AMS/ACSM
Ionization Efficiency Introduction

Tuesday May 9, 2017

14:00

Calibrations

How to convert mass spectrometric ion signals into meaningful quantities?

- Particle velocity-aerodynamic size
- Volumetric flow rate
- Ionization efficiency

AMS Reported quantity is particle mass loading

Particle Mass Loadings Reported by the AMS requires an Ionization Efficiency

From Mass Spectrometer
Ionization Efficiency calibration

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

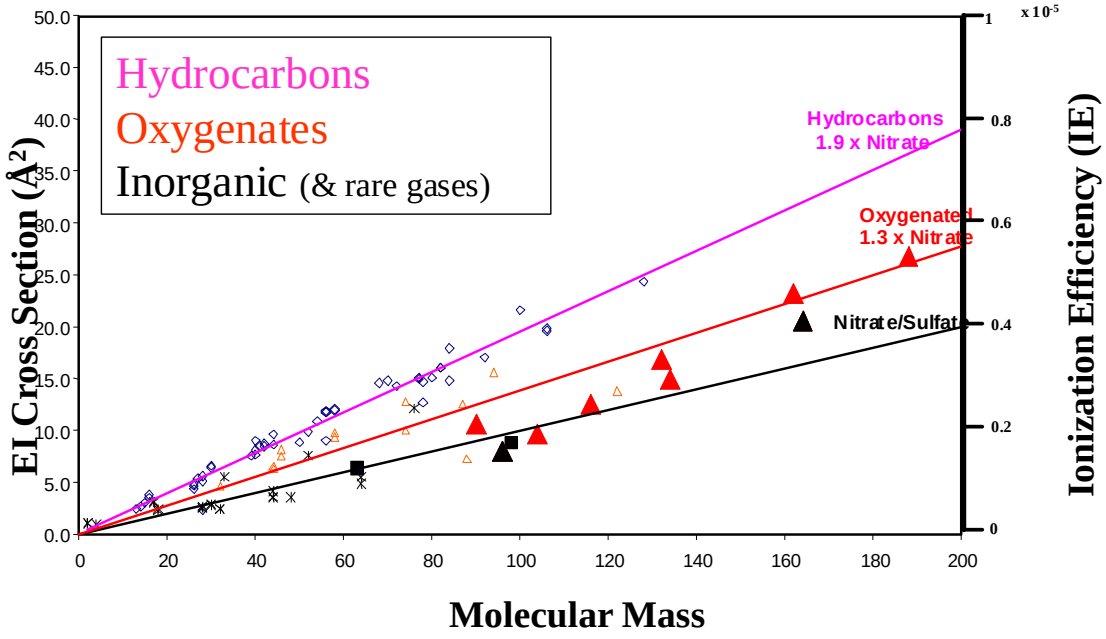
From volumetric flow rate

EI Ionization Cross Sections

$$A + e^{-}(70\ eV) \rightarrow A^{+}$$

Mass Loading A $\propto (MW_A/IE_A) \sum$ **(all Ion Signals)**

Calibration Factor $*(MW_{NO3}/IE_{NO3})$



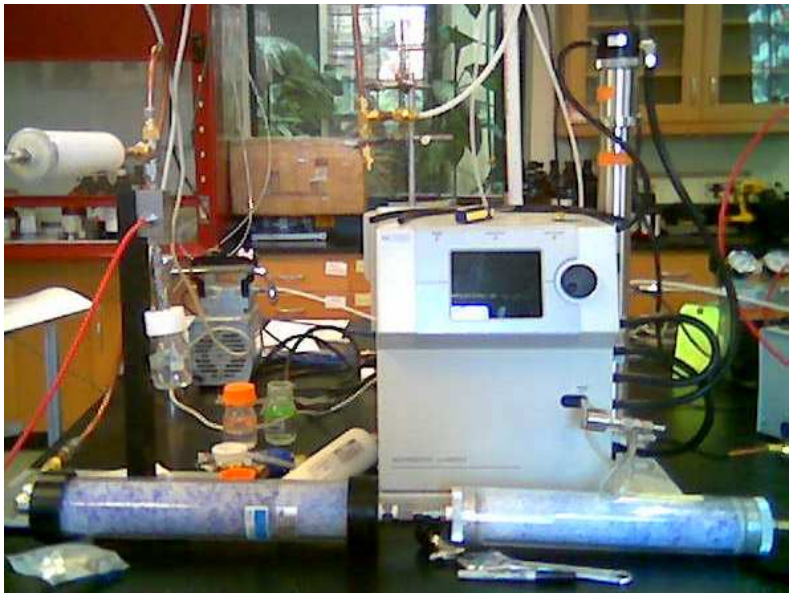
Determination of “Ionization Efficiency” IE Calibration

There are two methods:

1. DMA/CPC mass based method.
2. Single particle based method
   I. BFSP mode in V4 DAQ
   II. Event Trigger mode in V5 DAQ

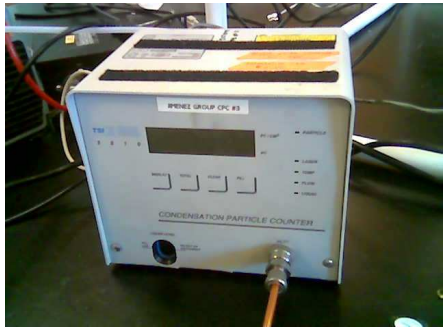
- ACSM systems are calibrated using the mass based method
- AMS systems can be calibrated using either method

