Single Particle Composition as a function of Hygroscopicity, Volatility and Density

June 2004

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Presentation Outline

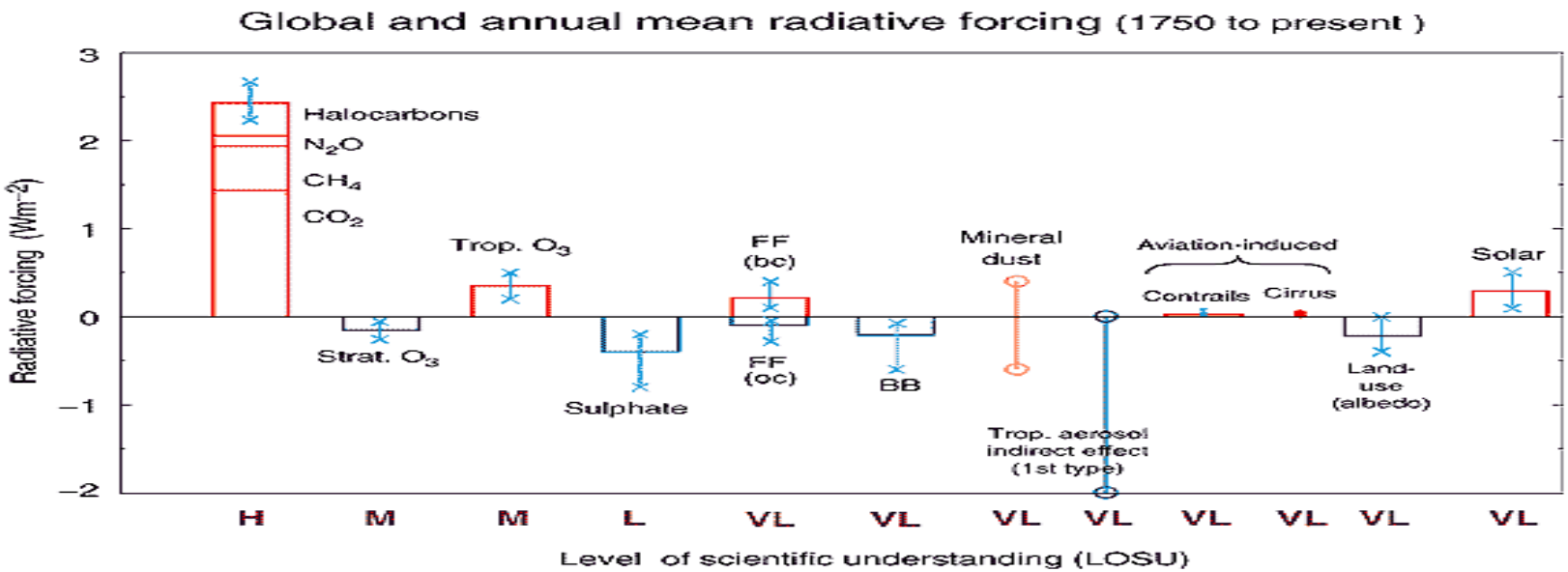
- Single Particle Mass Spectrometry background
- Characterization of our ATOFMS (Wallace)
- Atlanta-ANARChE and Diesel Studies

What are these aerosols we've been talking about anyway?

- Any mixture of gasses with suspended liquid or solid particles.
- Sizes range from single nanometers – tens of micrometers
  - Primary aerosols are directly emitted
  - Secondary aerosols form in the atmosphere

Atmospheric Aerosol

- Health Effects
- Visibility
- Largest uncertainty in climate forcing



IPCC 2001

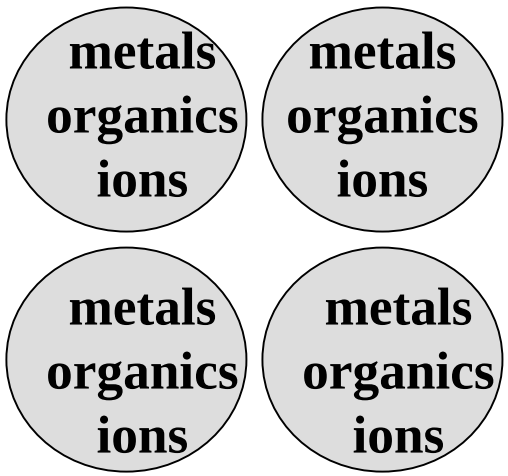
Single Particle Mass Spectrometry Background

What is Single Particle Mass Spectrometry?

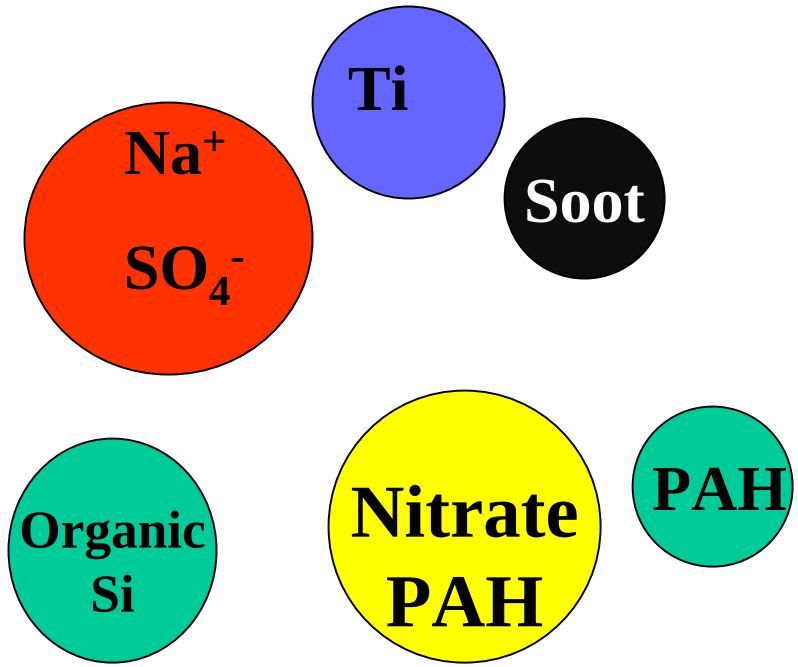
- Provides composition analysis on a particle by particle basis
- Usually coupled with particle size measurement

Why Single Particle Mass Spectrometry?

Traditional Bulk Chemical Analysis



Single Particle Analysis



Why Single Particle Mass Spectrometry?

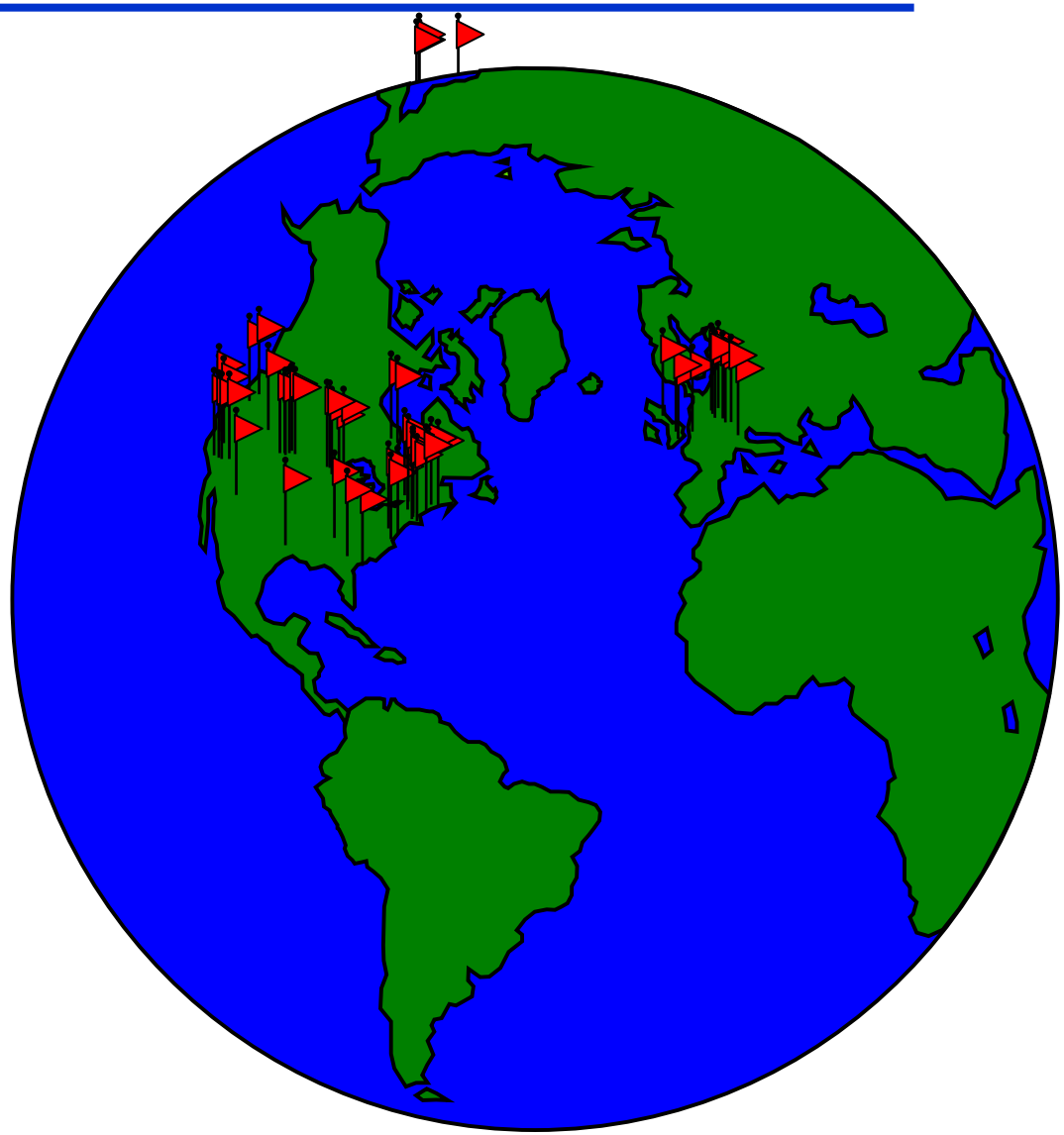
- No positive filter artifacts
- Better retention of volatile species
- Sensitivity (<1pg for mass spectra)
- “Real time analysis”
- Time resolution
- Source Apportionment

Groups doing single particle mass spectrometry

North America: ~35 groups

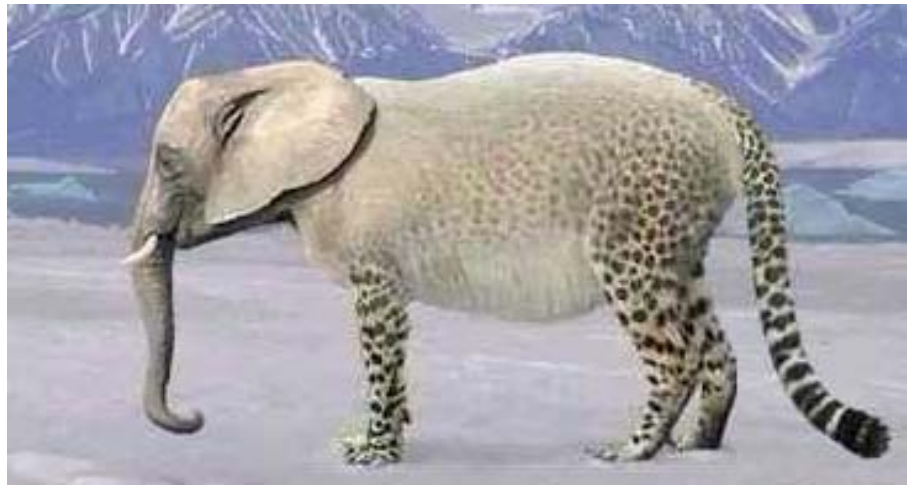
Europe: ~15 groups

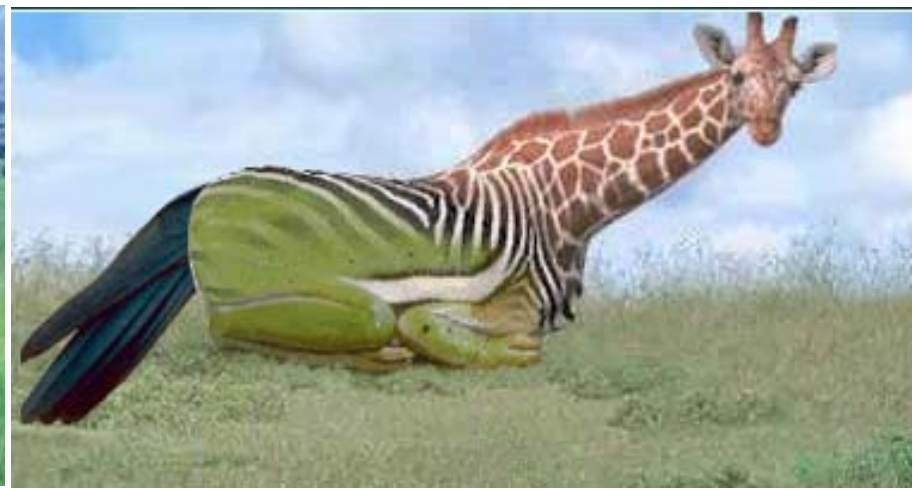
Asia: ~5 groups



Mix and Match Components

- **There are a variety of ways to build each component so mix and match…**
- **The basic components are the inlet, a sizing method, ablation/ionization, and mass spectrometry**





http://www.switcheroozoo.com

Single Particle Mass Spectrometry Techniques

Inlets

- Nozzle
- Aerodynamic Lens
- Size-selective Focusing Inlet

Sizing

- Particle Velocity
- Aerodynamic Sizing
- Optical Sizing

Single Particle Mass Spectrometry Techniques

Ablation-Ionization

- Laser Desorption/ Ionization
- Thermal Desorption/Electron Impact Ionization
- Thermal Desorption/Chemical Ionization

