AMS/ACSM Calibration Protocols

The Aerodyne Team
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Outline

Primary calibrations to quantify aerosol mass loading and size*

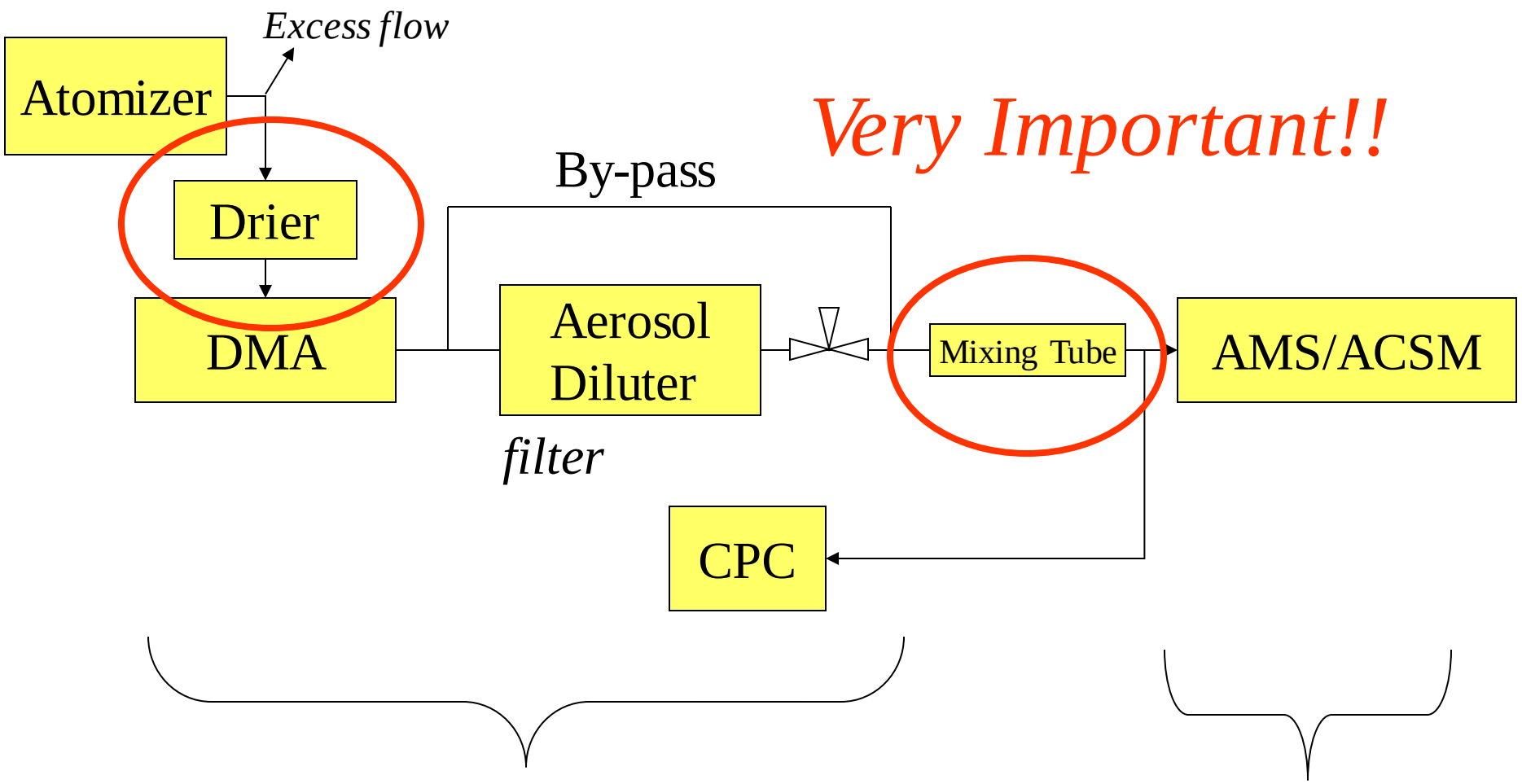
- IE and RIE Calibrations (AMS and ACSM)
  - Anita will talk about SP-AMS calibration on Wednesday 1/20/2021.
- Velocity calibration – particle time-of-flight to size (AMS)
- Vaporizer temperature calibration (AMS)

*After your instrument is well-configured (lens aligned, MS tuned, gain measured, flow rate calibrated). CU Boulder group working on manuscript on detailed procedures. See Ben's talk later today.

Ionization Efficiency for NO3 (IE_NO3)

- How to go from ions/s (what we measure) to mass loading (μg/m3).
- Mass-based method – compare MS signal to mass of particles sampled.
- Use NO3 from NH4NO3 for IE because
  - Vaporizes completely at 600 – 650 C
  - Doesn't bounce, particles well-focused by aerodynamic lens
  - Creates only two main ions (NO^+ at m/z 30 and $NO2^+$ at m/z 46)
  - Readily soluble in water, not especially hazardous
- Requires equipment
  - Atomizer to generate particles + dryer to remove water
  - DMA to size-select
  - CPC to count particles
  - New compact calibration module coming soon – see Phil's talk Wednesday 1/20/2021!

