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2012 AAAR Conference
Minneapolis, MN
Tutorial #3

Aerosol Mass Spectrometry: Instrumentation for Aerosol Scientists

Jose-Luis Jimenez
Associate Professor & CIRES Fellow
University of Colorado-Boulder

jose.jimenez@colorado.edu
http://cires.colorado.edu/jimenez/ams.html

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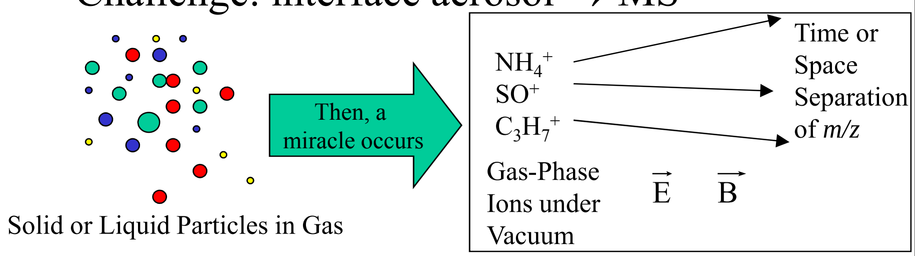
Outline

1. Building Blocks
   – Inlets and sizing
   – Mass spectrometers
2. Instrument Designs
   • Main properties & example applications

Note: focus on most common or useful instruments & last 10 years – don't have time to cover everything, or early work (see references)

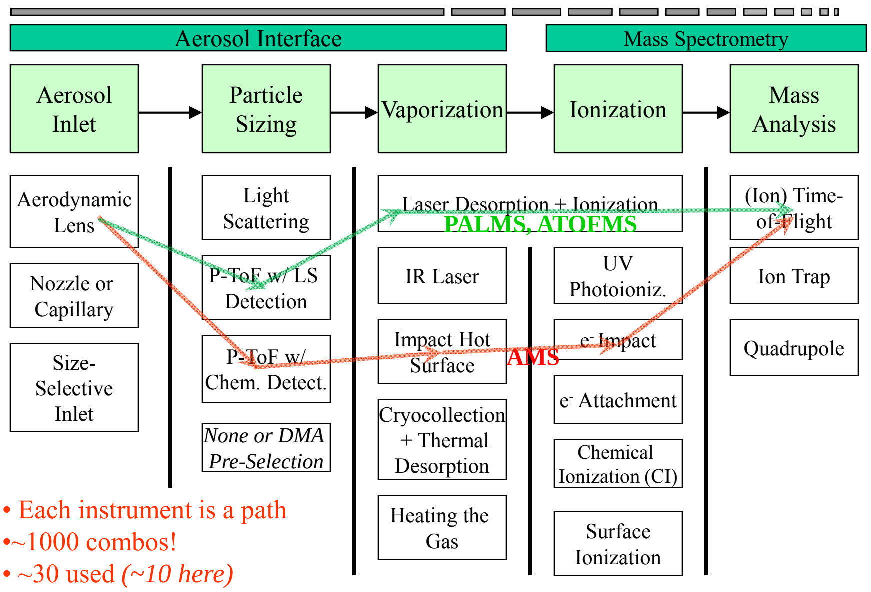
Why Aerosol Mass Spectrometry?

- Mass Spectrometry
  - Extreme sensitivity
  - Very fast response (down to 0.1 ms)
  - Universal detection
  - Field deployable
- Challenge: interface aerosol → MS