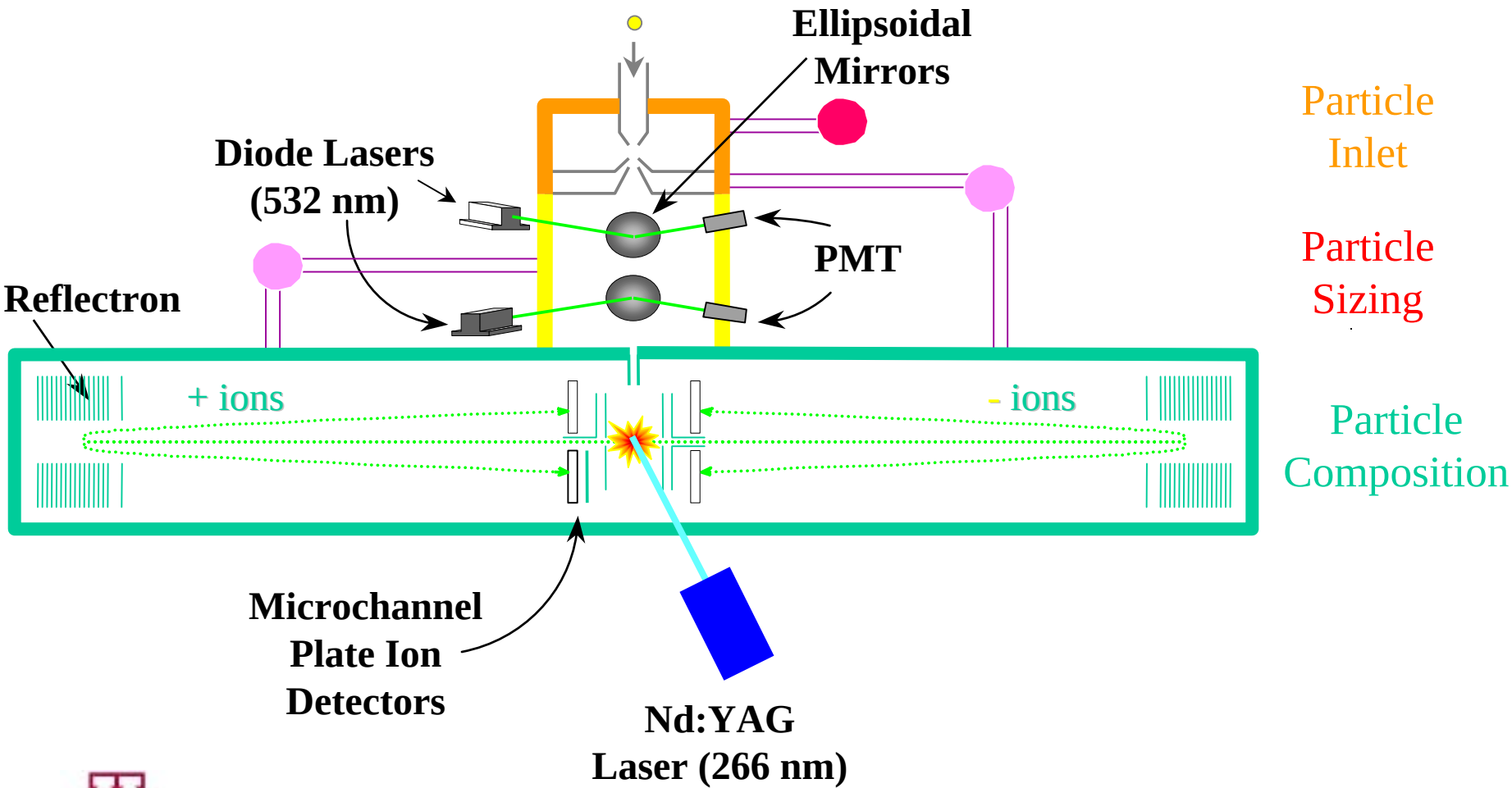
Mass Spectrometry Methods

- Time-of-Flight
- Quadrupole
- Ion Trap
- MS/MS

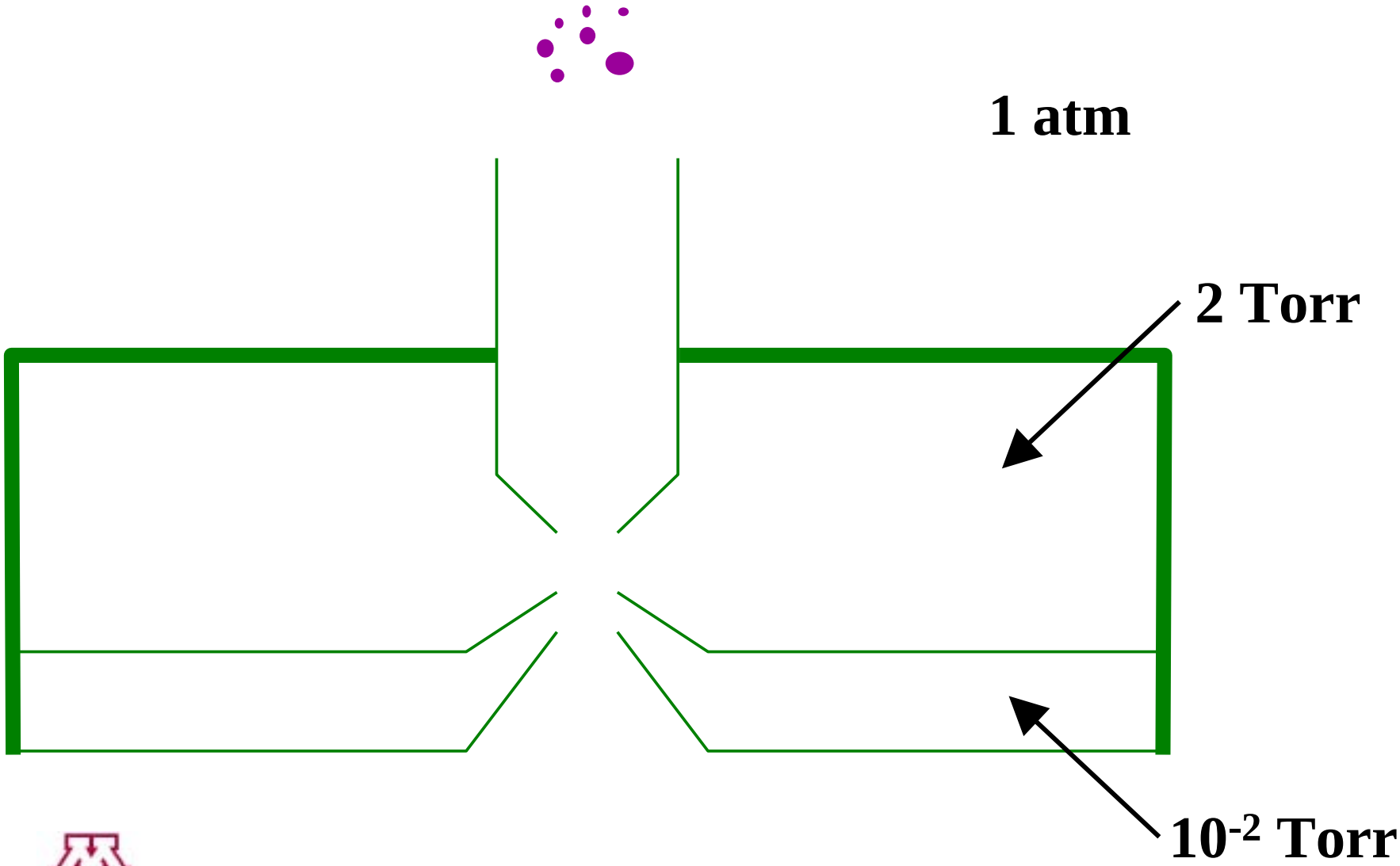
OUR ATOFMS (Wallace)