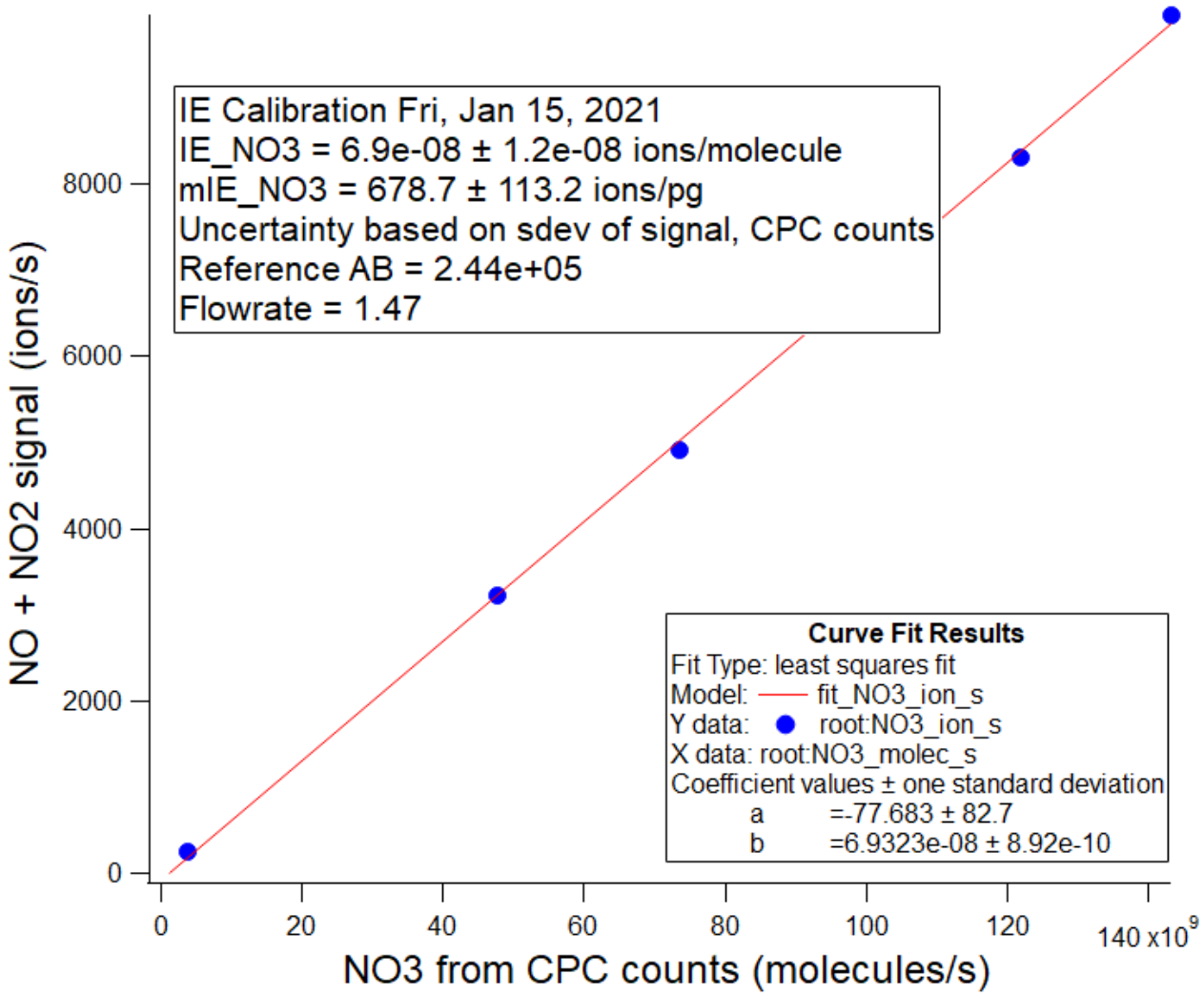
Setup for Mass-based IE Calibration



<u>Input Mass</u> = Eff. Density x Volume(size) x Number

<u>Instrument Response</u>

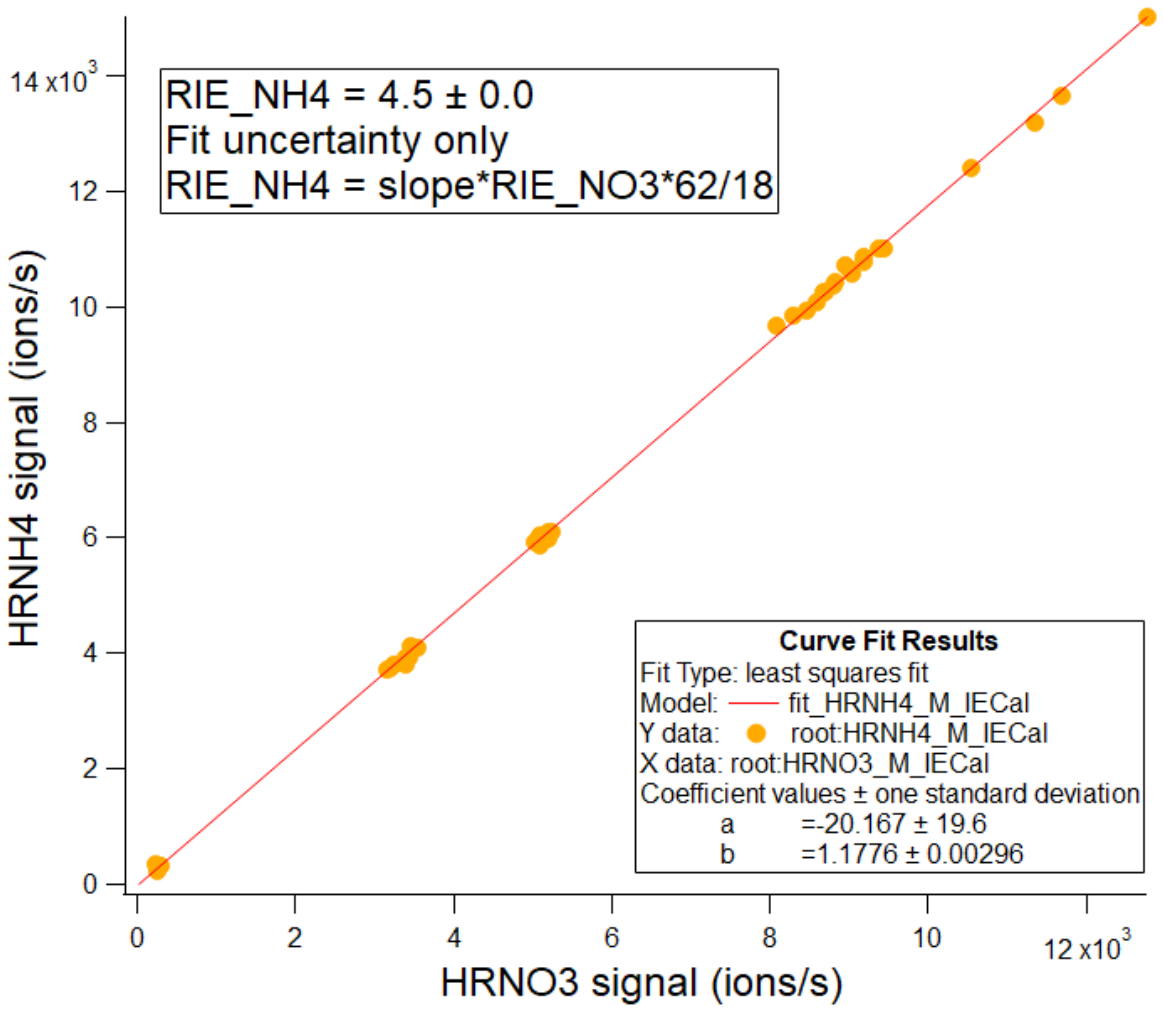
IE_NO3 Calculation with 300 nm NH4NO3, multiple concentrations



- Use mass loading similar to expected measurement, e.g., 0 – 20 μg/m3 NO3.
- IE Calibration units
  - Ions/molecule for AMS
  - Ions/pg for TOF-ACSM
  - Amps/(μg/m3) for Q-ACSM
- IE Analysis
  - Manual for AMS (in Squirrel or Pika)
  - Integrated in DAQ for ACSM
- Measure IE (and AB) at one point in time
  - Correct for variations in detector sensitivity (e.g., aging, temperature of instrument) with measured AB.