Part 1: Instrumentation Building Blocks

Conceptual Schematic of an Aerosol MS

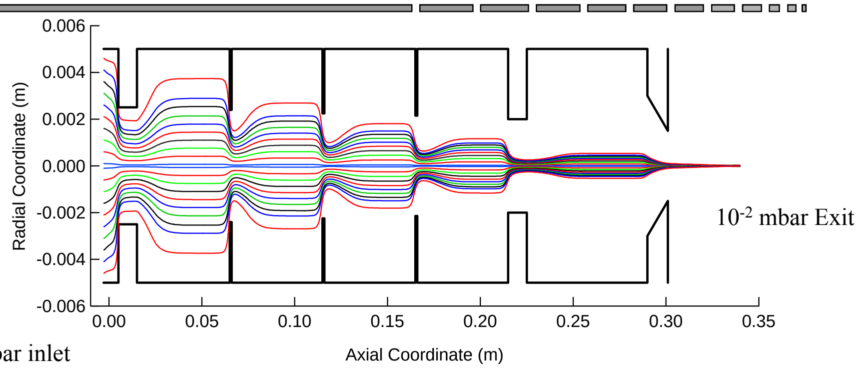


- Each instrument is a path
- ~1000 combos!
- ~30 used *(~10 here)*

Aerosol Inlets

- Particle Beam MS:
  - Introduce the particles into vacuum
  - Concentrate aerosols from gas-phase
    - ~10^{-8}: particle (10 µg m^{-3}) / gas (1 kg m^{-3})
    - Reduce gas-phase interferences
  - Impart size-dependent velocity
    - Use to measure size by *particle* time-of-flight
- Other custom inlets

Aerodynamic Lenses



2 mbar inlet

Calculated Particle Trajectories, 100 nm (Fluent ver 4.47)
Diameter Unit Density Spheres

Original lens design:
- Liu, P., Ziemann, P. L., Kittelson , D. B., and McMurry, P. H. *Aerosol Sci. Technol*. 22:293–313, 1995.
- Liu, P., Ziemann, P. L., Kittelson, D. B., and McMurry, P.H. *Aerosol Sci. Technol.* 22:314–324, 1995.

CFD Simulations:
- Zhang, X., Smith, K.A., Worsnop, D.R., Jimenez, J.L., Jayne, J.T., and Kolb, C.E. *Aerosol Sci. Technol.*, 36: 617, 2002.
- Zhang, X., Smith, K.A., Worsnop, Jimenez, J.L., Jayne, J.T., D.R., Kolb, C.E., Morris, J., Davidovits, P., *Aerosol Sci. Technol.*, 38: 619, 2004.

Aerosol Inlets: Aerodynamic Lenses

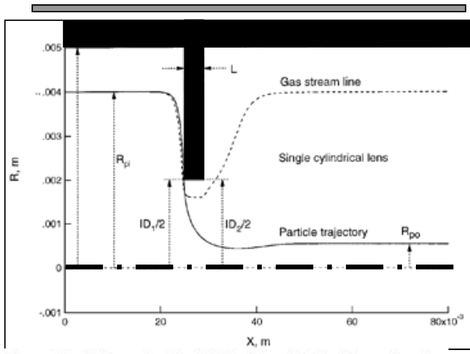


Figure 2. Schematic of a single thin cylindrical lens showing a gas streamline and the trajectory of a 500 nm particle. Q = 60 scc/min, L = 4 mm, $ID_1 = ID_2$ = 2 mm, OD = 10 mm, Re_0 = 12.5, P_{up} = 280 Pa, R_{pi} = 4 mm, R_{po} = 0.5 mm.

Note: original lens design by Liu, Ziemann, and McMurry (1995).

Xuefeng Zhang, Kenneth A. Smith, Douglas R. Worsnop, Jose Jimenez, John T. Jayne, and Charles E. Kolb. A Numerical Characterization of Particle Beam Collimation by an Aerodynamic Lens-Nozzle System: Part I. An Individual Lens or Nozzle Aerosol Science and Technology 36: 617–631 (2002)

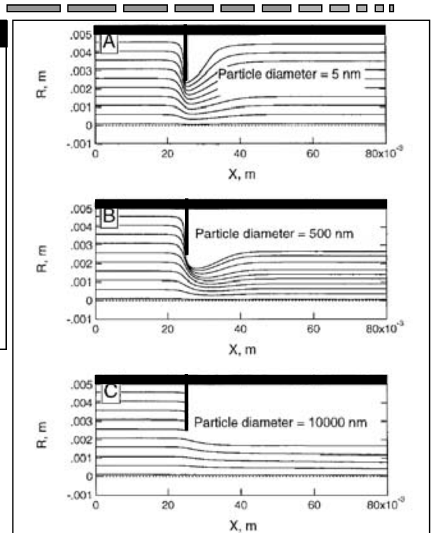


Figure 3. Particle trajectories through a single thin cylindrical lens (D_p = 5,500, 1000 nm). L = 0.5 mm, $ID_1 = ID_2$ = 5 mm, OD = 10 mm, Q = 60 scc/min, Re_0 = 12.5, and P_{up} = 280 Pa.