- Background
- Customization
- Characterization

TSI 3800 ATOFMS

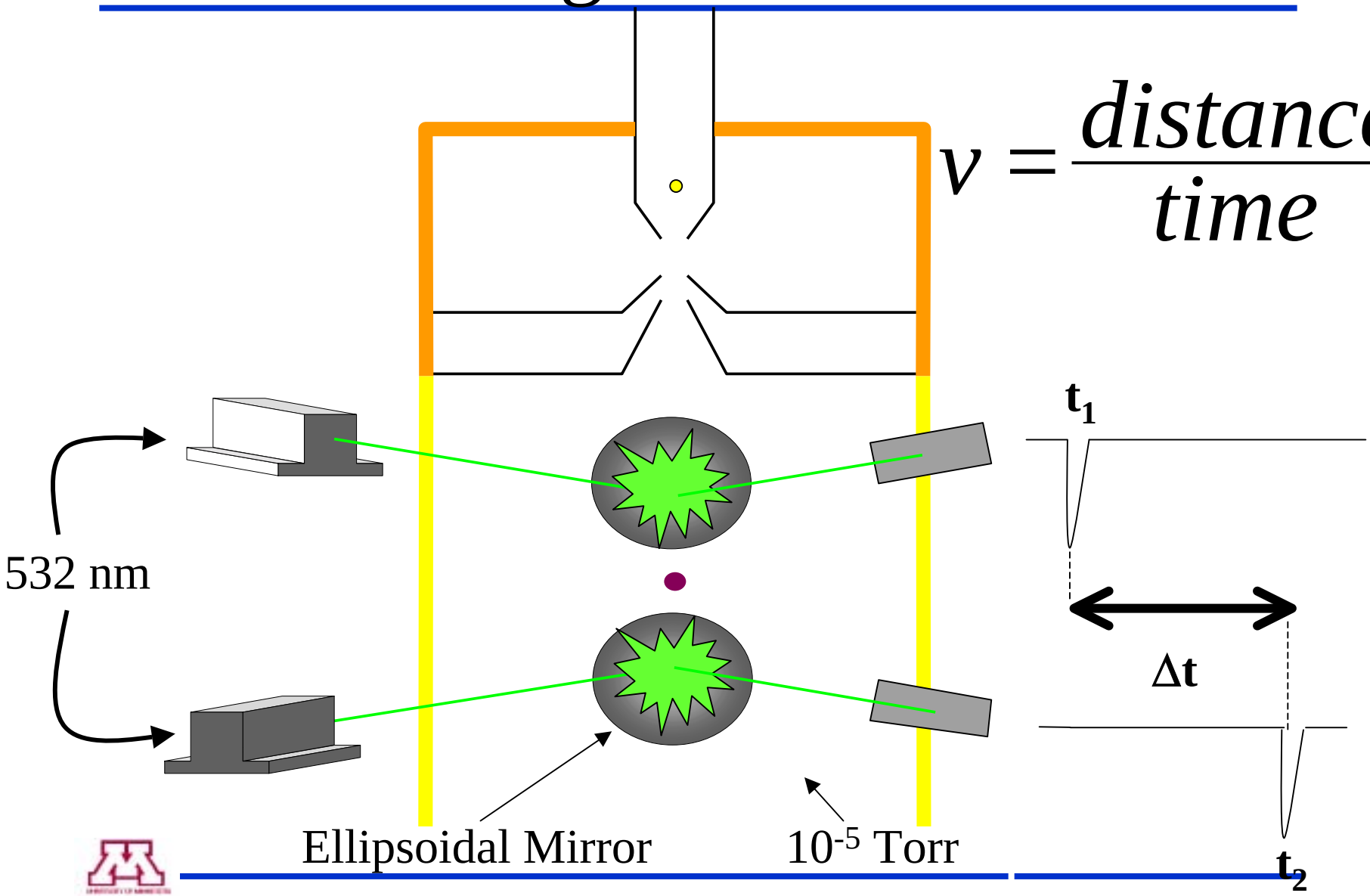


Inlet

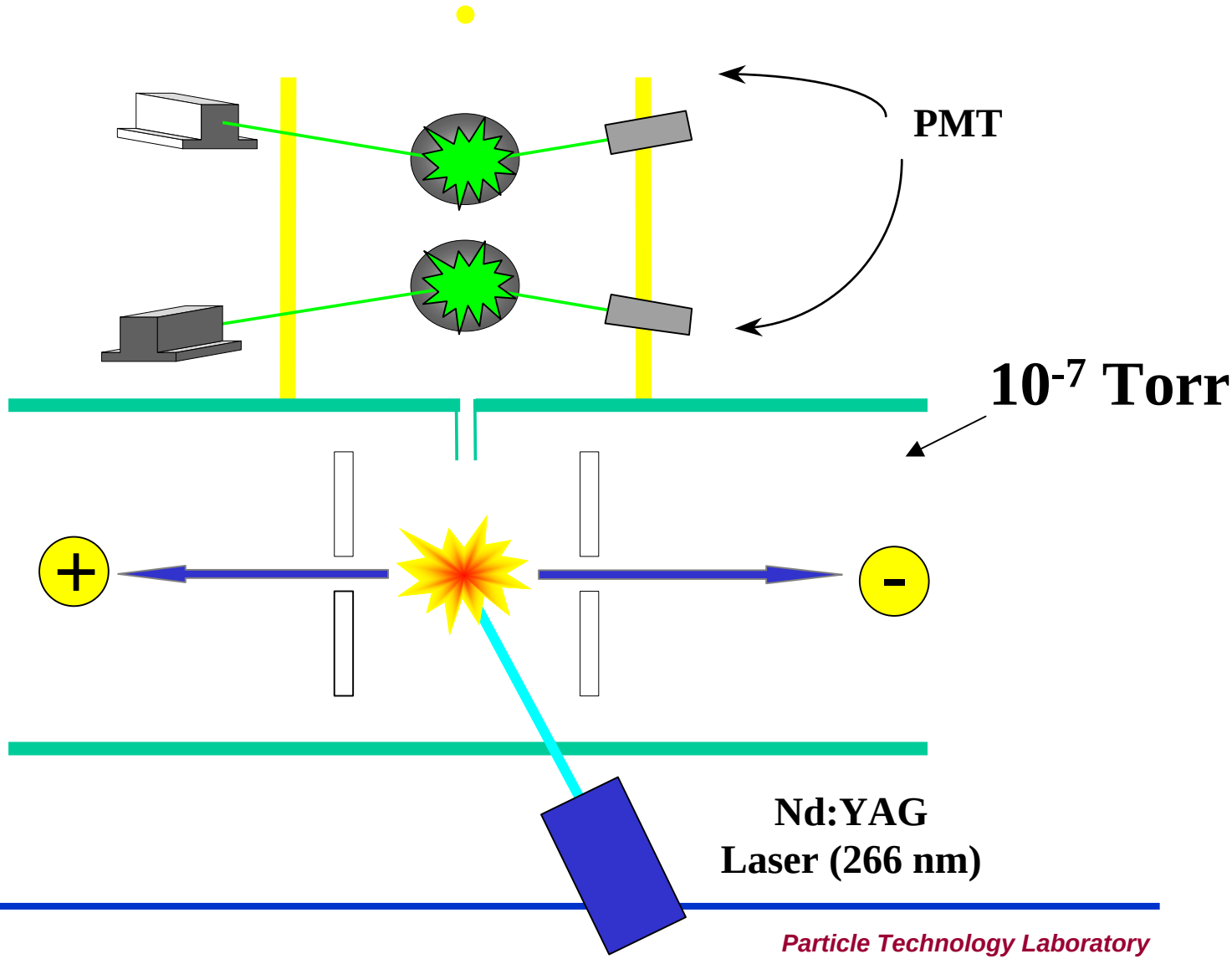


Particle Sizing

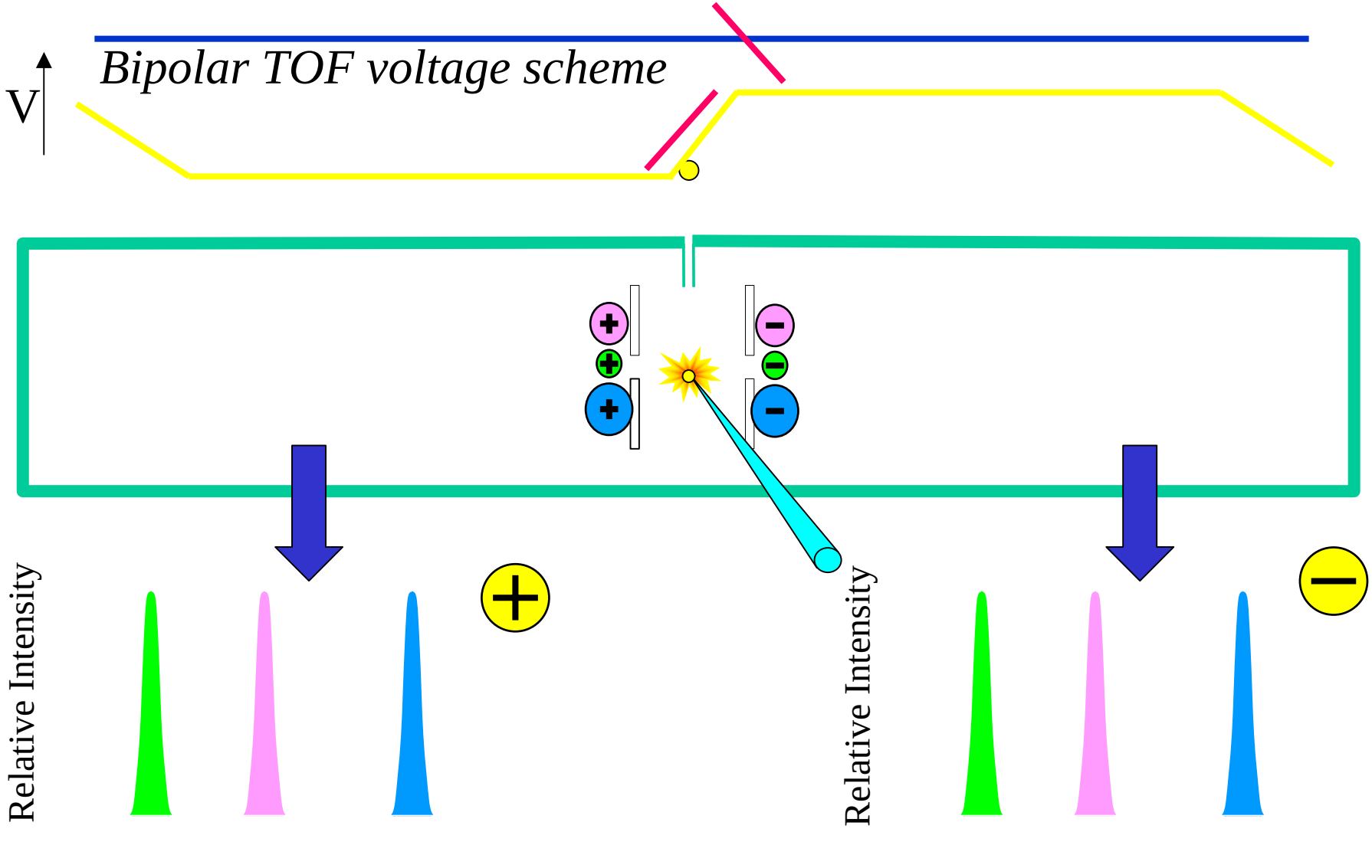
$$v = \frac{distance}{time}$$



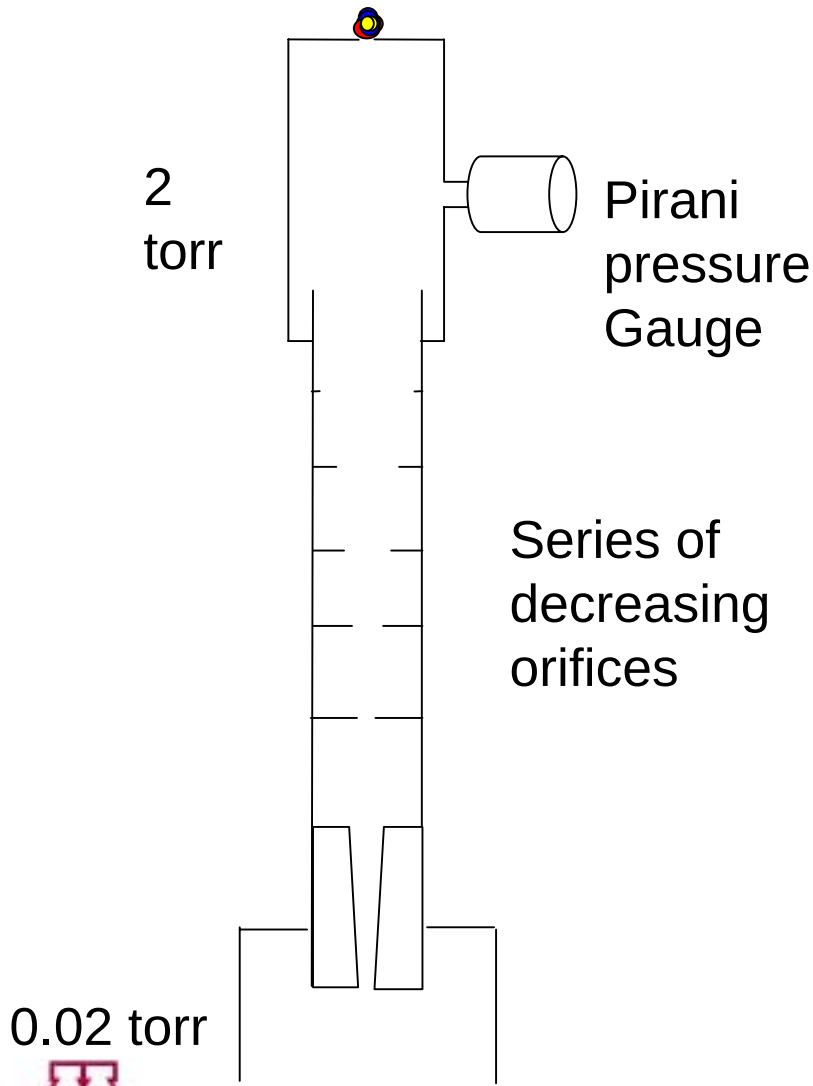
Ionization

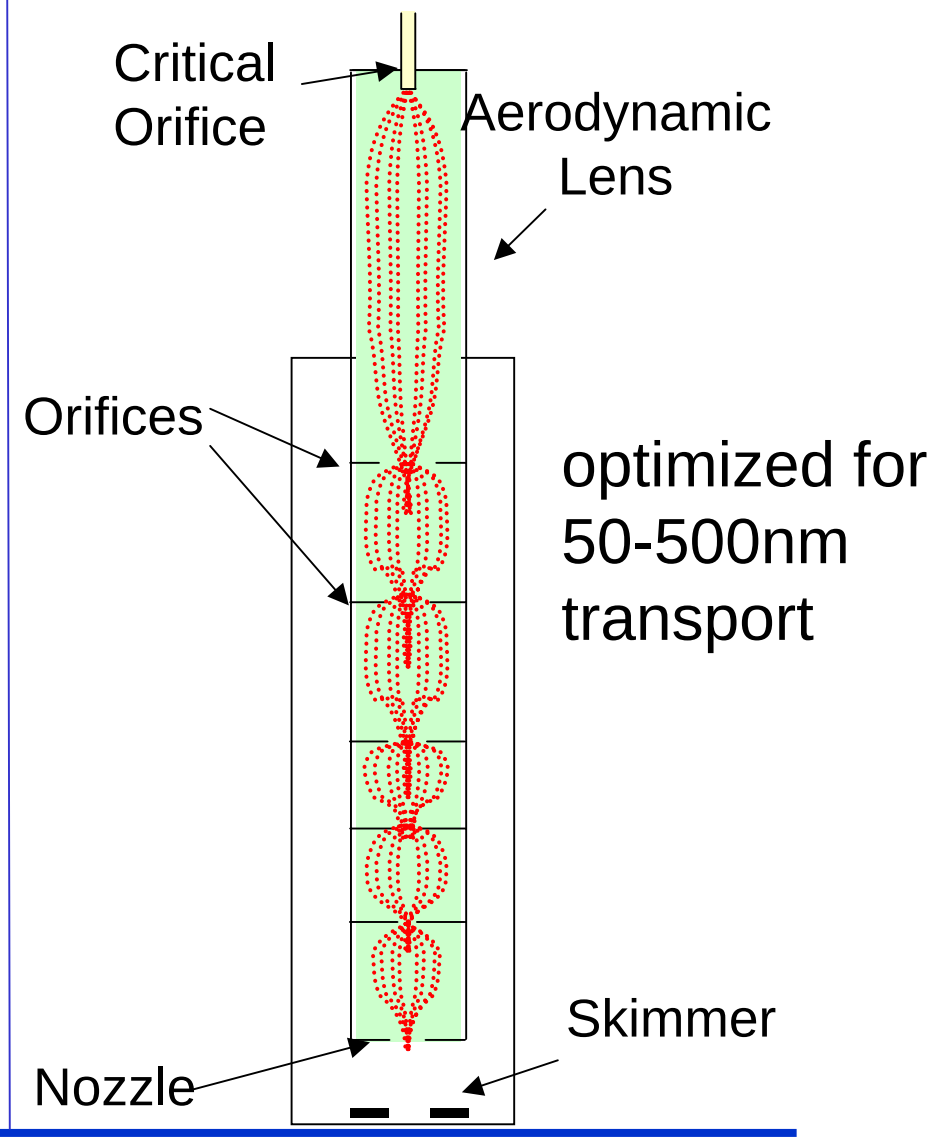


TOF Mass Spectrometry

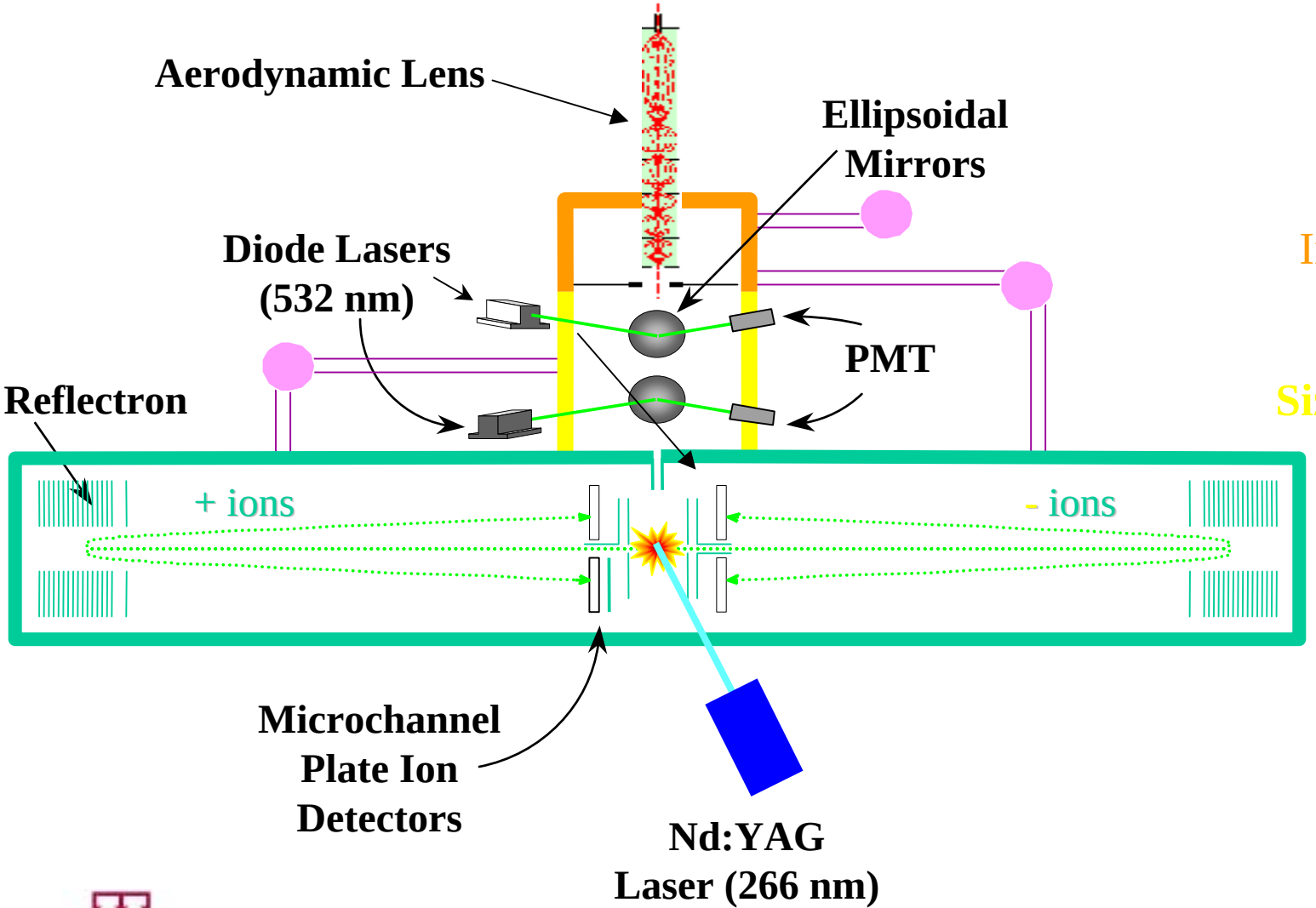


Aerodynamic Lens Inlet