Typical Calibration Set Up



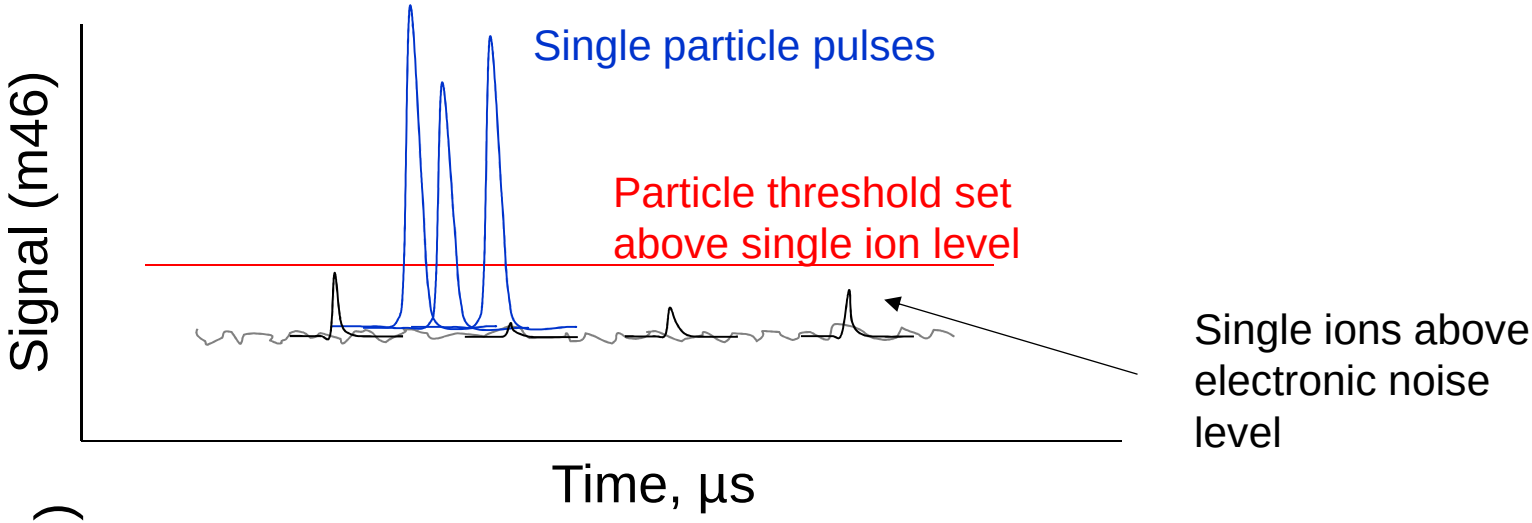
Requires:

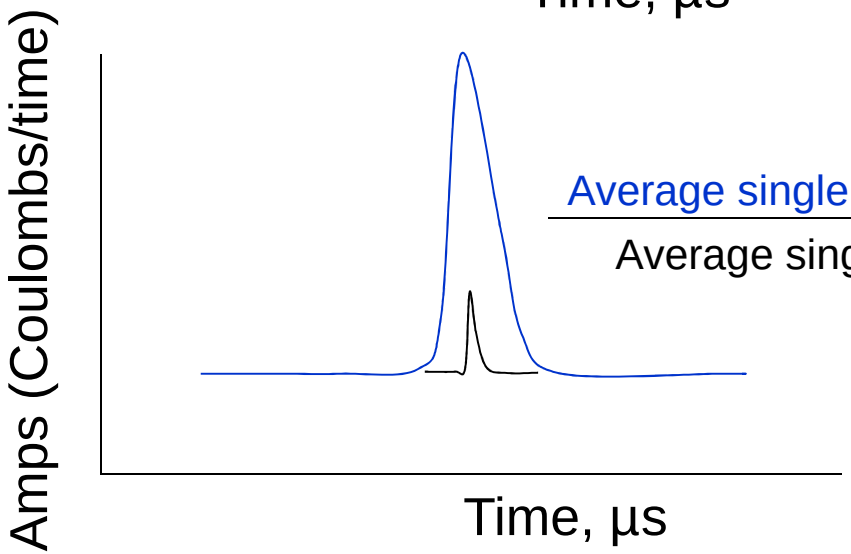
- Atomizer/dryer
- DMA
- CPC



CPC

Single Particle Based IE Calibration

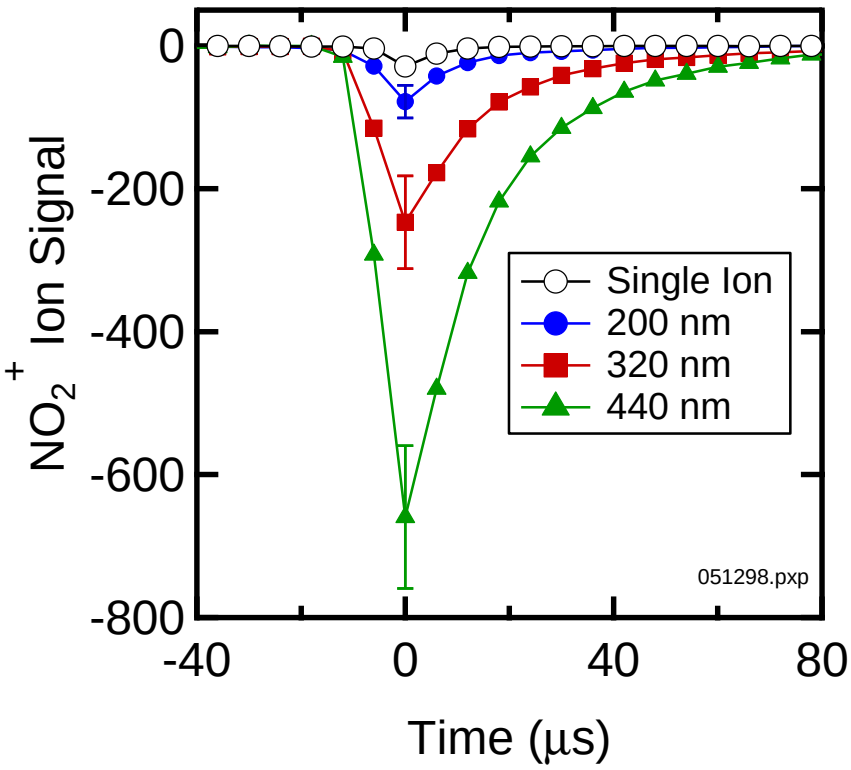


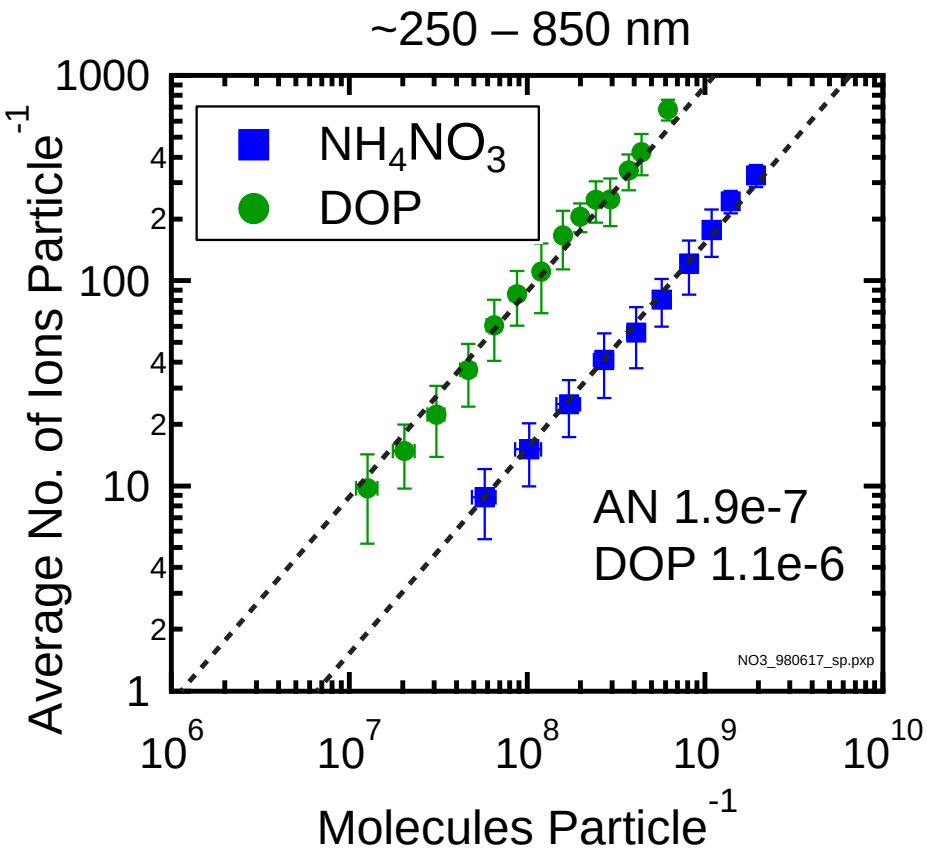


$$\frac{\text{Average single particle pulse}}{\text{Average single ion pulse}} = \text{Ions per particle (IPP)}$$

Ionization Efficiency = IPP / Molecules per Particle

Average Single Particle Signals





For Details on SP Based IE Calibration See Presentation from 2006 AMS Users Meeting