IEandVelCal_18Dec2020.pxp

Bonus! Relative Ionization Efficiency for NH4 (RIE_NH4)



- NH4NO3 also gives RIE_NH4
- Acquire and analyze IE and RIE calibration data in the SAME way as your regular data acquisition
  - If you will do HR analysis on HR-AMS data, then analyze IE and RIE data in Pika.
- If NH4 vs NO3 is very noisy, you might have a high background of water interfering with NH4. Wait a few days and try again.

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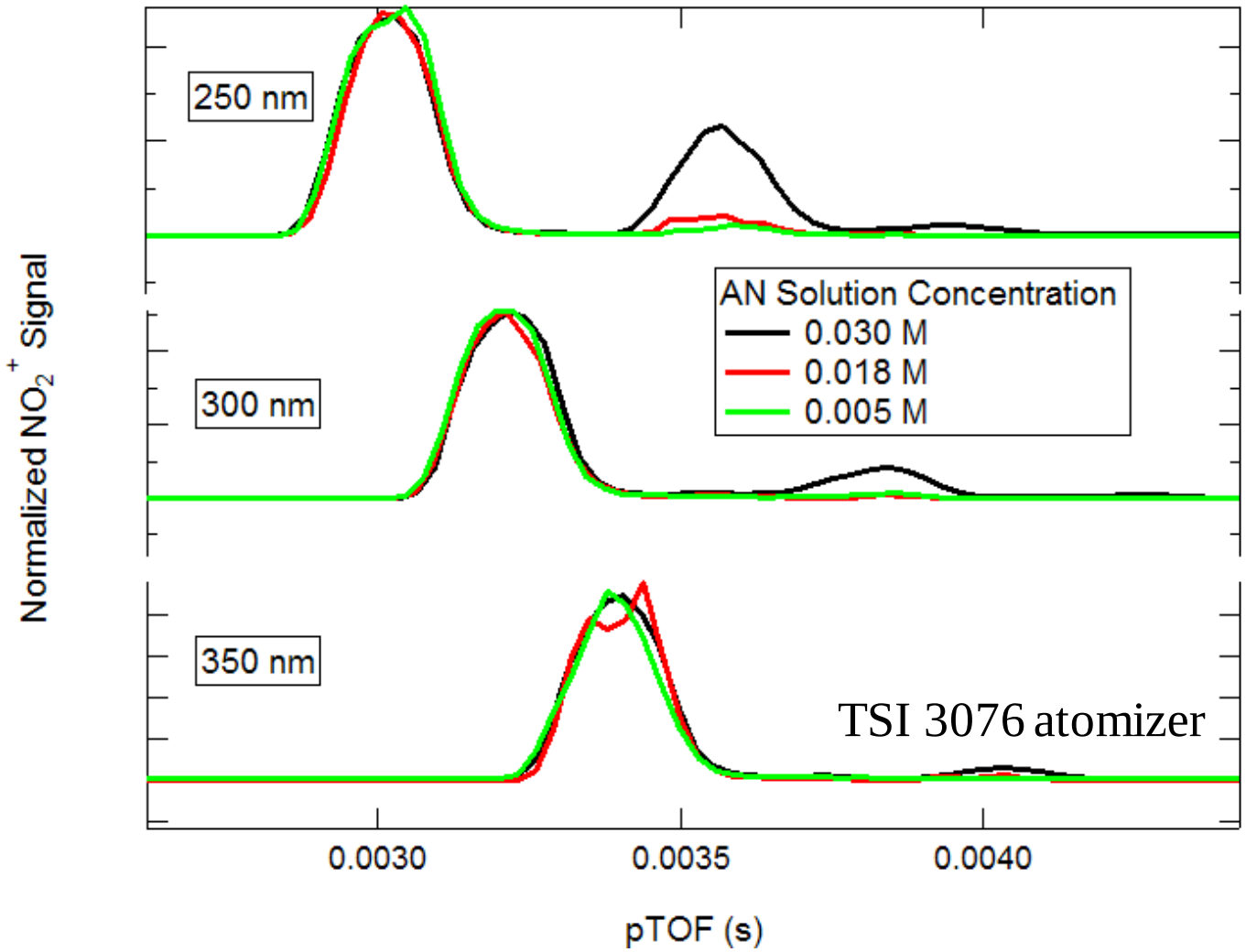
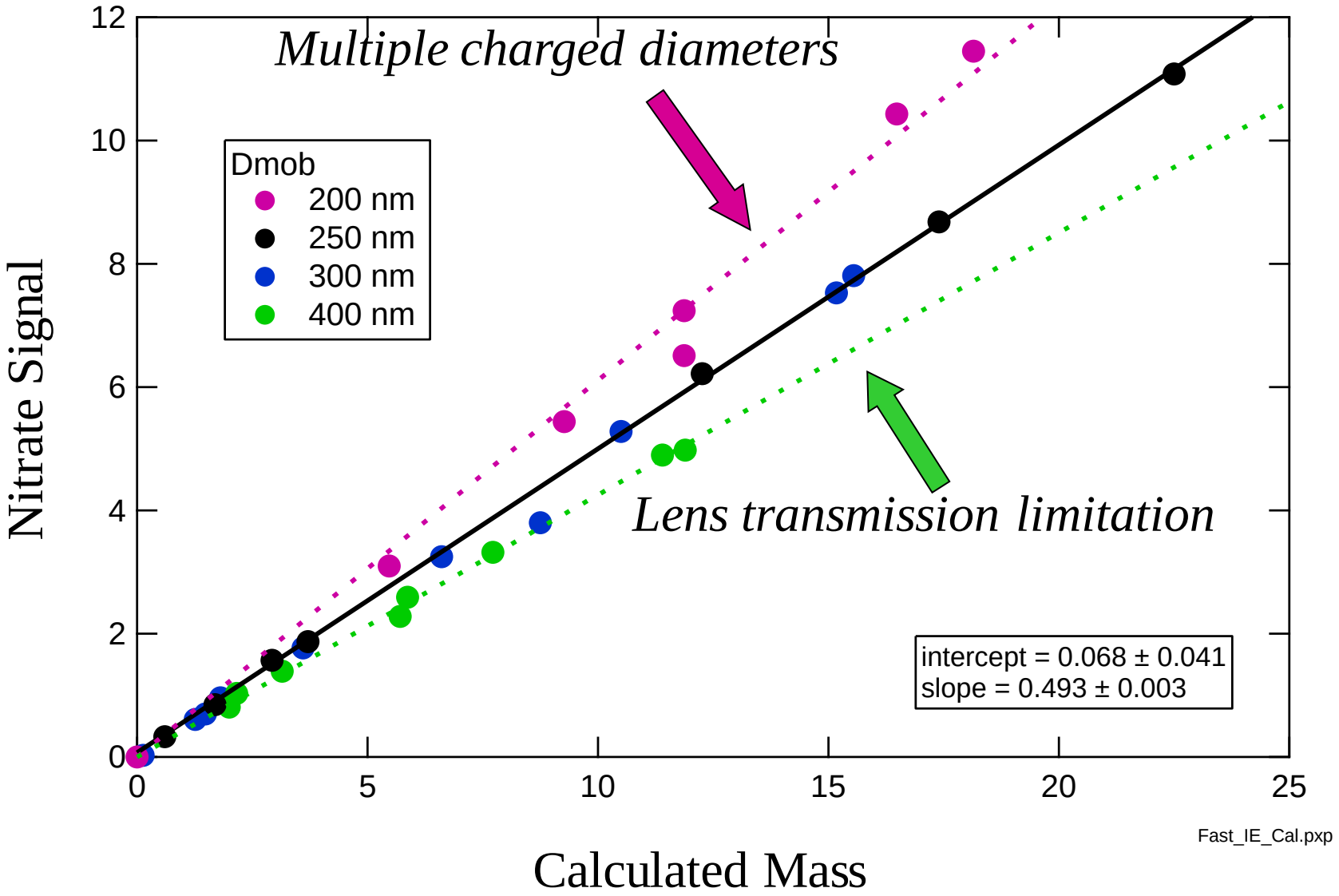
Note About Particle Size and Solution Concentration