Wallace



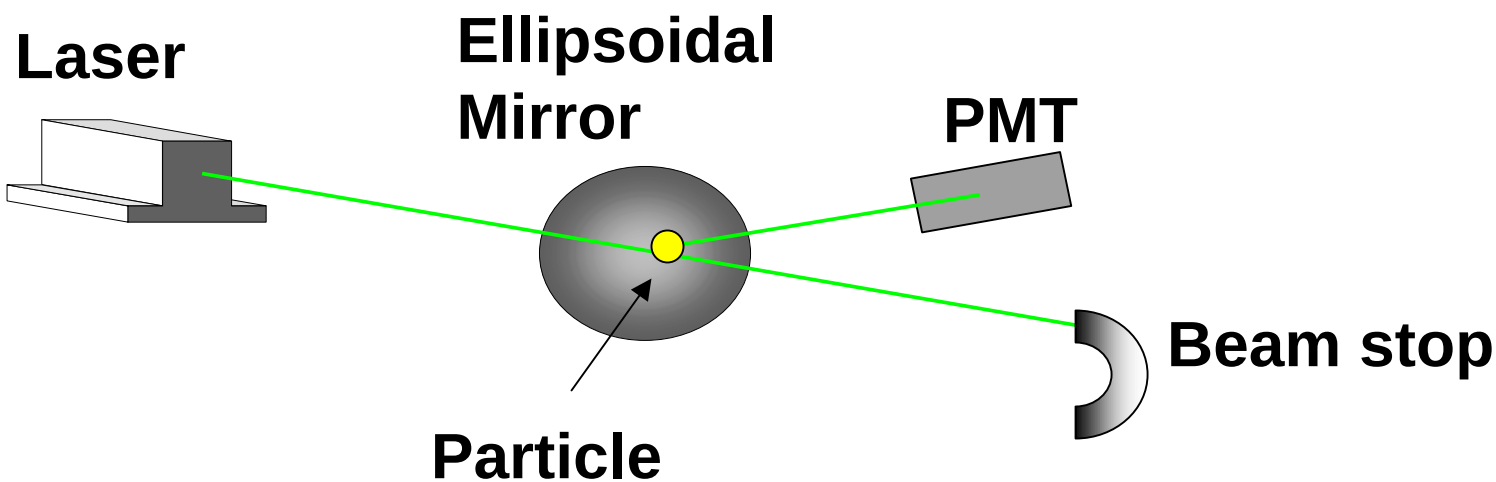
Lens
1 torr

Particle
Inlet 10^{-2} torr

Particle
Sizing 10^{-4} torr

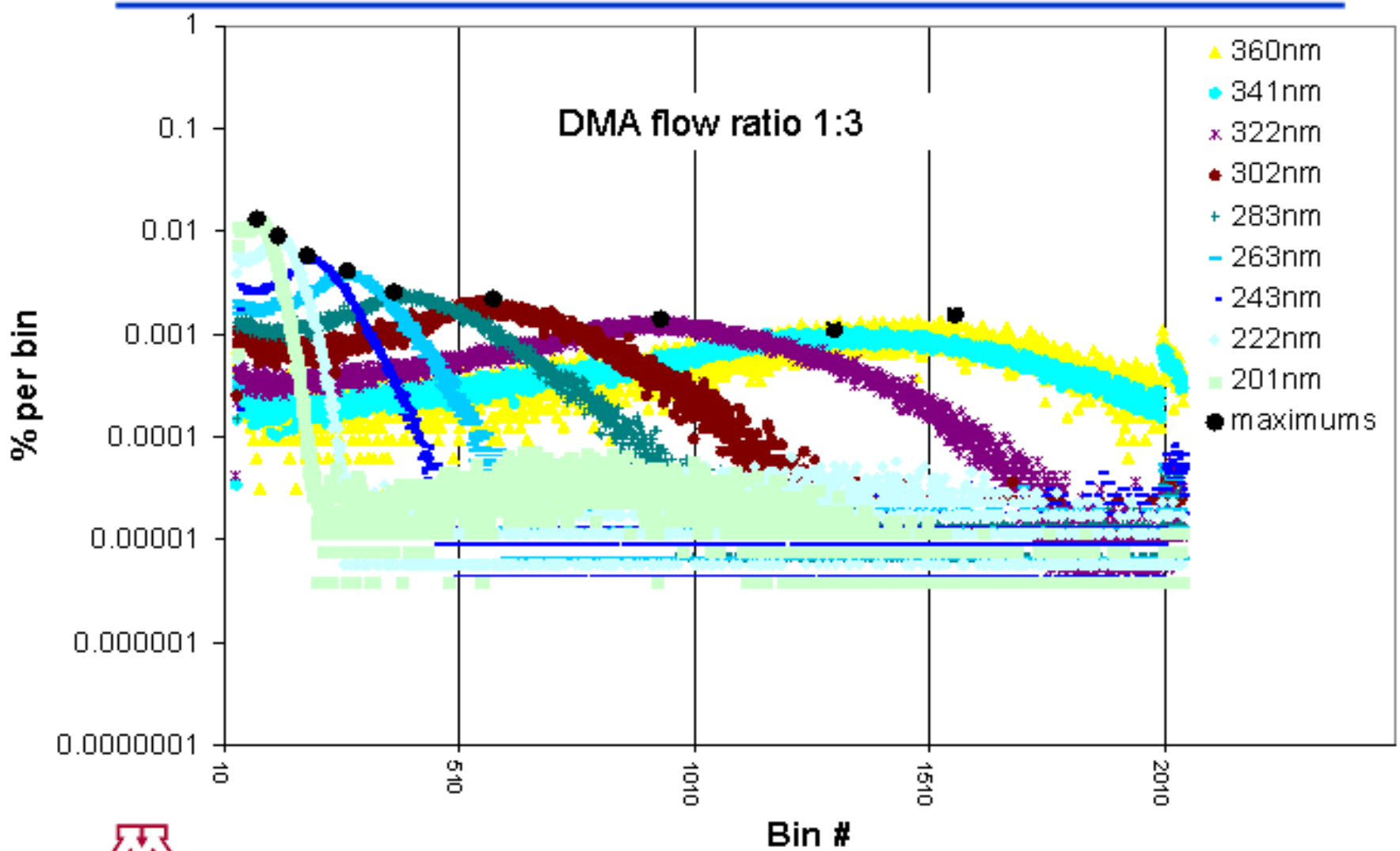
Particle
Composition
10^{-7} torr

Characterization of Sizing System

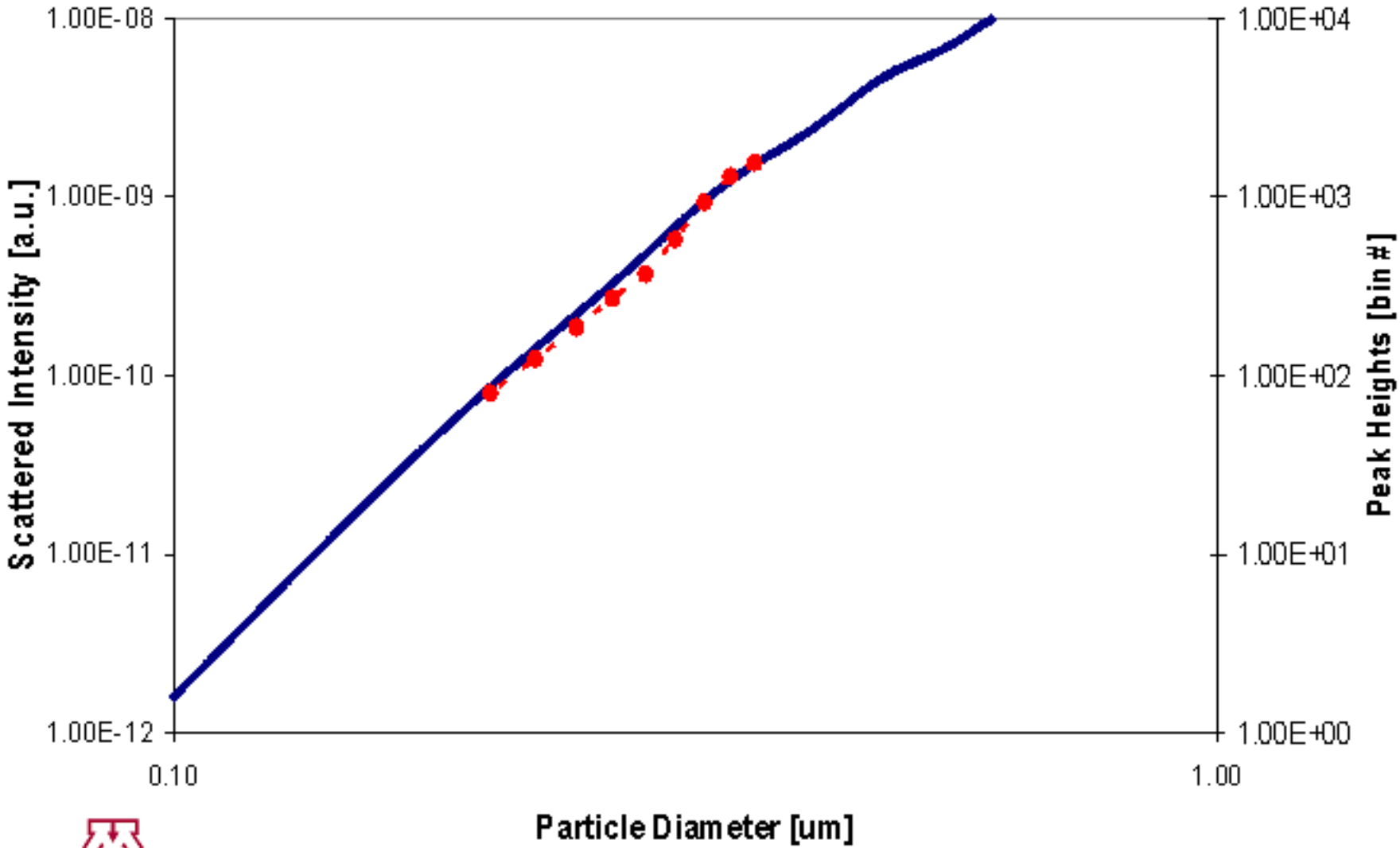


- **All the necessary OPC components**

Nomalized Scattering Curves for DOS
PULSE HEIGHT ANALYSIS



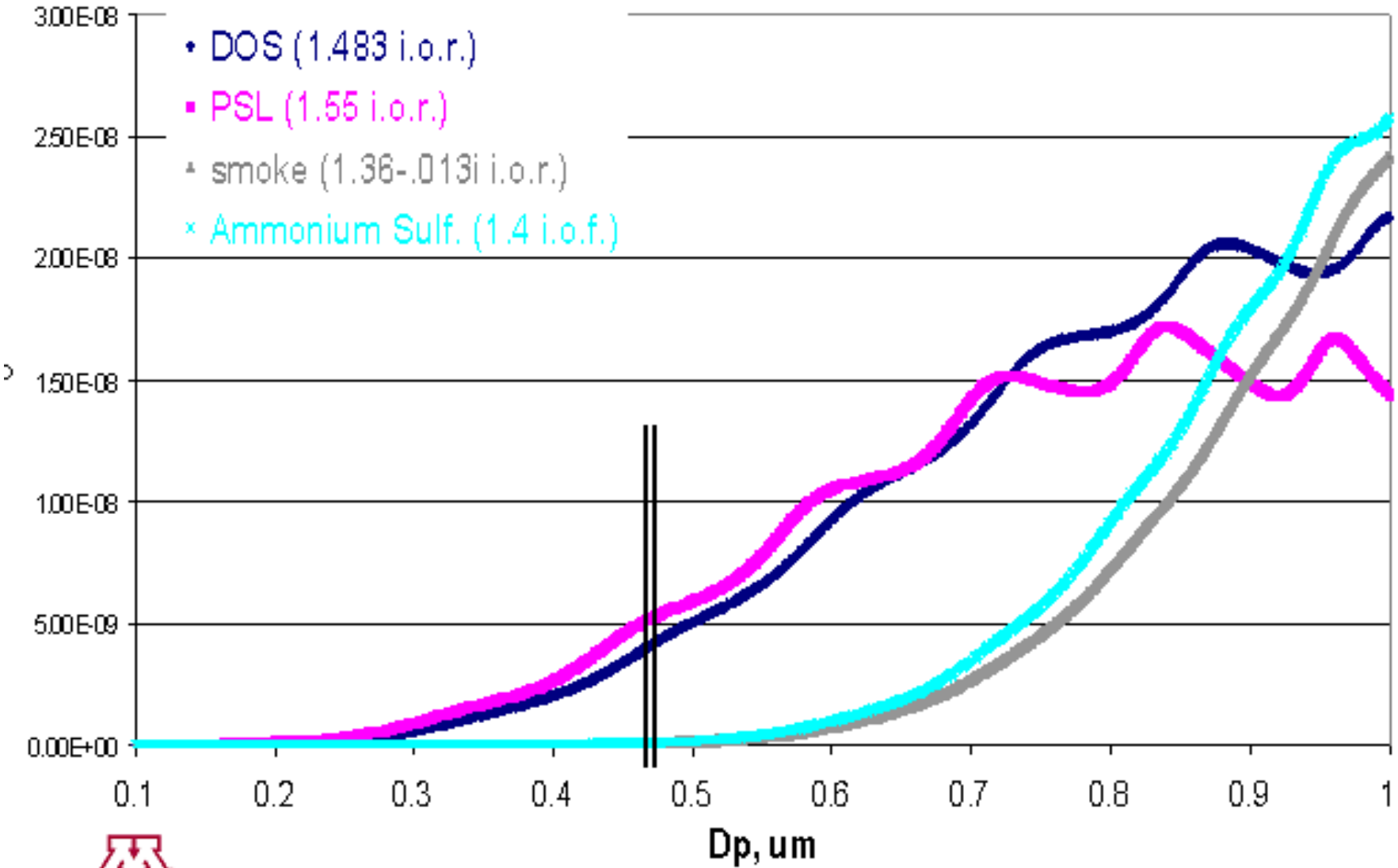