Ionization Efficiency Calibration Tutorial for the ToF-AMS

AMS Users Meeting
September 17, 2006
Edward Dunlea, University of Colorado

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

The purpose → Quantification!!!

General page: http://cires.colorado.edu/jimenez-group/UsrMtgs/

Ipf: http://cires.colorado.edu/jimenez-group/UsrMtgs/UsersMtg7/ams_tof_ie_calibration_v3.0.4.ipf

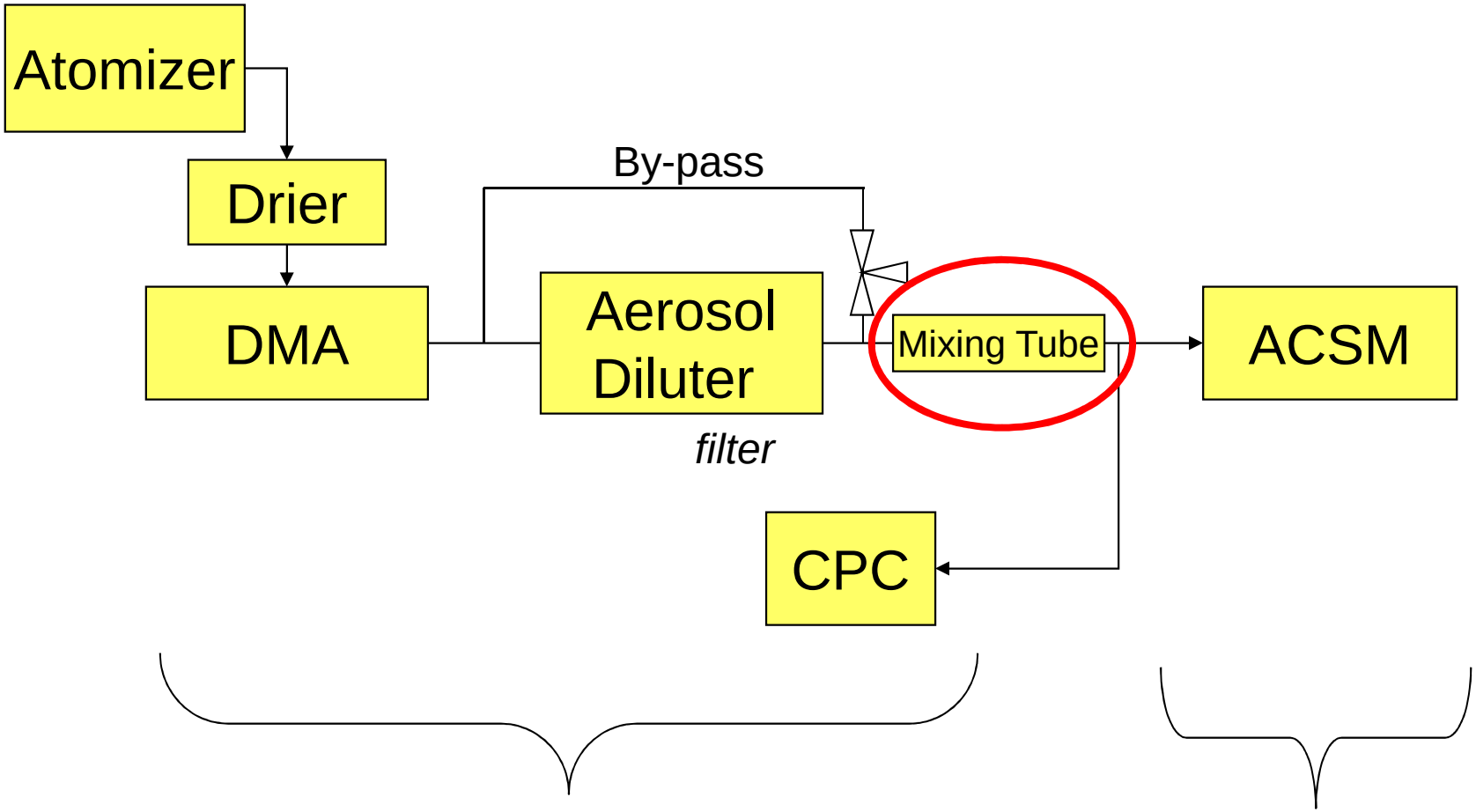
Data: http://cires.colorado.edu/jimenez-group/UsrMtgs/UsersMtg7/IE_tutorial_sample_data.zip