Beam Width w/ Aerodynamic Lenses

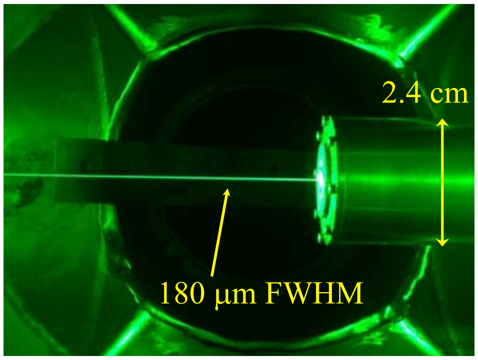


Figure courtesy of Guiseppe Petrucci, Univ. Vermont
http://www.uvm.edu/~gpetrucc

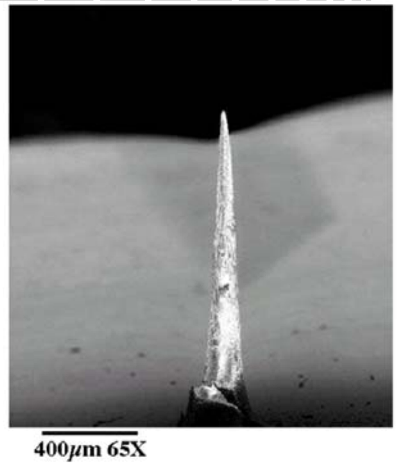
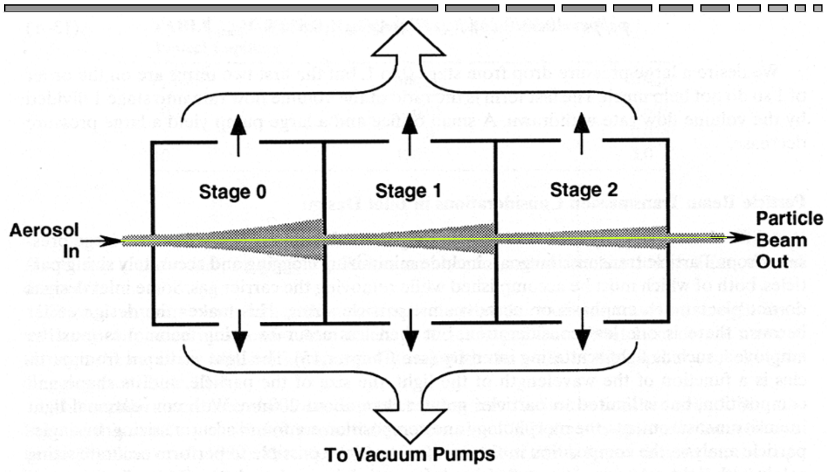


Fig. 6. SEM image of a silicon carbide 'tower' deposited by a focused nanoparticle beam [18].

Heberlein, J., O. Postel, S. Girshick, P. McMurry, W. Gerberichc, D. Iordanoglou, F.D. Fonzo, D. Neumann, A. Gidwani, M. Fan, and N. Tymiakc, Thermal plasma deposition of nanophase hard coatings. *Surface and Coatings Technology*, 2001. **142-144**: p. 265-271.

Differential Pumping of the Gas

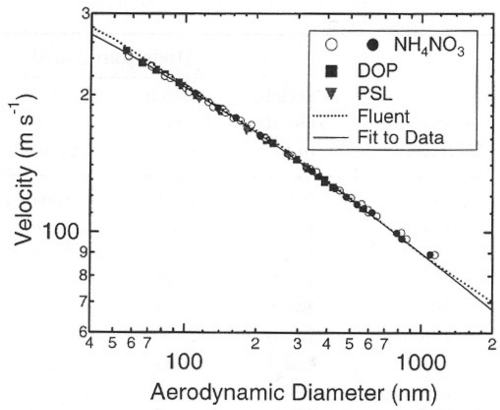


• E.g. in AMS: particles concentrated by 10^7 with respect to gas

Wexler, A. S., and Johnston, M. V. (2001). "Real-time single-particle analysis." Aerosol Measurement: Principles, Techniques, and Applications, P. A. Baron and K. Willeke, eds., Wiley-Interscience, New York, 365-386.