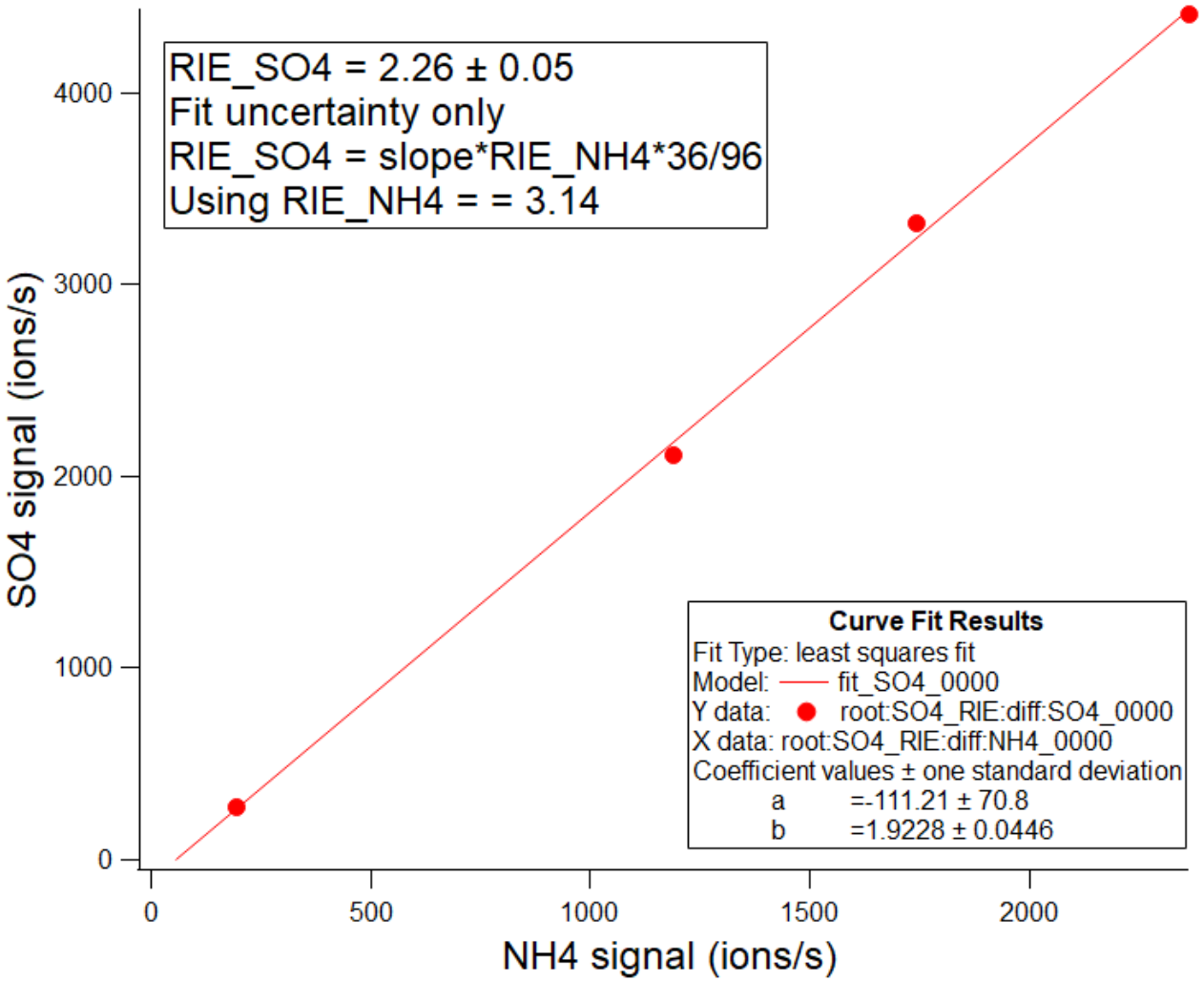


- 300 nm / 5 mM.
- Want to avoid Q2 particles from DMA (~ twice the mass, but only count as 1 particle).
- In AMS, can remove Q2's in analysis based on pToF.
  - Cannot remove Q2's in ACSM data.
- Aim for maximum of 1,000 p/cc at 300 nm (with TSI 3076 atomizer).