Calculated and Measured Scattering for DOS using the ATOFMS



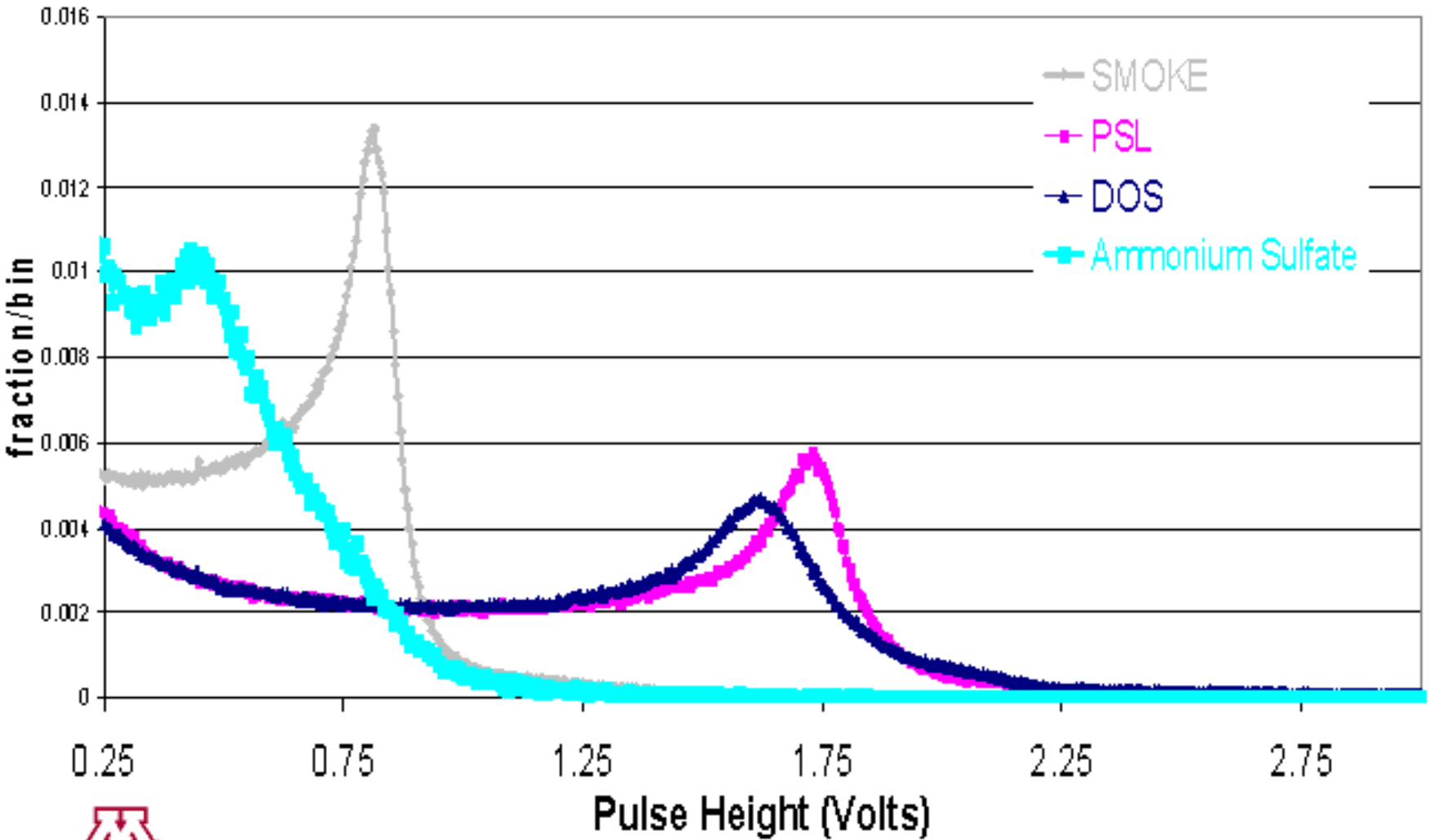
Why is index of refraction important?

- Scattering and absorption characteristics
  - Radiative forcing
  - Haze/visibility
- Optical measurement calibration

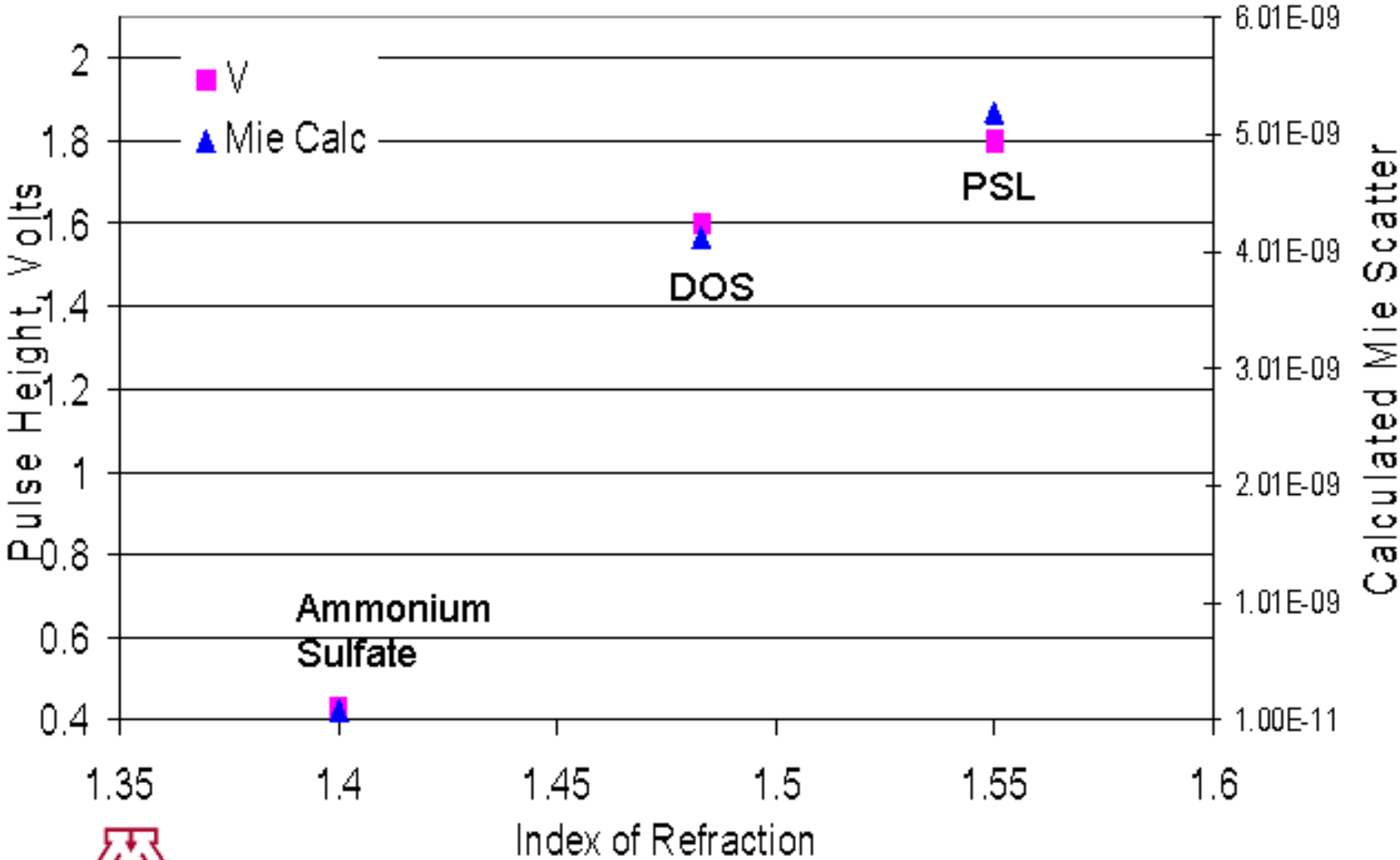
Calculated MIE Scattering



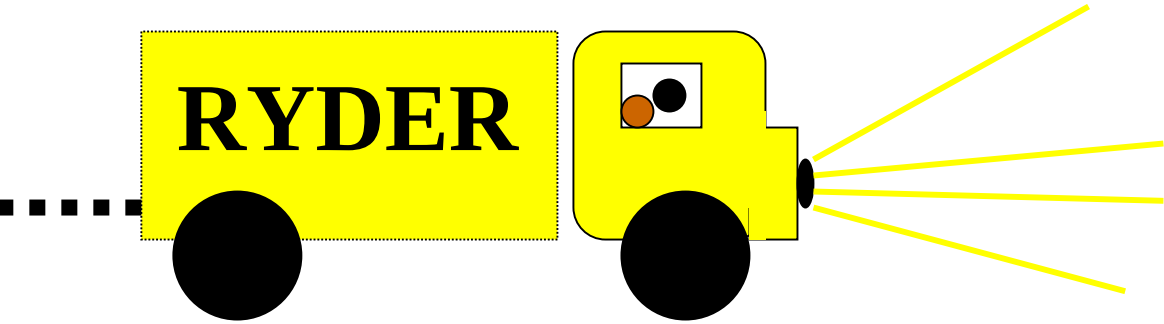
Pulse Height Distibutions
470nm mobility size