Drag: Size-Dependent Velocity

- Upon expansion into vacuum, particles acquire size-dependent velocity
- It's there, so you may as well use it to measure particle size



Jayne, J.T., D.C. Leard, X. Zhang, P. Davidovits, K.A. Smith, C.E. Kolb, and D.R. Worsnop, Development of an aerosol mass spectrometer for size and composition. analysis of submicron particles, Aerosol Sci. Technol., 33, 49-70, 2000.

Lift: Beam Broadening for Irregular Particles

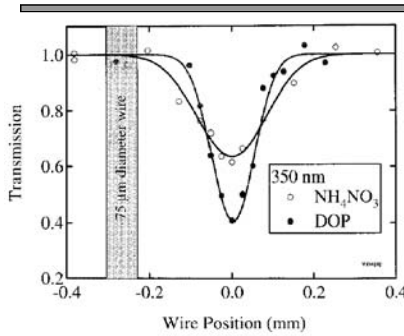


FIGURE 11. Particle beam width measurement for spherical DOP and nonspherical NH$_4$NO$_3$ particles. Beam widths are determined by passing a 75 µm diameter wire across the particle beam path and calculating particle transmission from the ratio of the single particle count rates measured by the mass spectrometer to the count rates measured by the CPC. Beam broadening is observed for nonspherical particles. The solid lines represent a Gaussian fit to the inverted data yielding FWHM values of 0.13 mm for DOP and 0.23 mm for NH$_4$NO$_3$.

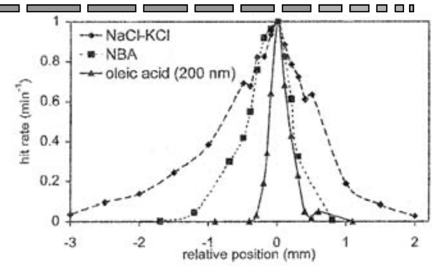


Figure 2. Particle beam profile measurements for NaCl-KCl, NBA, and oleic acid aerosols. NaCl-KCl and NBA aerosols are polydisperse with the average diameter of the detected particles approximately 85 nm. The oleic acid aerosol is monodisperse with a diameter of 200 nm.

(1) This effect can bias the detection of any instrument against irregularly shaped particles. The smaller the solid angle of collection, the worse the potential bias. (2) This effect may be used to obtain a surrogate particle irregularity measurement

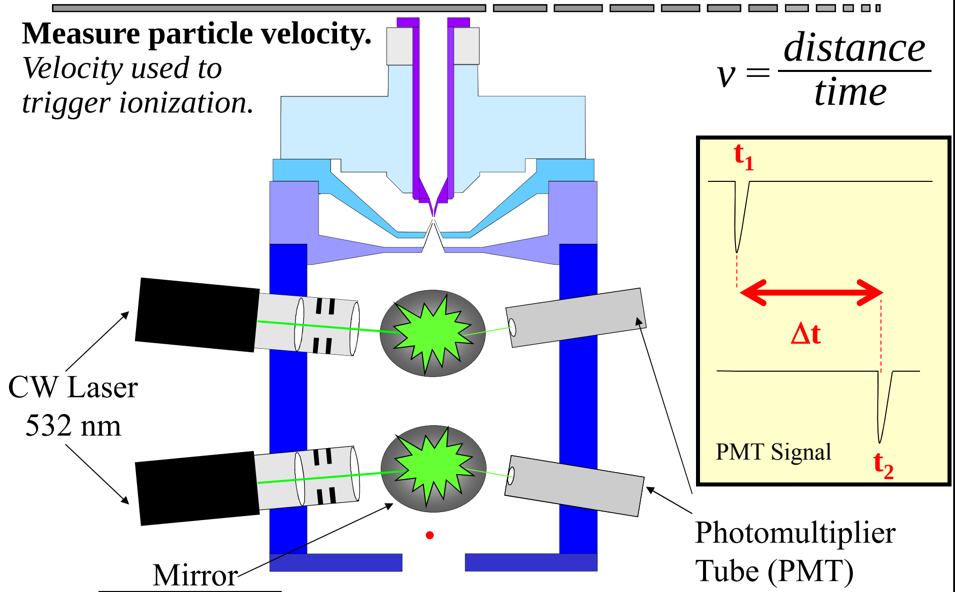
- Jayne, J.T., D.C. Leard, X. Zhang, P. Davidovits, K.A. Smith, C.E. Kolb, and D.R. Worsnop, Development of an aerosol mass spectrometer for size and composition. analysis of submicron particles, Aerosol Sci. Technol., 33, 49-70, 2000.
- David B. Kane, Berk Oktem, and Murray V. Johnston. Nanoparticle Detection by Aerosol Mass Spectrometry. Aerosol Science and Technology 34: 520–527 (2001)