Use 300 nm NH4NO3 Particles!

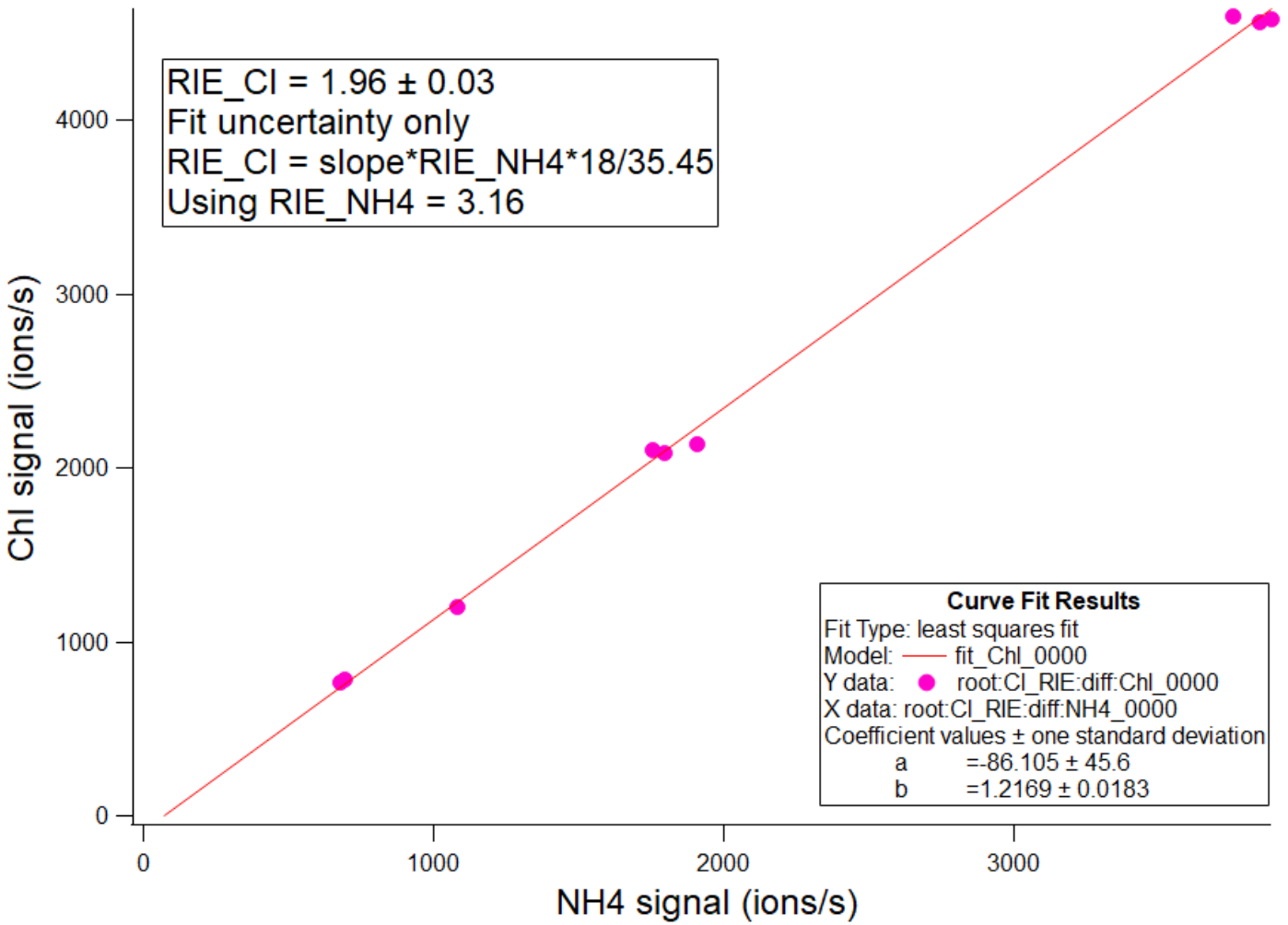


Do Measure RIE_SO4 for Your Instrument!



- Use size-selected (NH4)2SO4 particles.
- NH4 is internal reference, so CE does not matter.
- But make sure you have a good RIE_NH4 from NH4NO3 cal!
- Use similar mass loading to ambient.
- Default RIE_SO4 = 1.2 is not correct for many instruments.

Can measure RIE_Cl with NH4Cl Particles



- Use size-selected NH4Cl particles.
- NH4 is internal reference, so CE does not matter.
- But make sure you have a good RIE_NH4 from NH4NO3 cal!
- Use similar mass loading to ambient.
- Default RIE_Cl = 1.3 is not correct for many instruments.
- NOTE: NaCl has a different RIE_Cl! See Hongyu Guo's talk on Thursday 1/21/2021.

Single Particle IE Calibration (AMS only)

- Single particle method (record data when signal crosses a threshold)
  - Brute Force Single Particle (BFSP) (AP240 – old data card)
  - Event Trigger (ET) (ADQ – new data card) – Ben will talk more about this later.
- Always measure mass-based IE, too!
  - If they don't agree, trust the mass-based IE.
  - Pitfalls with getting enough signal per particle.
  - Only need ET IE measurement if taking ET data.
- Mass-based method only as good as your DMA and CPC
  - Spot check DMA sizing with PSLs.
  - Compare CPC to others.

Velocity Calibration (AMS only)

- How to go from particle time of flight (what we measure) to size (what we care about)
- Semi-empirical equation (somewhat meaningful parameters)