Determination of Index of Refraction

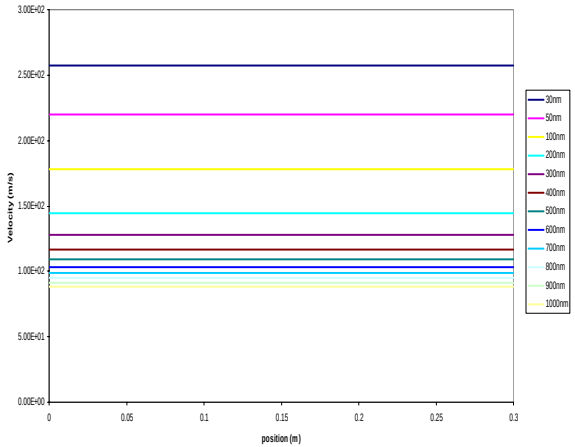


Particle Transport Efficiency

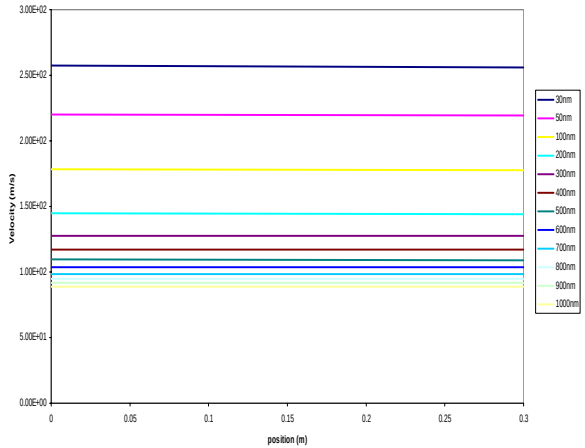


Position Dependant Particle Velocities

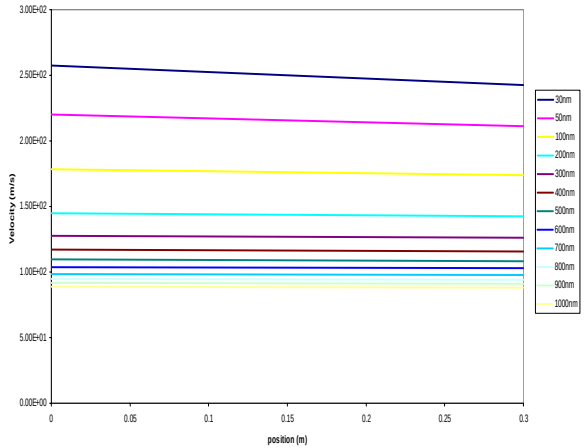
P=7.6E-6 Torr



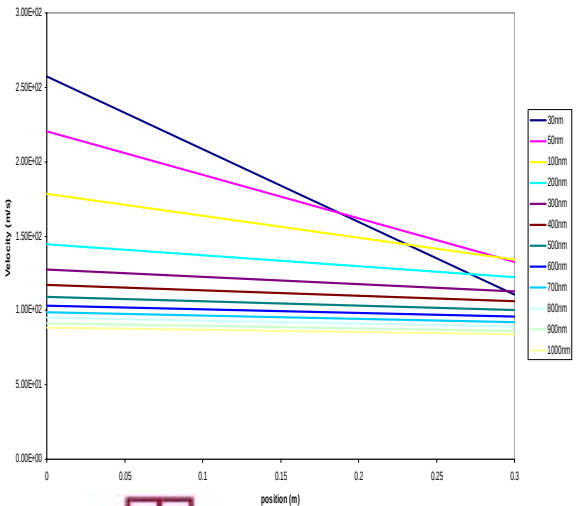
P=7.6E-5 Torr



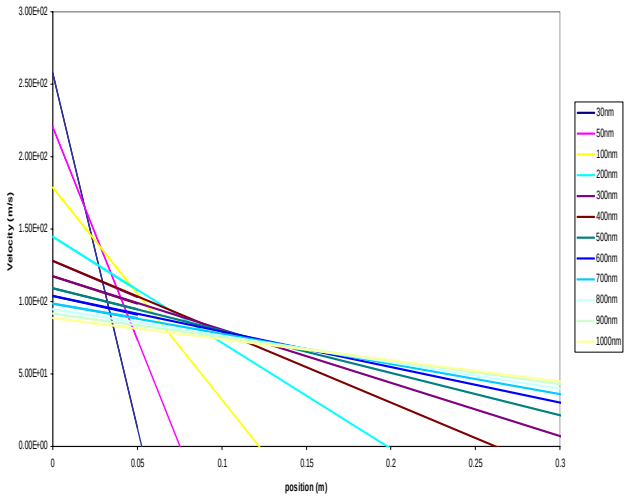
P=7.6E-4 Torr



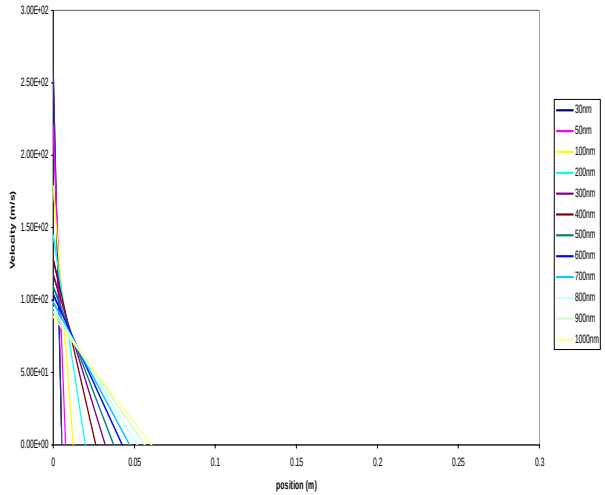
P=7.6E-3Torr



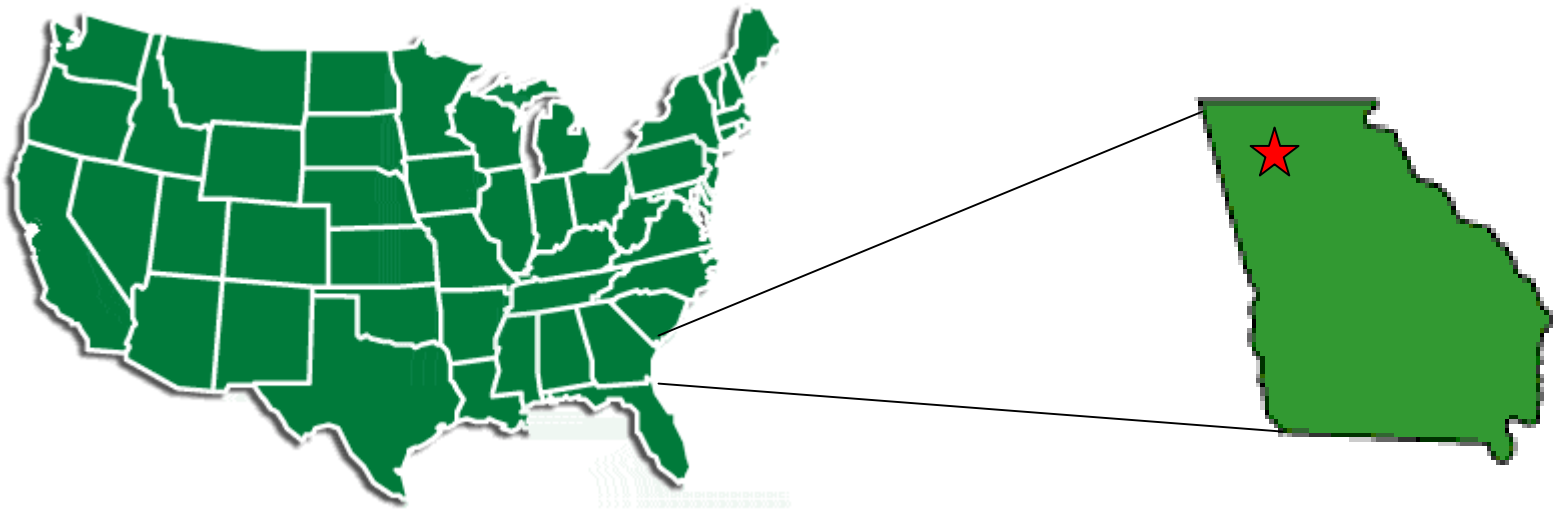
P=7.6E-2Torr



P=7.6E-1Torr



Atlanta-ANARChE
(Aerosol Nucleation and Real-time Characterization Experiment)



Site Conditions

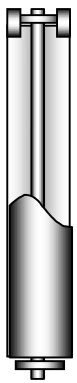
Atlanta, GA, August 1999

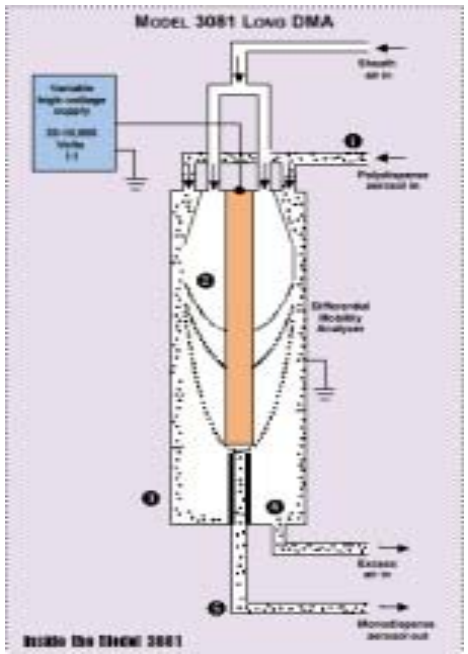
Day 1, ~4:50 PM

Day 2, ~3:30 PM

The additional instruments…

Differential Mobility Analyzer (DMA)

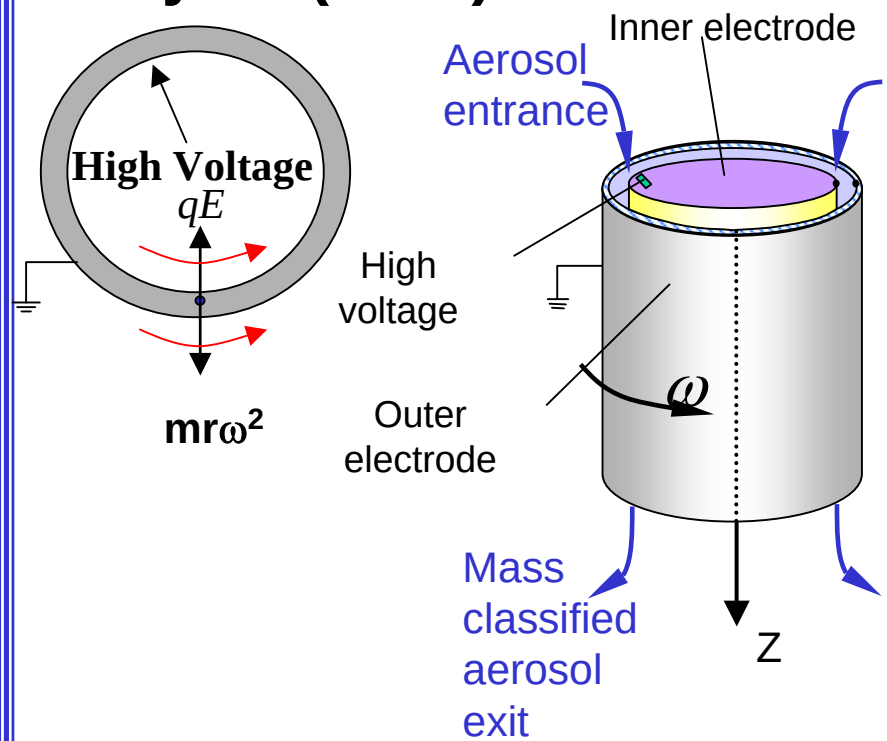




•Particles of a certain mobility size are selected for a certain flow and voltage.

