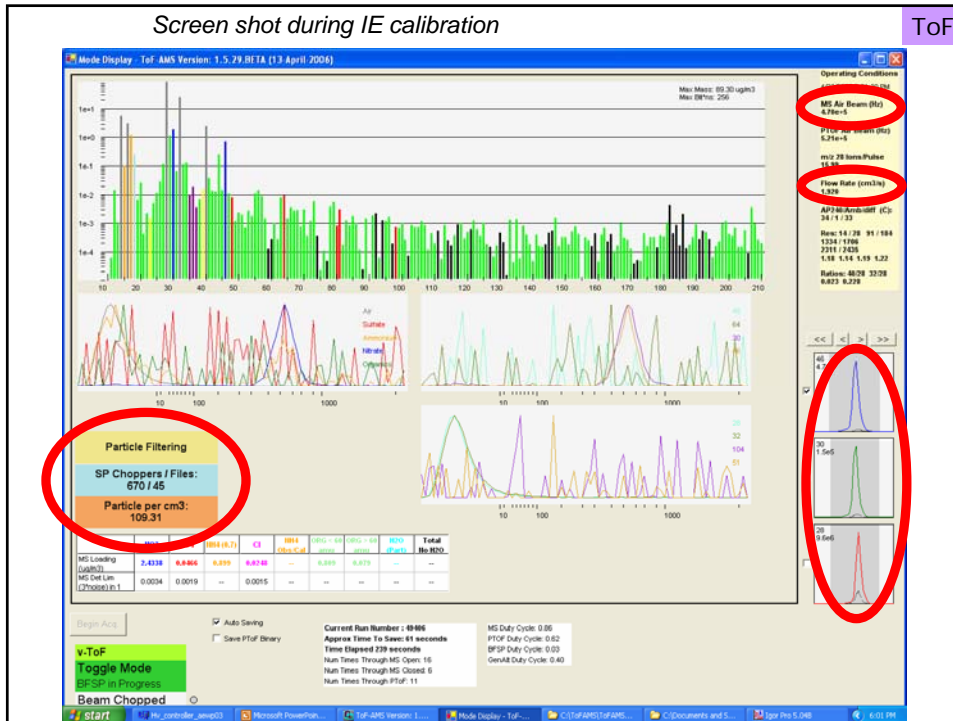
Acquisition Software Parameter Menu

Set timing to include PTOF, MS and BFSP data

Menu switching off

Set BFSP filters
• Filter for particles
• Chemical species filtering

ToF-AMS Data Acquisition Software

Version: 1.7.0.BETA (16-Sept-2006)

Copyrighted by P.F. DeCarlo, J.R. Kimmel, J.L. Jimenez,
M. Canagaratna, J.T. Jayne, D.R. Worsnop 2004-2006

9/17/2006 10:45:22 AM

Researchers Operating: Joel Kimmel
Experiment Being Conducted: AMS Users Meeting

Parameters
Parameter Menu | Default Settings

Measurement Modes
Particle-Time-of-Flight (PTOF) | Mass Spectrum (MS) | BFSP | General Alternation (GenAlt)

Diagnostic and Tuning Windows
m/z Calibration | Servo Movement | Threshold Analysis | m/z Ratio Diagnostics

9/17/2006 10:43:17 AM: Software Started
9/17/2006 10:43:17 AM: Menu 1 Loaded
9/17/2006 10:43:17 AM: Menu 2 Loaded
9/17/2006 10:43:17 AM: Menu 3 Loaded
9/17/2006 10:43:17 AM: Menu 4 Loaded
9/17/2006 10:43:17 AM: Menu 1 to TPS-RC
9/17/2006 10:43:17 AM: Exact mass file loaded.
9/17/2006 10:43:17 AM: Heater Bias set to 5.60 V
9/17/2006 10:45:14 AM: Menu 1 to TPS-RC

Means that MS and BFSP data will have same run number

Screen shot during IE calibration

BFSP

Difficult to get BFSP signal in W-ToF mode

- BFSP = Brute Force Single Particle
- BFSP = single pToF file
- Save of BFSP particle file triggered when 2 *m/z*s from same compound > 10 bit*ns
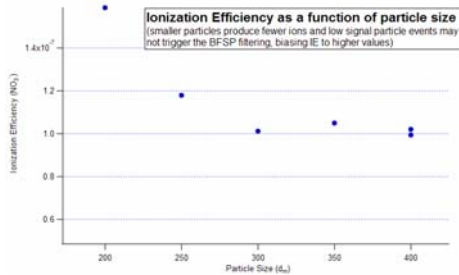 - E.g., NH_4NO_3 → *m/z* 30 and 46

BFSP Software Versions

- Version 1 – Created by Roya Bahreini
- Version 2.0.1 - Created by Edward Dunlea
  - Making the panel
- Version 2.1.0 - Updates from Ed
  - Functional and cosmetic updates to panel
- Version 2.2.0 – Updates from Ed
  - More updates to panel
- **Version 3.0.4 – Critical updates from Ed**
  - **Inclusion of duty cycle correction to IPP calculation**
  - **Inclusion of proper definition of RIE**
  - **Must use this version of code or later**

Stop. Open Igor and go through panel.

IE as Function of Size and Pulser Period

Ionization Efficiency as a function of particle size
(smaller particles produce fewer ions and low signal particle events may not trigger the BFSP filtering, biasing IE to higher values)

- •Stable IE down to certain size particle
- •Threshold biases towards larger particles (higher IE)
- •Ion signal scales with pulser period

No Constraints Fit:
1.024e-07 ± 2.04e-09

Fixed 0 Intercept:
9.64e-08 ± 1.85e-09
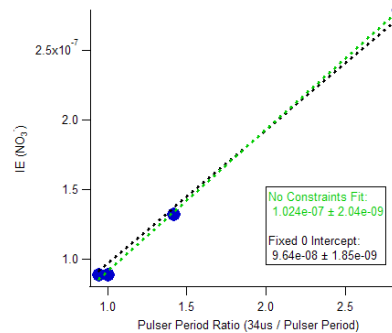
Recommendations

- All instruments
  - Monodisperse dried NH_4NO_3
- Q-AMS
  - Use of IE calibration window
- C-ToF-AMS & V-ToF-AMS
  - Record in BFSP
    - with same pulser frequency as your normal operation if using C-ToF
    - with higher pulser frequency if using V-ToF, but scale it with ratios of pulser frequencies during calibration and normal operation
  - Check with more than one particle size
    - Make sure no thresholding bias
  - Check IE using MS data with calibration particles
- W-ToF
  - Record in MS mode
  - As check, calibrate in V mode
    - Use ratio of AB in W and V modes

$$IE\ (W) = IE\ (V)\ \frac{AB\ (W)}{AB\ (V)}$$

**If you have questions, email Donna (donna.sueper@colorado.edu)
after you've read the "Readme file"!!**