In DAQ 5 we now use Event Trigger Mode for Single Particle based IE cal.

Donna and Joel will mention this later in this meeting.

http://cires1.colorado.edu/jimenez-group/wiki/index.php/AMSUsrMtgs#7th_AMS_Users.27_Meeting

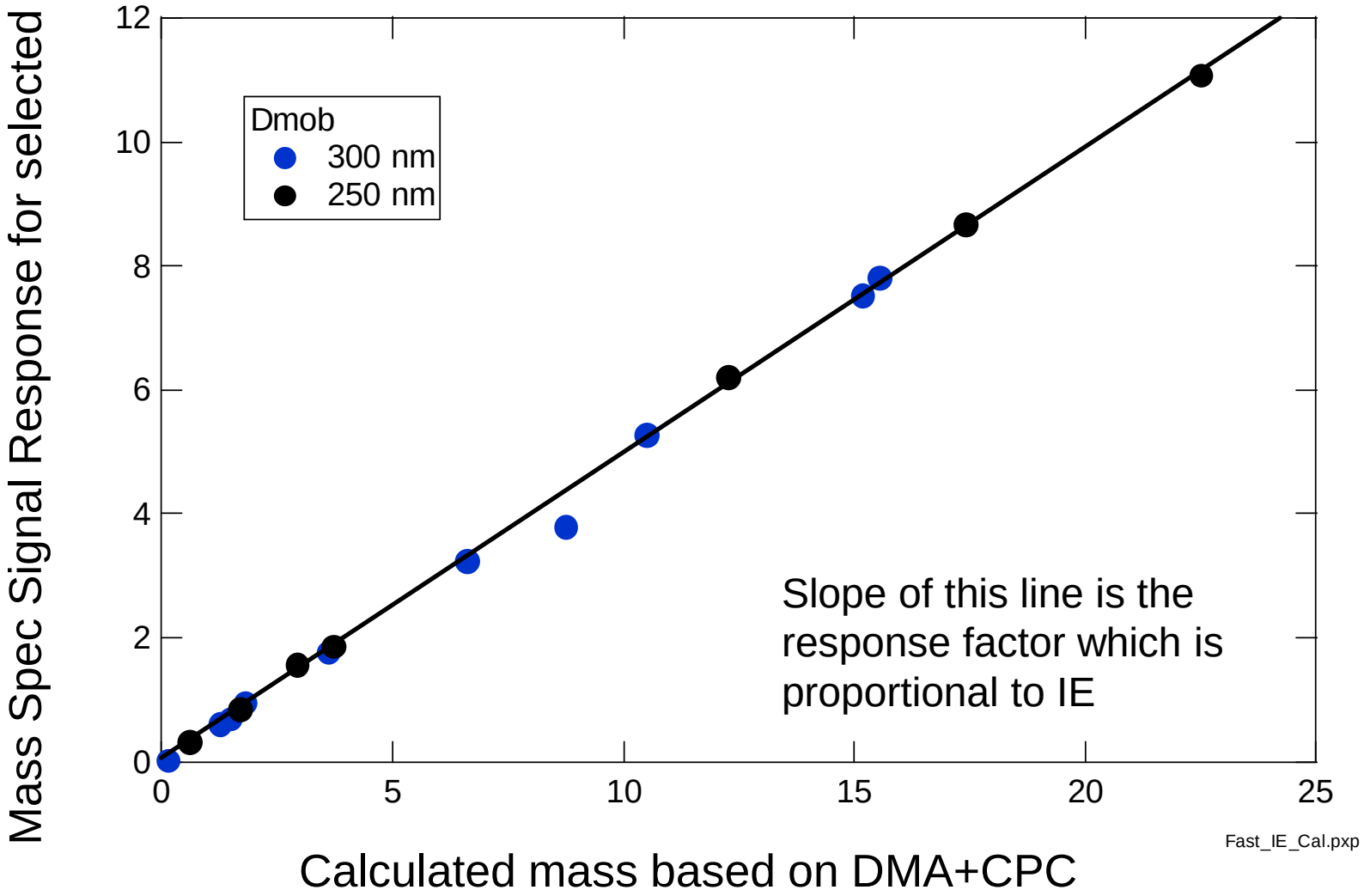
Setup for Mass Based IE Determination



<u>Input Mass</u> = ρ x Volume(size) x Number <u>Reported Mass</u>

Plot Measured Mass vs Input Mass