•Electrostatic force = Drag Force

Aerosol Particle Mass analyzer (APM)

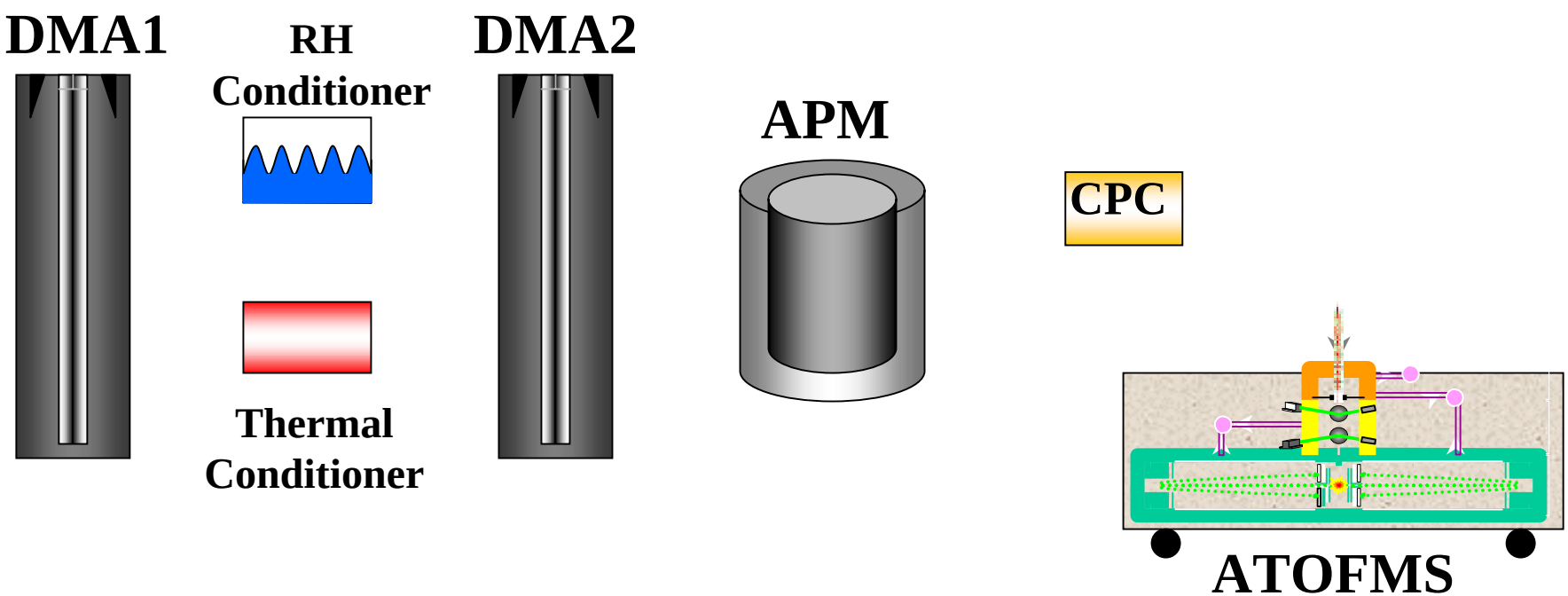


• Particles of a certain mass can penetrate through the APM for a fixed rotational speed and voltage.

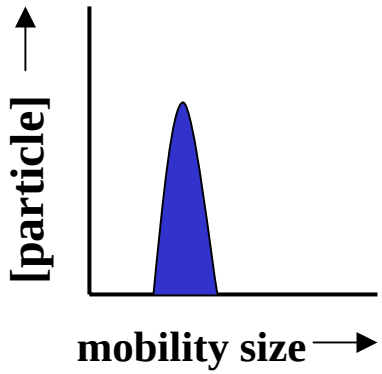
• Electrostatic force = Centrifugal force

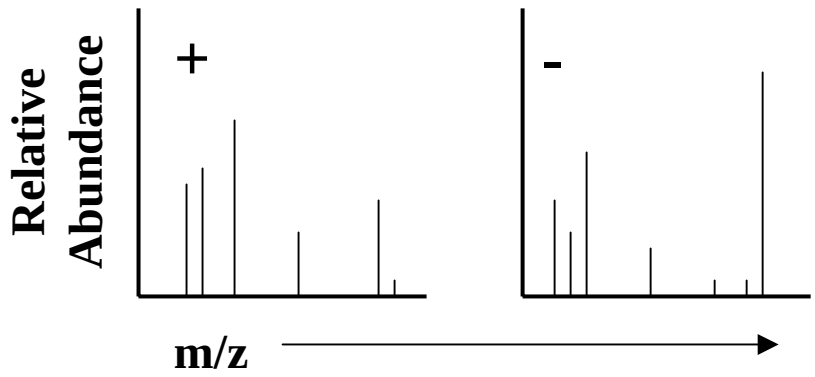
Experimental Set-up

the available toys….



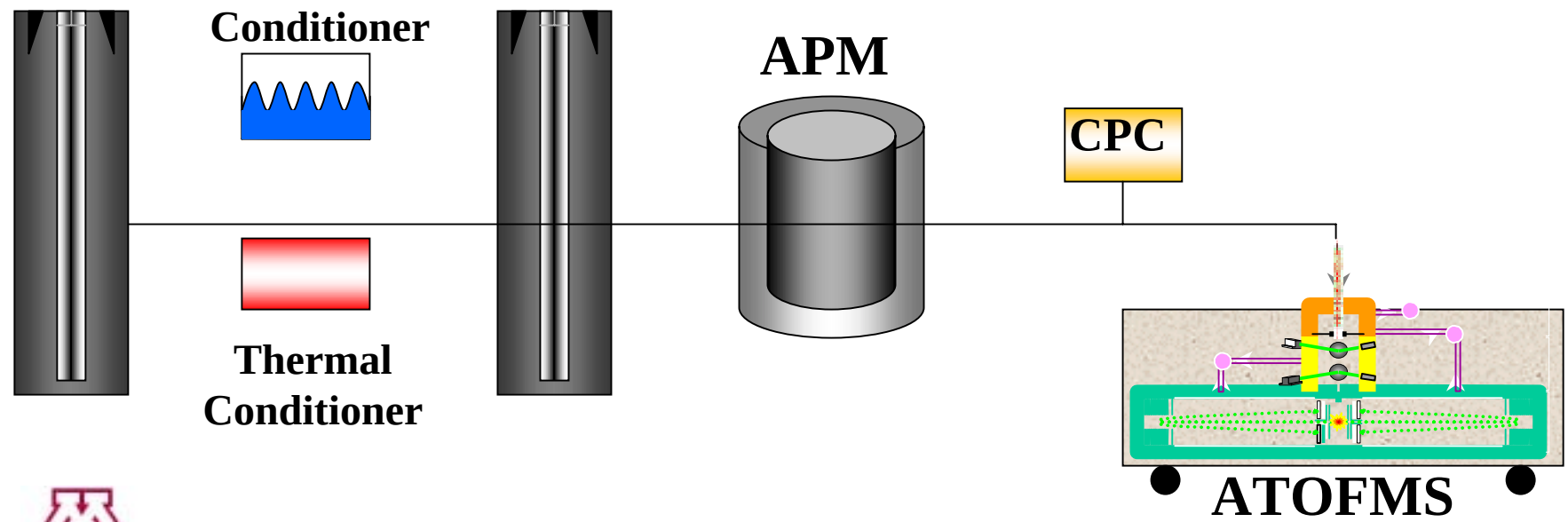
Composition of particles of known mobility size…