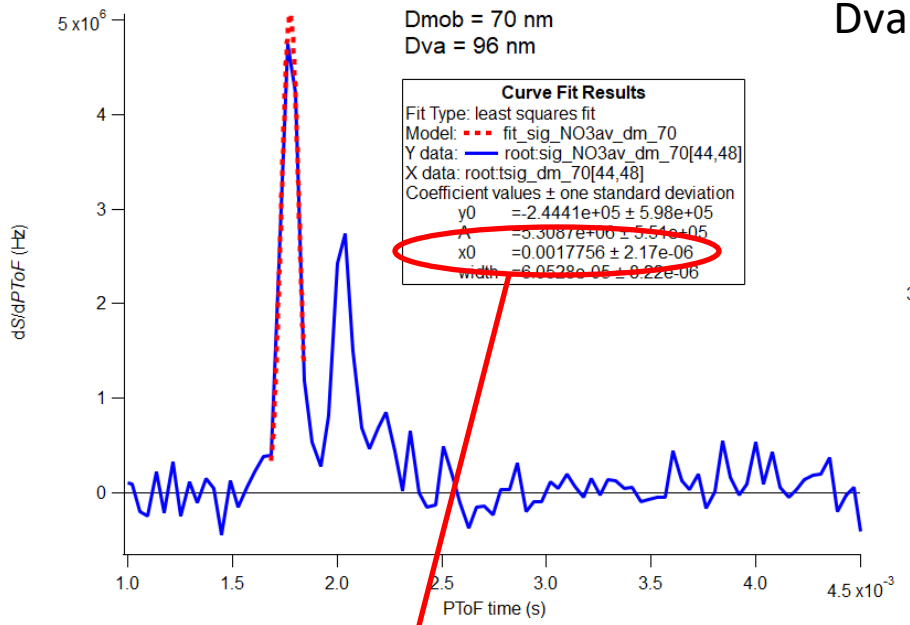
$$Vel(D_{va}) = V_{gas,lens} + \frac{V_{gas,exit} - V_{gas,lens}}{1 + \left({D_{va}}/{D^*}\right)^b}$$