Animation courtesy of Deborah Gross Carleton College

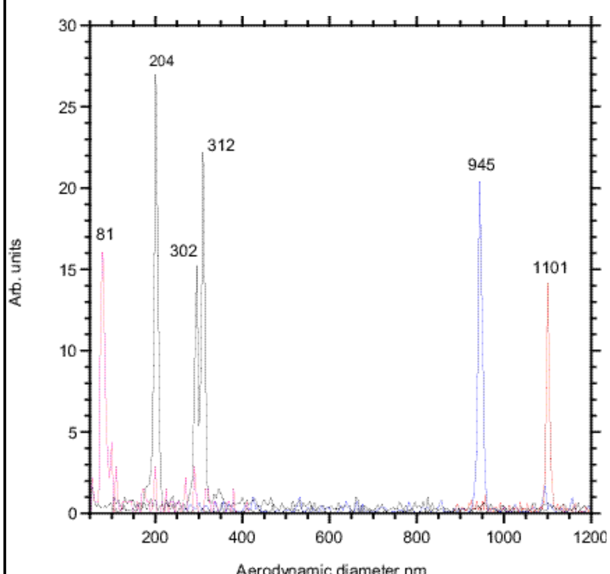
Particle TOF with LS Detection

Measure particle velocity.
Velocity used to trigger ionization.

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



Two-Laser Particle TOF: Resolution



- Very high size resolution
  $R_d = d_{va}/\Delta d_{va} \sim 30$

$$d_{va} = \frac{\rho_p}{\rho_0}\frac{d_{ve}}{\chi_v}$$

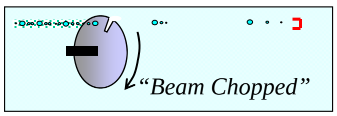
d_{va}: vacuum aerodynamic diameter (see DeCarlo et al., *Aerosol. Sci. Technol.*, 2004)

Zelenyuk, Alla and Imre. Beyond single particle mass spectrometry: multidimensional characterisation of individual aerosol particles, *International Reviews in Physical Chemistry*,28:2,309 -358, 2009.

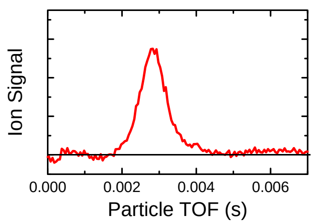
Figure courtesy of Dan Imre.

Size measurement: chopper + chemical detect.

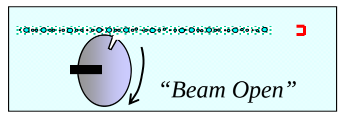
Size Distribution



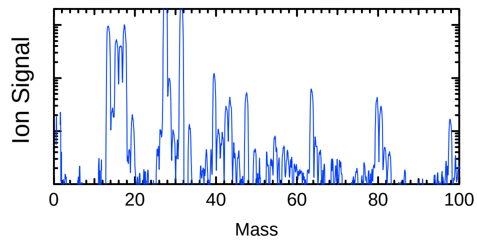
- Size distribution at each *m/z*
- Lower resolution than laser PToF
- But signal cut by ~25!