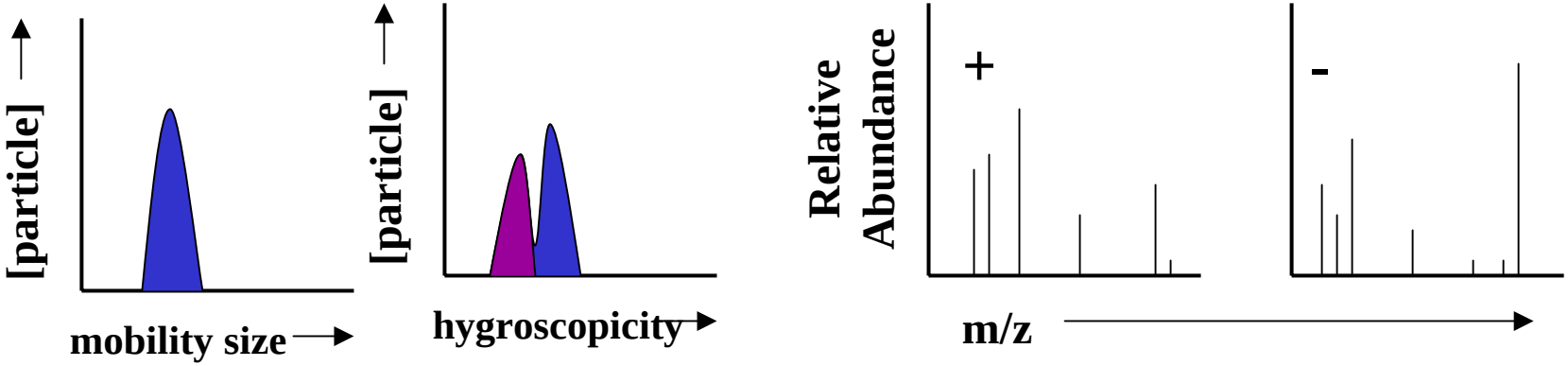


size

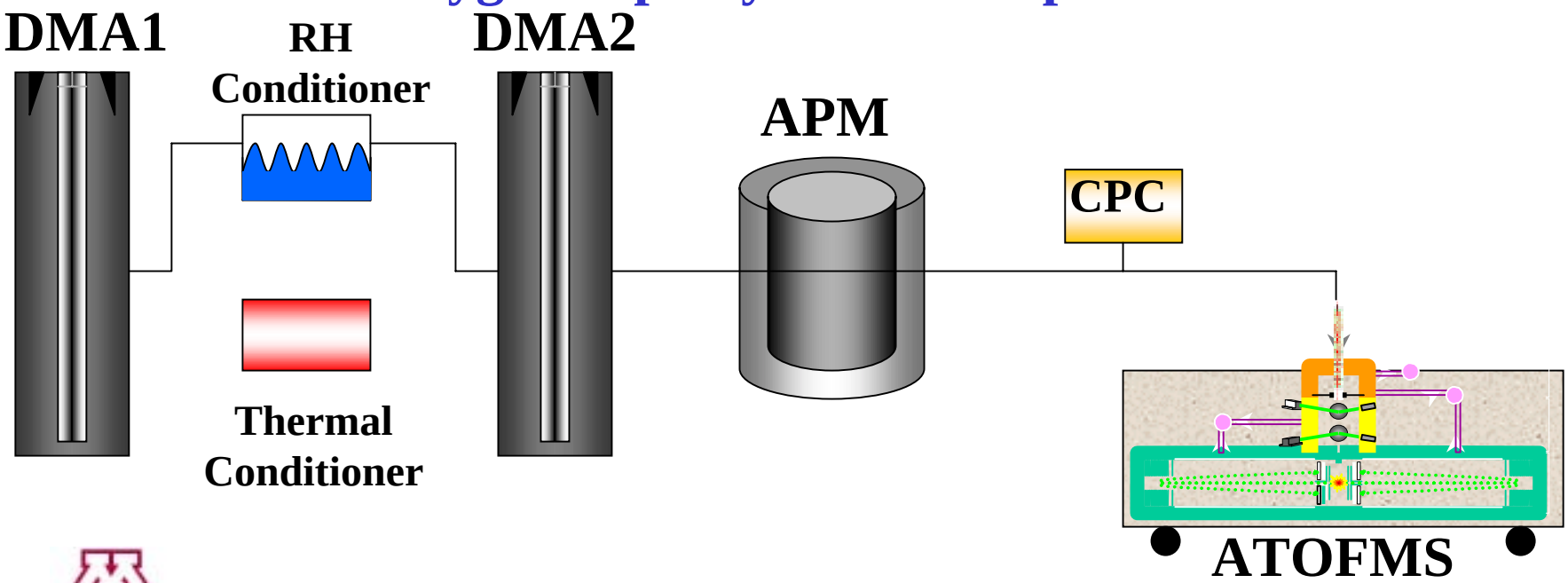
composition



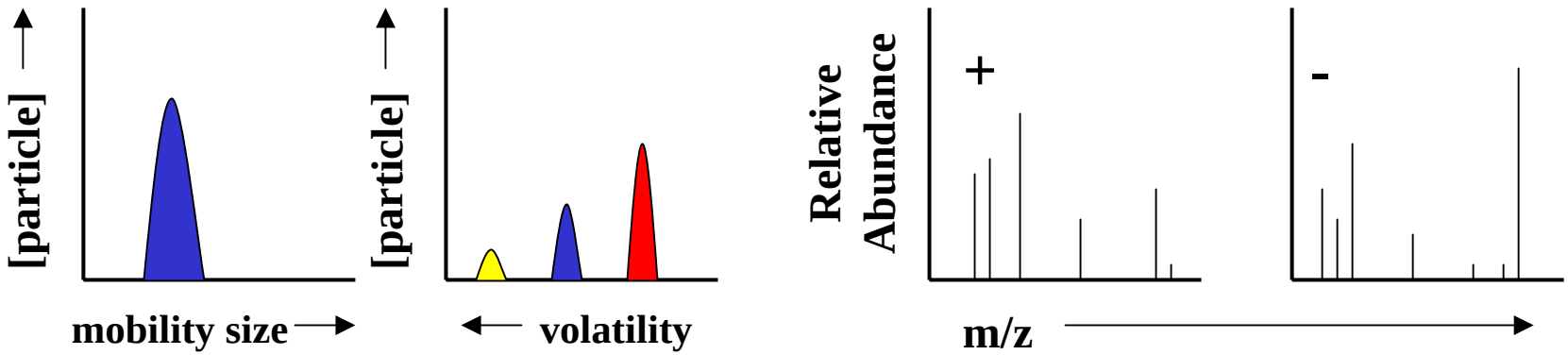
Composition of particles of known size and hygroscopicity…



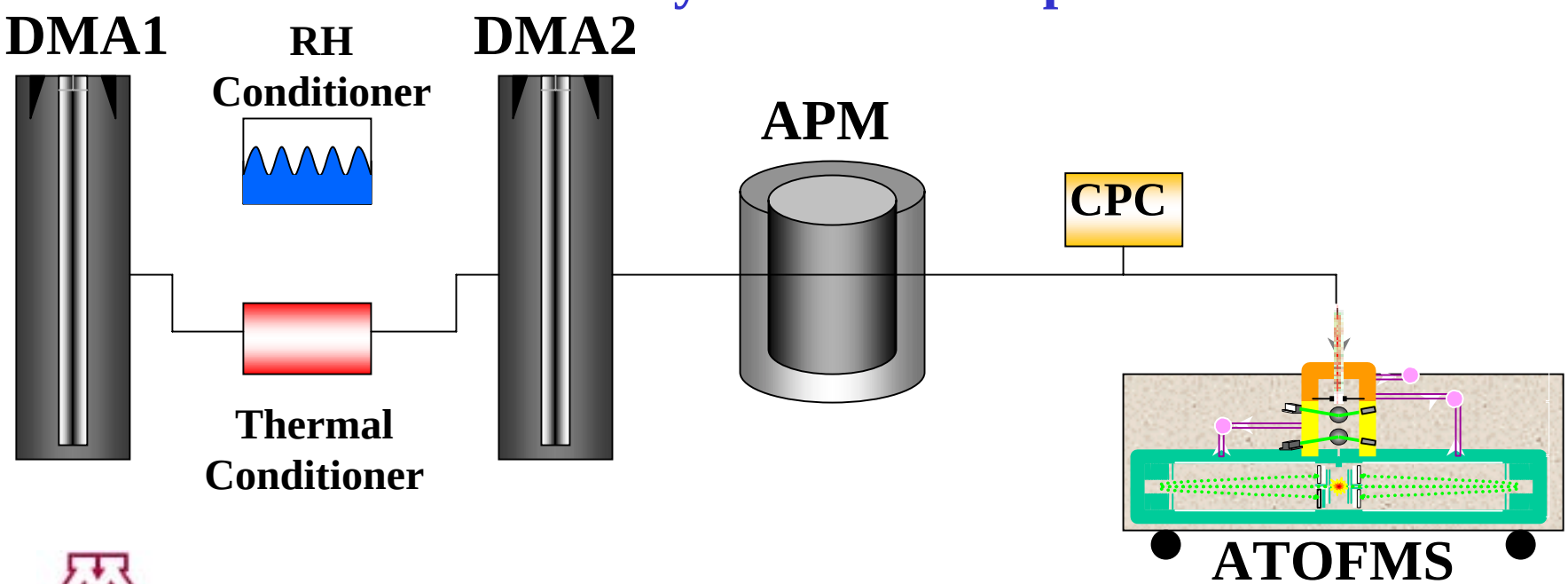
size **hygroscopicity** **composition**



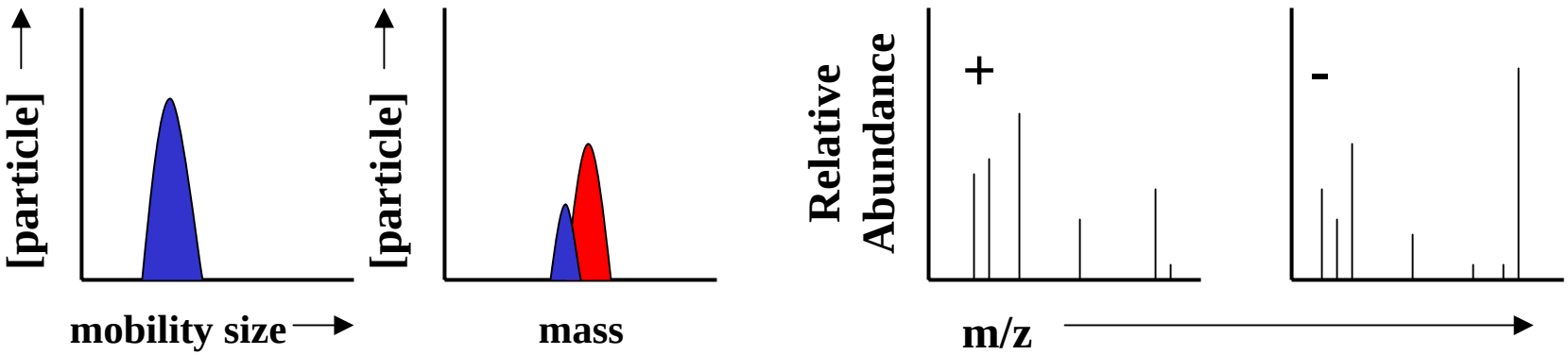
Composition of particles of known size and volatility…



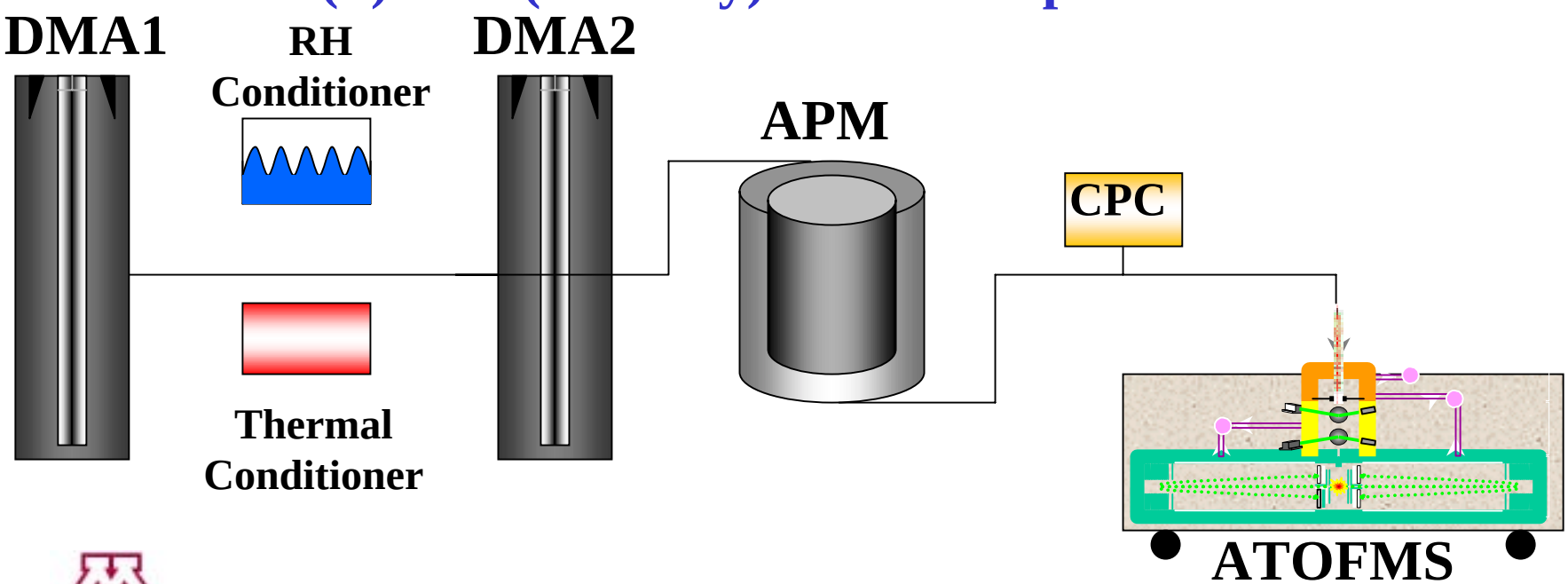
size **volatility** **composition**



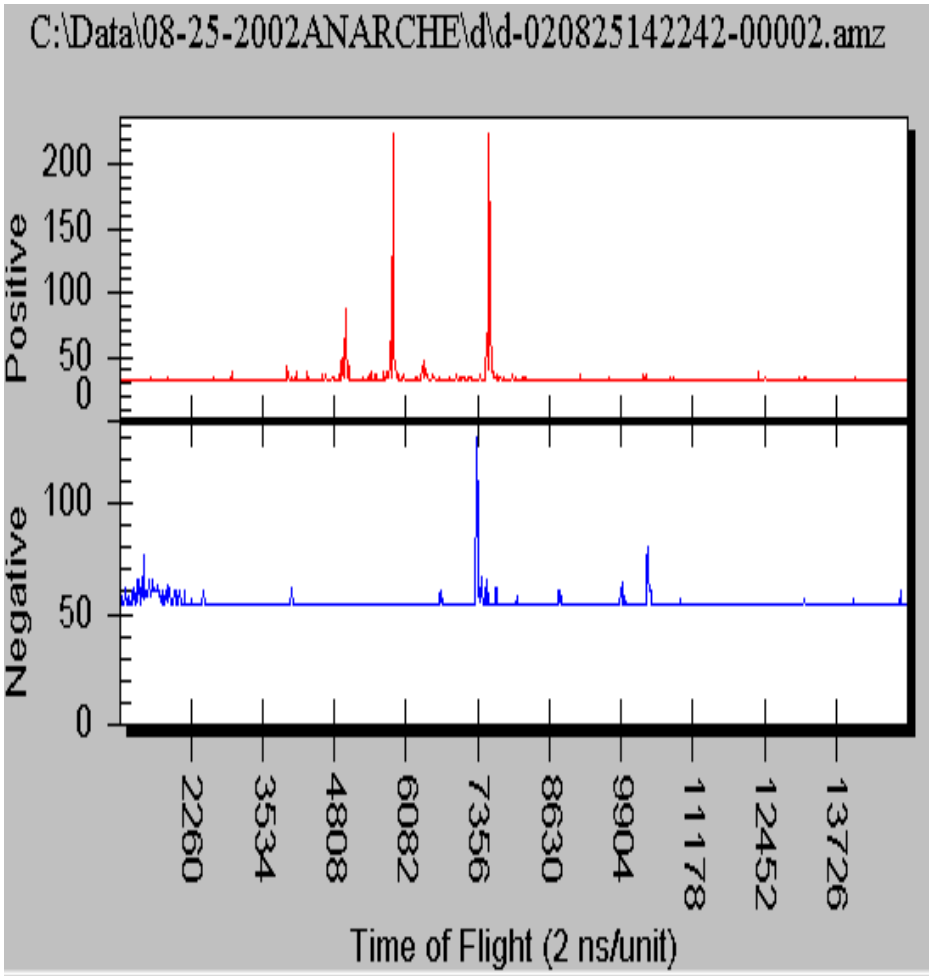
Composition of particles of known density…



size (+)mass (=density) composition



Contaminant or Silver Lining…



- Secondary Amine w/HSO_4
- Heterogeneous Reaction?
- Gas Source → Tygon Tubing, Trailer, Regional???

Future Work

- Smaller Particles
  - Pumping
  - Alignment
- Contaminant
  - Source
- Data Crunching
  - Spectral Averages
  - …

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- Peter McMurry
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- Alla Zelenyuk