$$Velocity = \frac{Distance}{pToF}$$

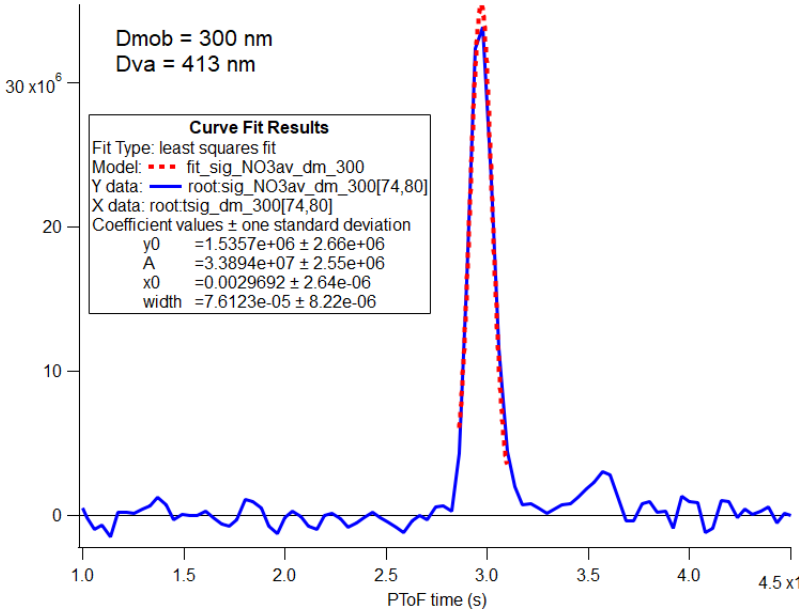
215-series:
Distance = 0.295 m

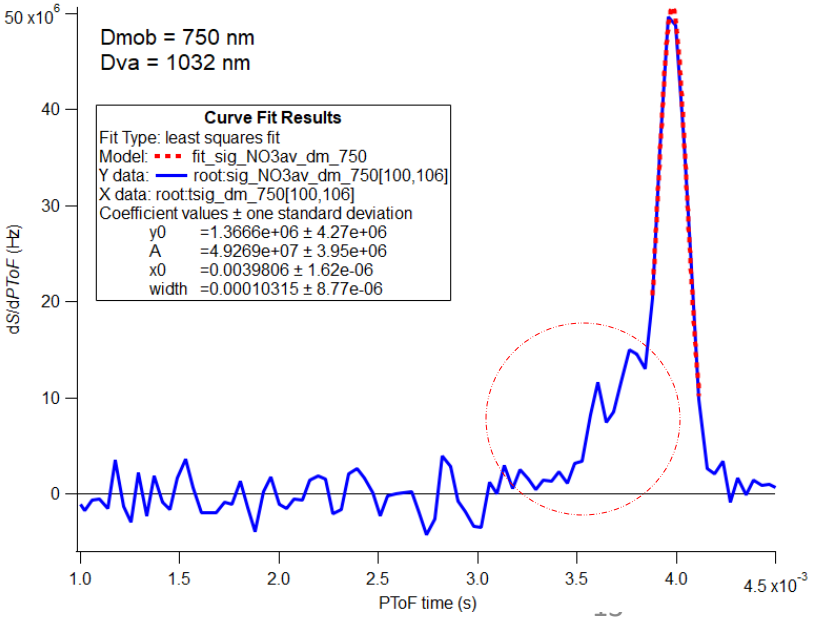
255-series:
Distance = 0.395 m

Velocity Calibration with Size-selected NH4NO3 Particles at Many Dmob



Dva = Dmob * Density * Shape Factor
= 70 nm * 1.72 * 0.8
= 96 nm



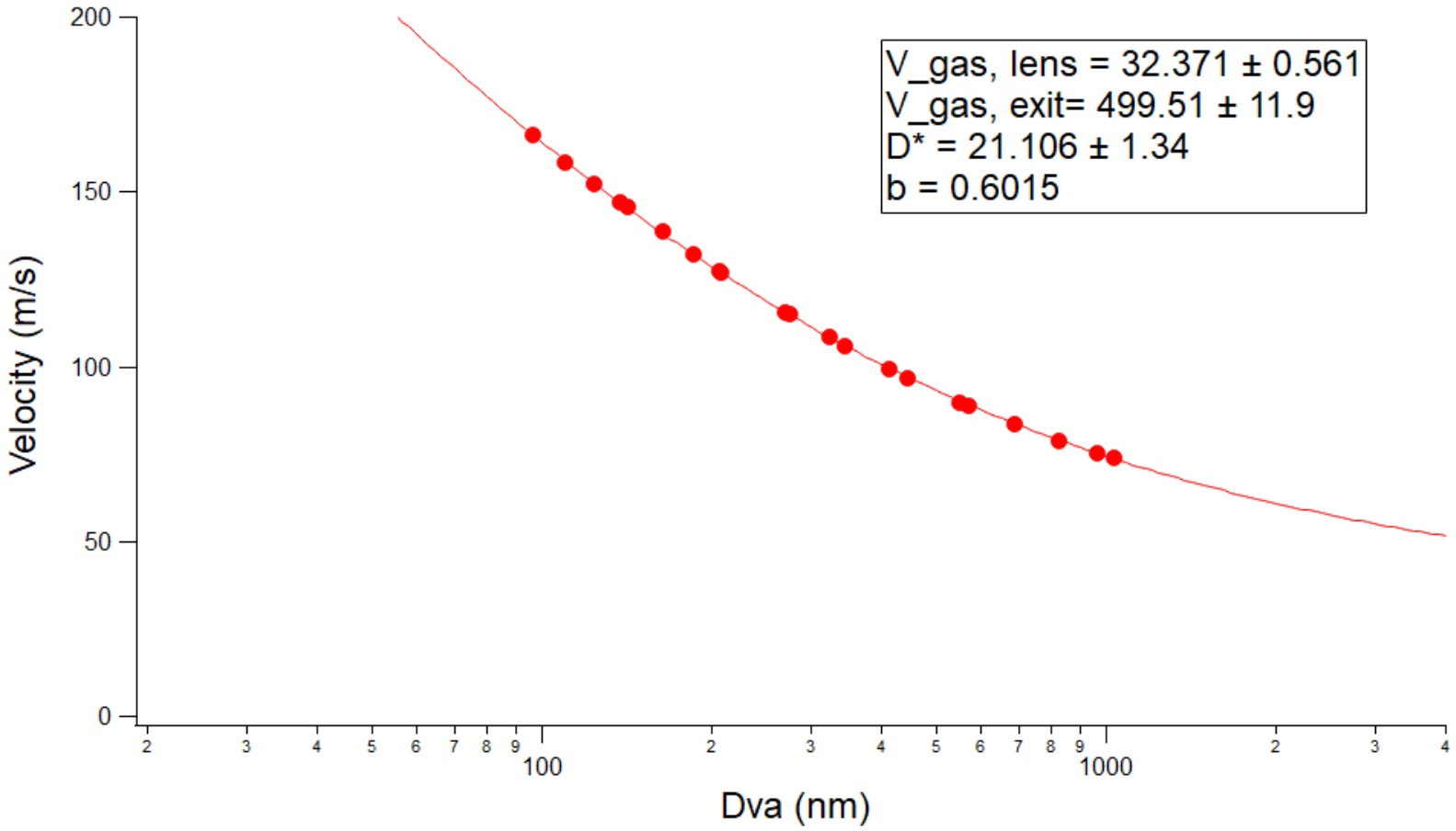


pToF = 0.00178 s
Vel = Chamber Length/pToF
= 0.295 m/0.00178 s
= 166 m/s

IEandVelCal_18Dec2020.pxp

Velocity Calibration

$$Vel(D_{va}) = V_{gas,lens} + \frac{V_{gas,exit} - V_{gas,lens}}{1 + \left({D_{va}}/{D^*}\right)^b}$$



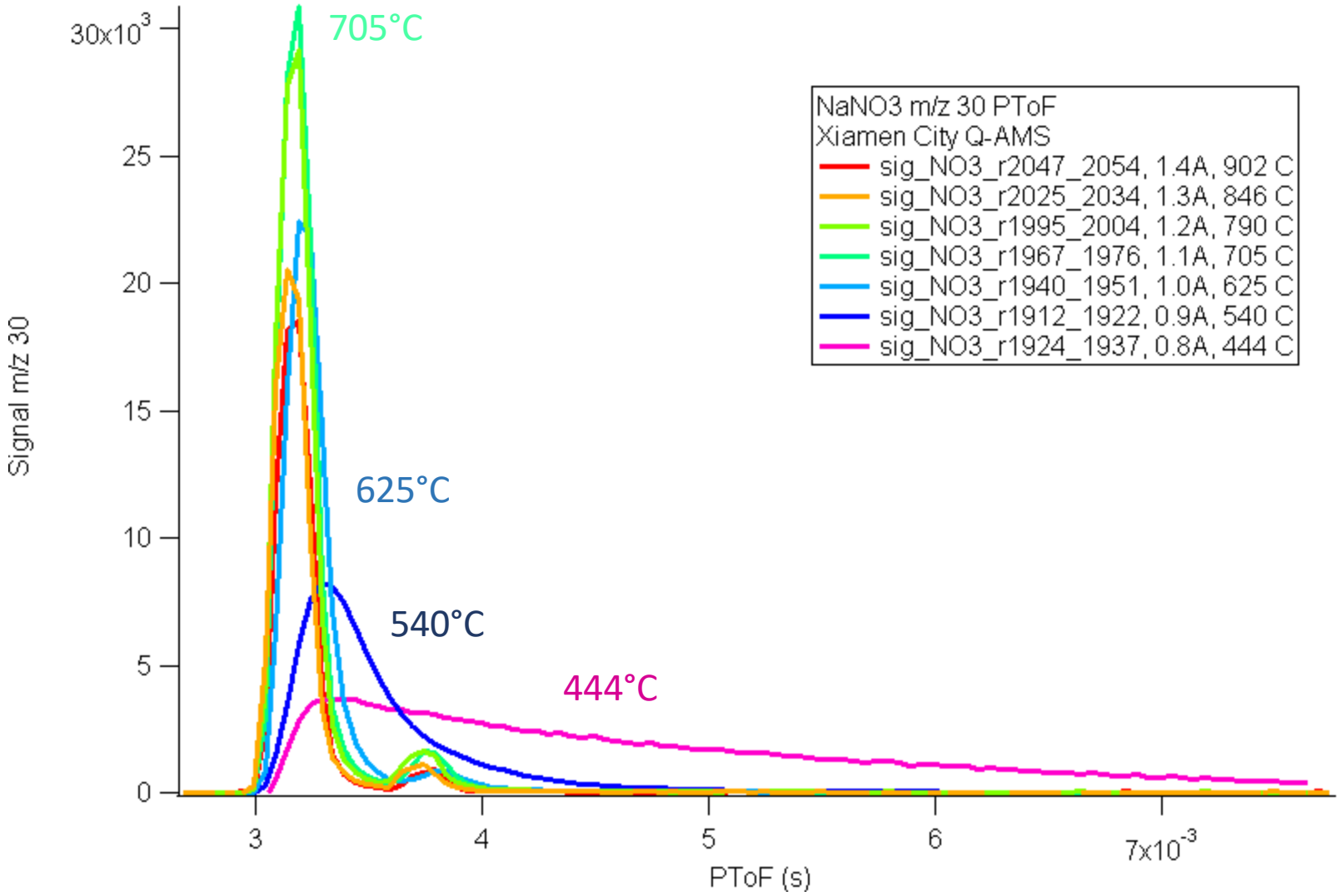
- Remember to enter parameters in DAQ!
- Or Squirrel if you need to correct sizing after data is collected.