Mass Based IE Determination



ACSM Mass Based Calibration

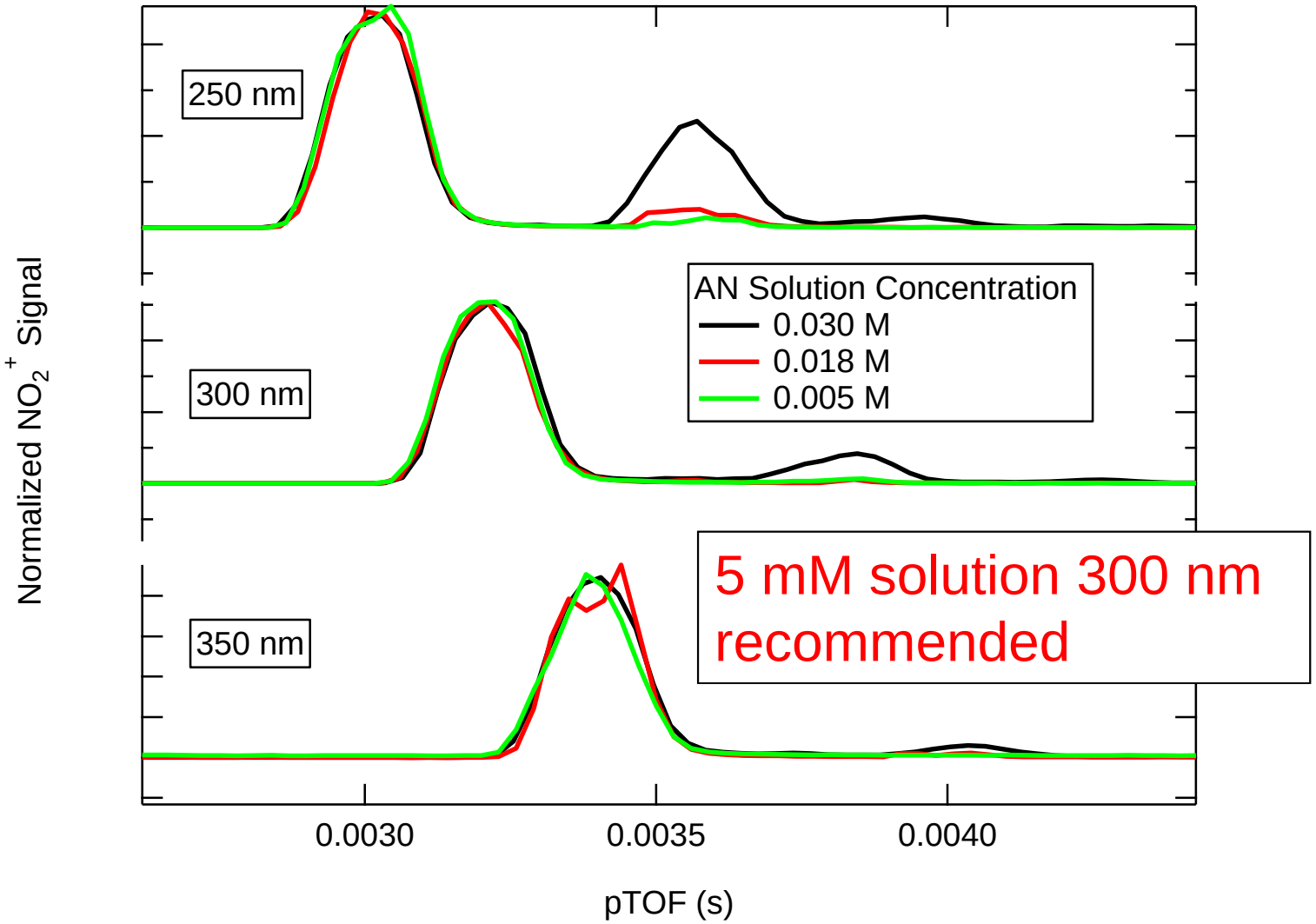
The ACSM response is calibrated using the mass based method

There are two practical concerns:

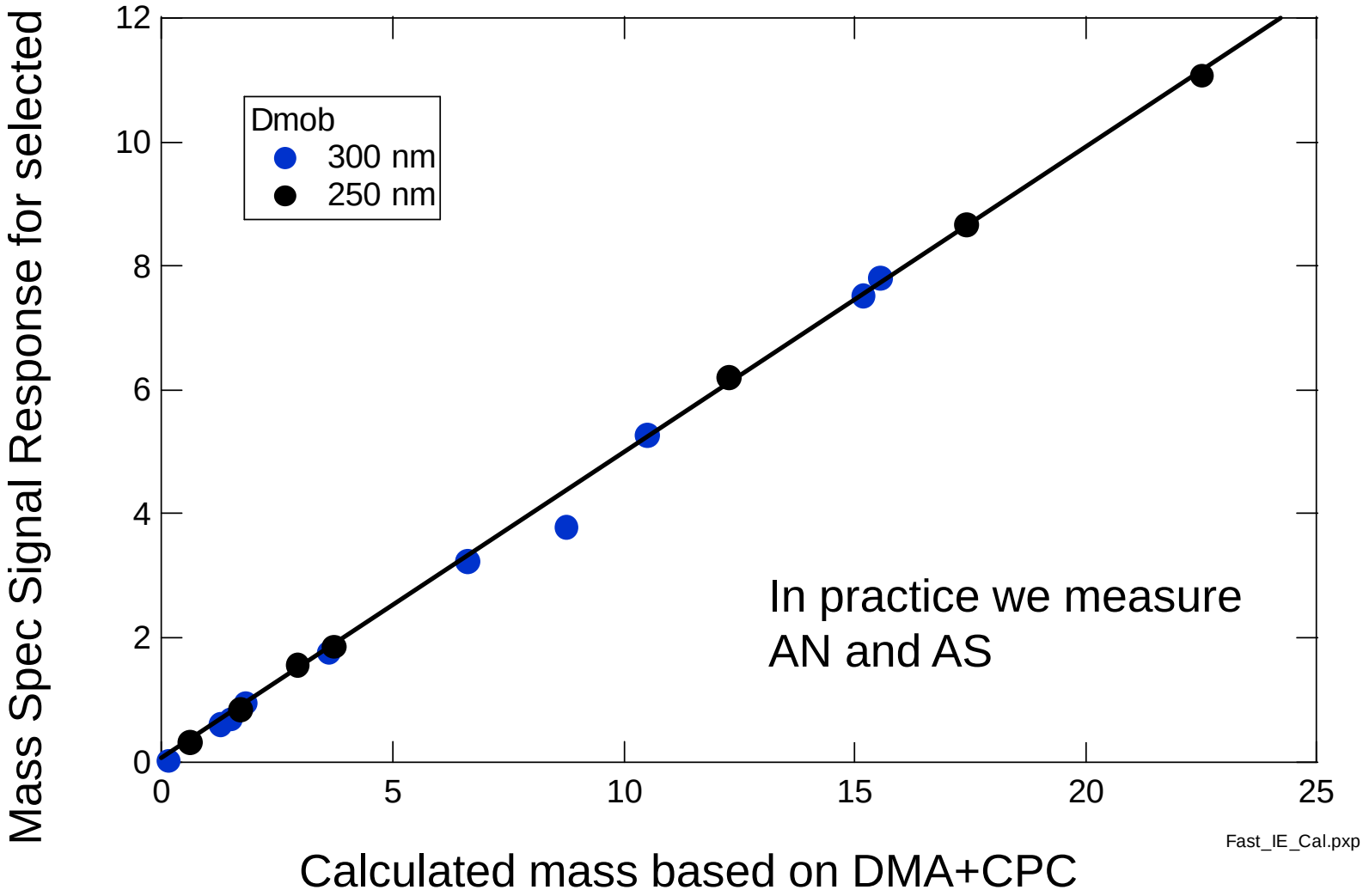
1) the primary DMA size selected should not be larger than 350 nm, 300 nm is suggested. This is to avoid particle loss due to limited transmission in the aerosol (standard) lens system.

2) One must be careful about the atomizer solution concentration. Too high a concentration can result in a significant mass at the higher charged diameters (Q2, Q3 etc.) NH_4NO_3 solution concentration of 0.005M (molar) is recommended.

Minimize multiple charged mobility diameters by decreasing NH_4NO_3 atomizer concentration

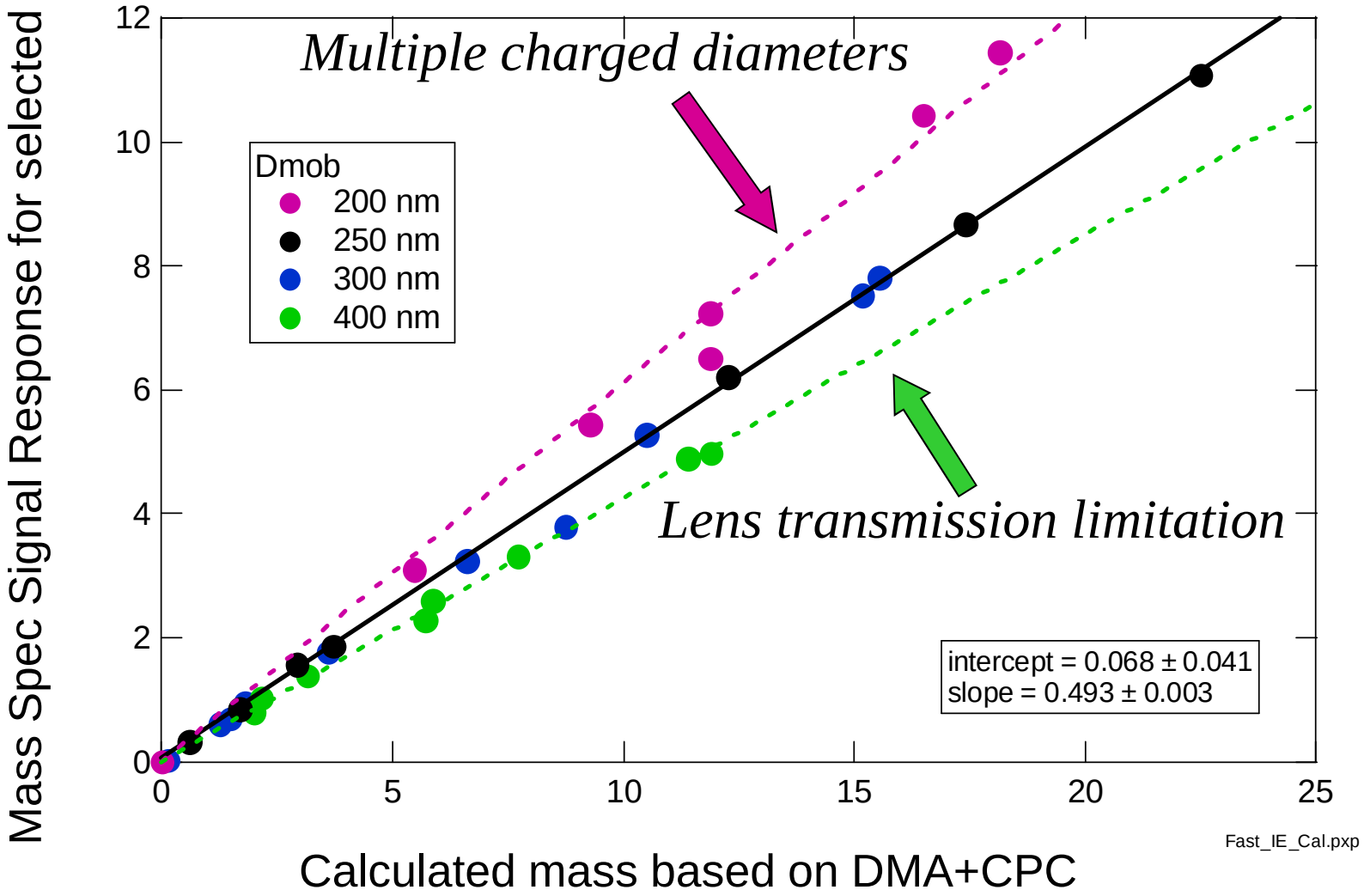


Mass Based IE Determination



Need to consider fragmentation pattern for NH_4NO_3

Mass Based IE Determination



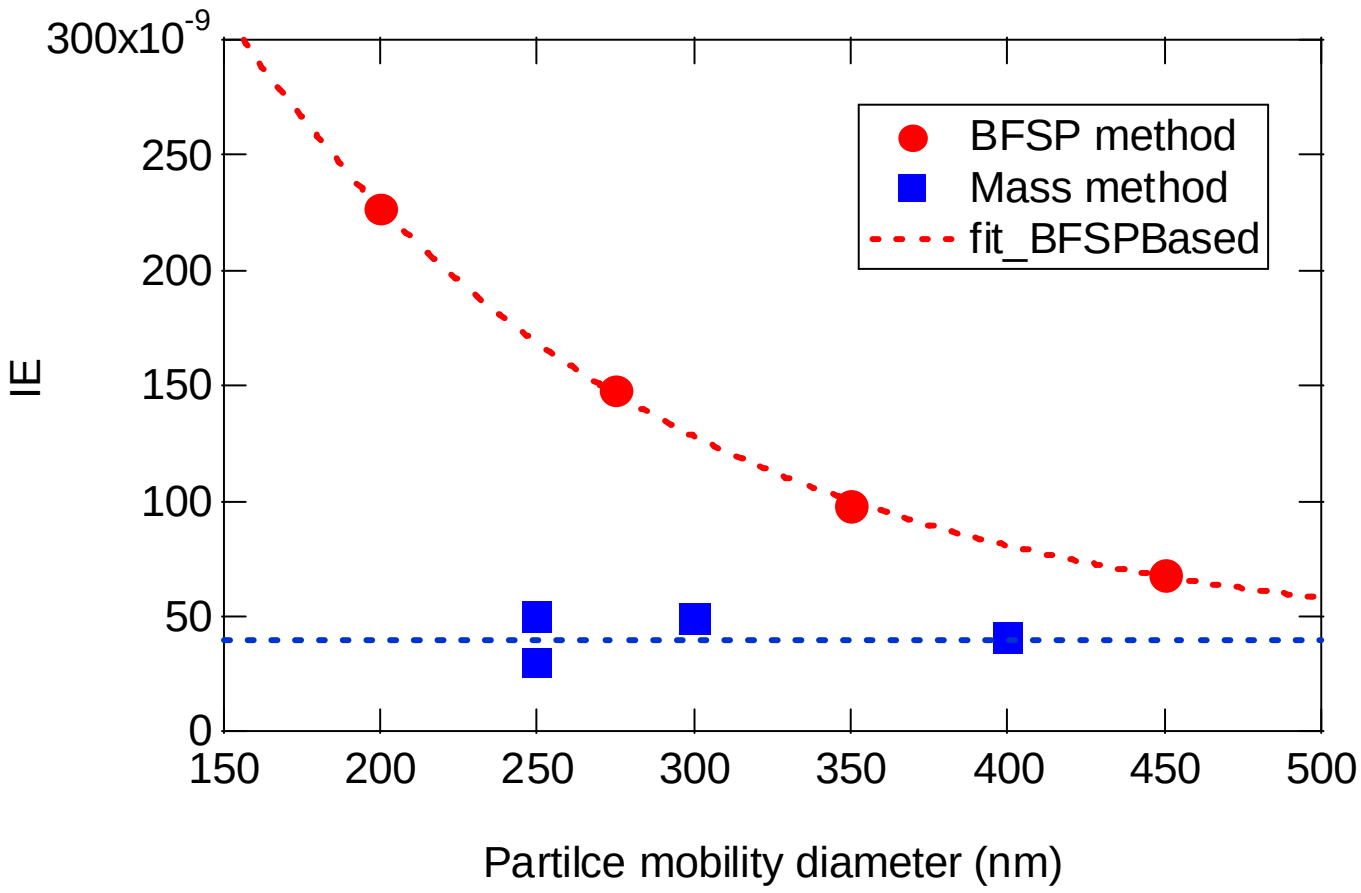
Comparison of Mass and CPC Based Ionization Efficiency Determination

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	Difficult for species that produces many ions (ie, organics)
	Could be performed without a DMA	