IEandVelCal_18Dec2020.pxp

Velocity Calibration Tips

- Velocity calibration only changes if lens P changes!
  - Different elevation, aircraft campaign, new lens
- Or you change your chopper servo and aren't careful about rotational alignment of chopper flange.
- Every time you do an IE calibration, double check your velocity calibration. 300 nm NH_4NO_3 should be Dva = 413 nm!
- Use the widest possible range of particle sizes
  - Curve does not extrapolate well.
  - Be careful on the small particle side that you actually see Q1's.
  - Be careful on the large particle side that you have a clean pToF signal (NH_4NO_3 tends to break up at sizes > 450 nm).
  - Can use PSLs (at Vaporizer T = 800 C) or $NaNO_3$ (at Vaporizer T = 750 C) for larger sizes. Use half height on rising edge for pToF. Remember to use correct density and shape factor to calculate Dva.
- Fit is underdetermined, so don't worry about exact values of parameters.

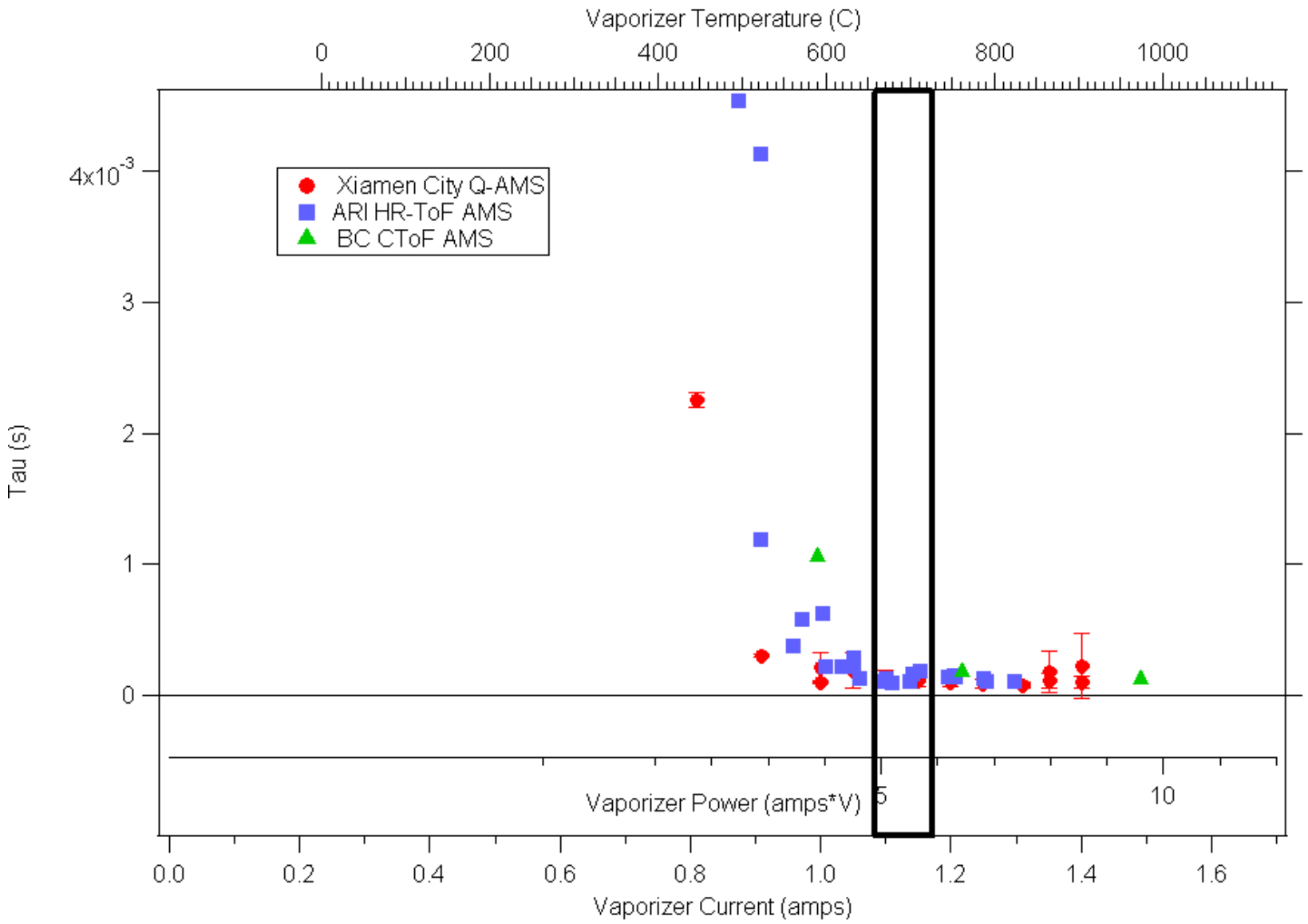
Measuring Vaporizer Temperature with pToF for 300 nm NaNO3 particles (AMS only)



- Want 600 to 650 C for complete vaporization of non-refractory and long life for vaporizer.
- pToF traces for NaNO3 (m/z 30) get narrower as vaporizer T increases.

VapT_SN_100805.pxp

Determine amp setting where pToF gets narrow.



- Fit falling edge of PToF with single exponential.
- Plot tau vs amps.
- pToF are narrow at 700 to 750 C, usually ~ 1.1A.
- Vaporizer is glowing dull orange from back (front is cooler than back).
- Subtract 0.1 A to get operating T of 600 to 650 C.

Summary_VapT.pxp

Vaporizer Temperature Tips

- Warning: For older AMS instruments, T readout can be off by 100's of degrees due to thermocouple detachment.
- If your measured vaporizer T is dropping with time, don't just turn up the current/power.
- If vaporizer current is NOT about 1 to 1.1 A, need to check true vaporizer temperature! Probably should check it anyway.
- Look at NaNO3 mz30 pToF. Sharpens up at 700 to 750 C. Subtract 0.1 from amps to get operating current.
- Look at back of vaporizer. If glowing dull orange, 700 to 750 C. Too hot for normal operation.
- ACSM: We calibrate temperature vs power. If T is unexpectedly low, trust the calibration curve.
- Working on chemical vaporizer T calibration for ACSM – ideas welcome!