END

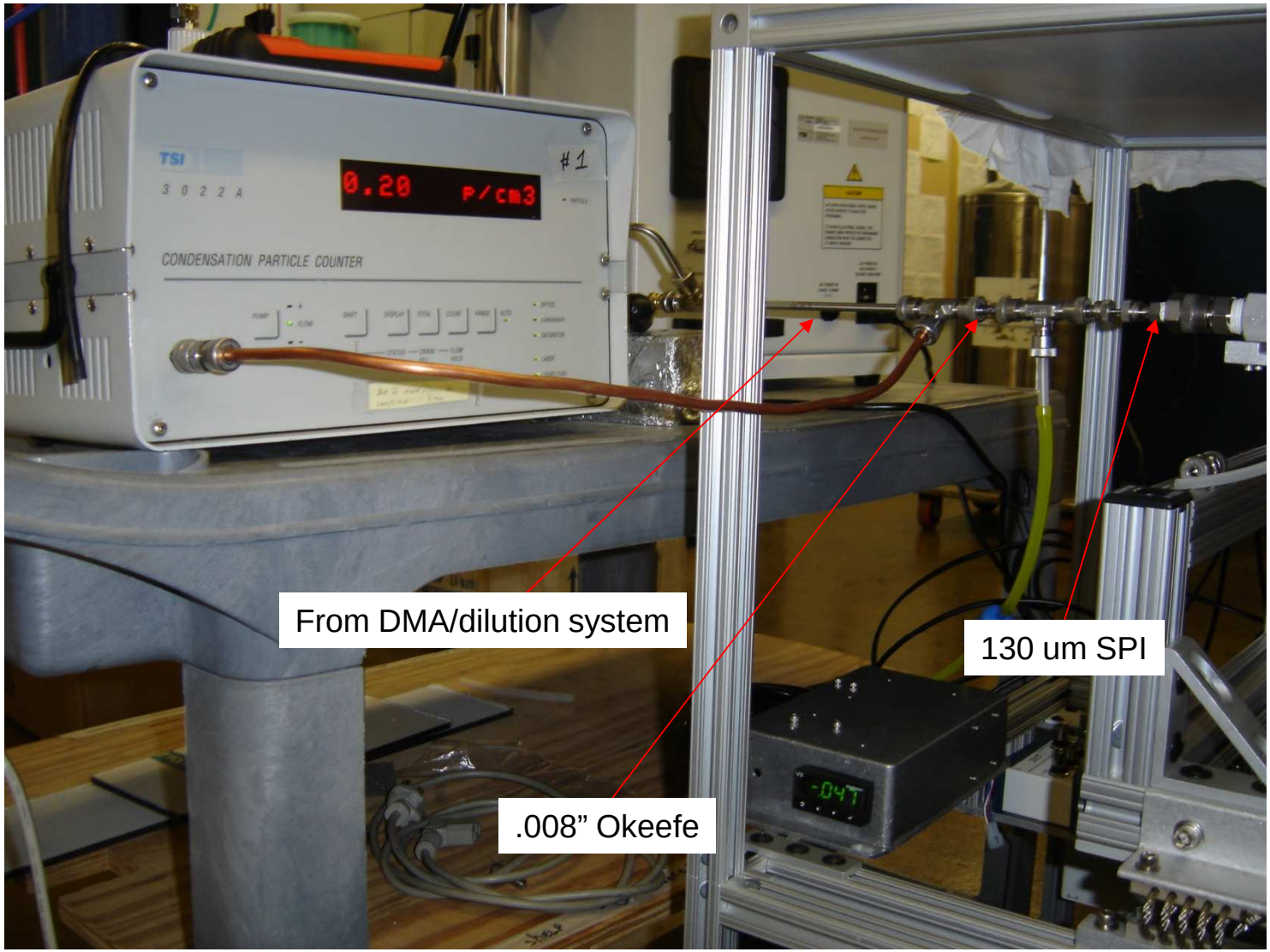
IEs Measured by Harvard Group wTOF AMS

J. Shilling, Qi Chen - Ver2.2.0 May 2006

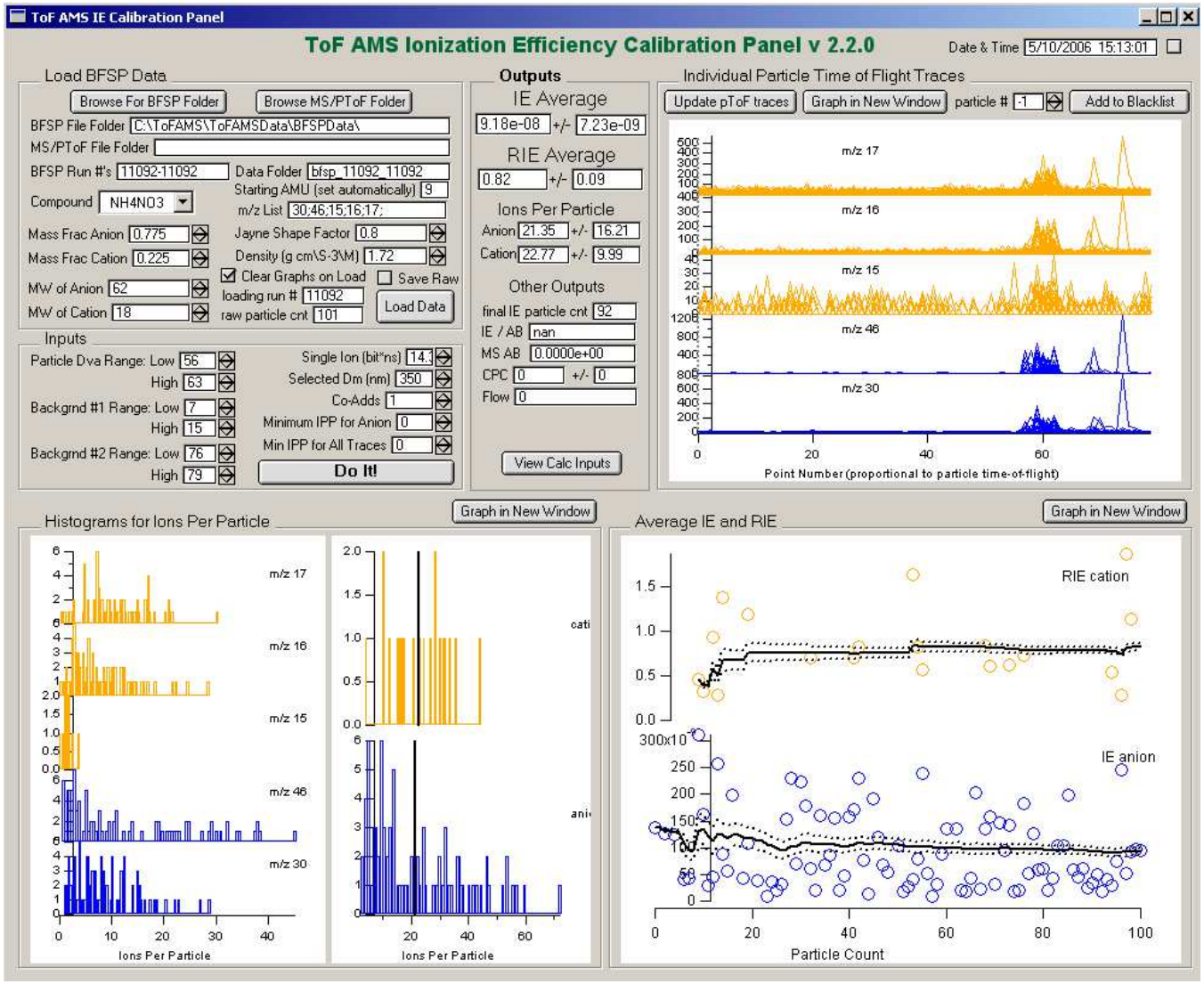


Aerosol transmission tests were performed using this plumbing arrangement.

QAMS, standard lens, 215 series chamber.



BFSP Analysis Panel for IE Determination



Edward Dunlea

Slide of SP signals from Igor plot
D:\Igor\SP_Data

D:\IgoDOS_Single.pxp
NO3_051298.pxp AN data
NO3_980617_sp.pxp use this