Ensemble Composition



- No size information
- Much higher signal-to-noise



Size Distribution Quantification

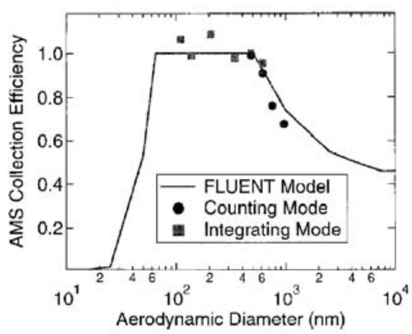
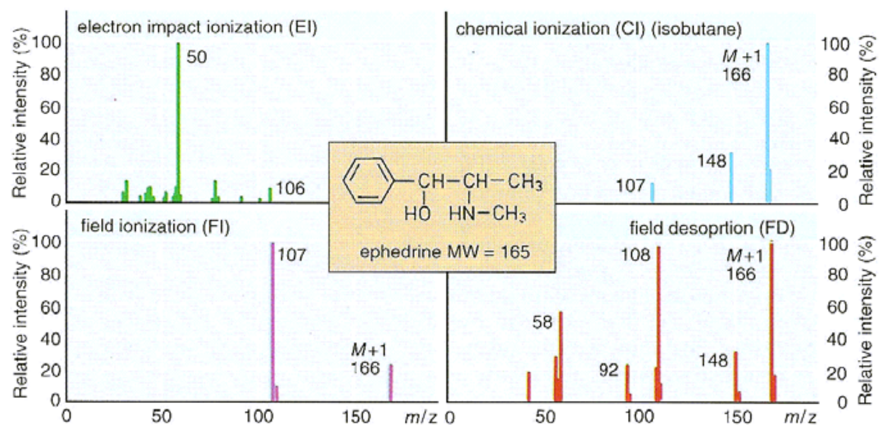


FIGURE 9. Summary of the AMS particle collection/detection efficiency as a function of aerodynamic diameter. Solid line is FLUENT model prediction. Circles are efficiencies determined by comparing AMS and CPC counting rates (data from Figure 8). Squares are collection efficiencies determined from the ratio of the measured to the calculated integrated area of the TOF data shown in Figure 4 (note that the data points originating from Figures 4 and 8 have been converted from mobility to aerodynamic diameter using particle density of 1.72 and a shape factor of 0.8).

- No inlet can transmit all sizes
- Most common: submicron lenses
- Some custom lenses & others

Jayne, J.T., D.C. Leard, X. Zhang, P. Davidovits, K.A. Smith, C.E. Kolb, and D.R. Worsnop, Development of an aerosol mass spectrometer for size and composition. analysis of submicron particles, Aerosol Sci. Technol., 33, 49-70, 2000.

Effect of Ionization Techniques



K. Comparison of mass spectra following different ionization methods

- Information is complementary
- Obtain data from more than one technique

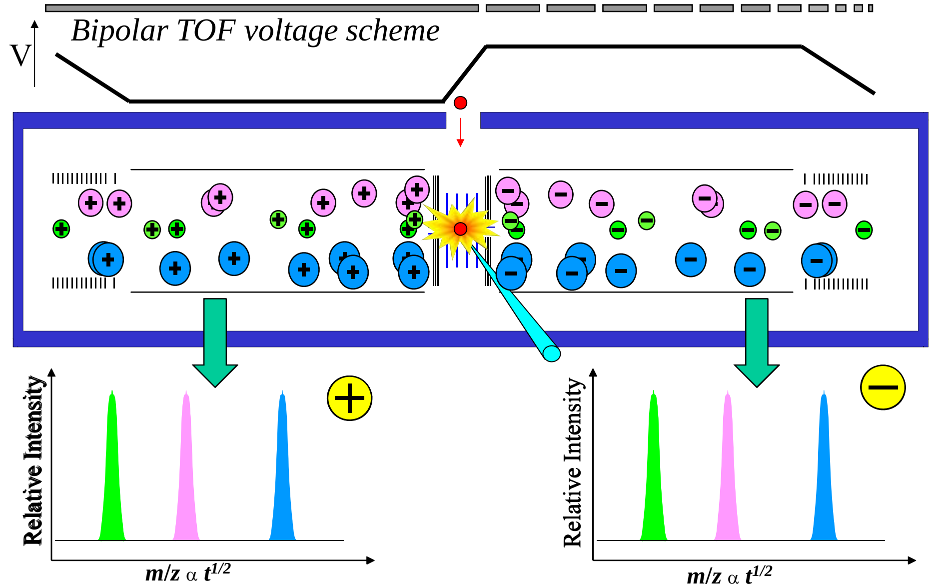
From Schewdt, The Essential Guide to Analytical Chemistry, Wiley, 1997

Mass Spectrometer

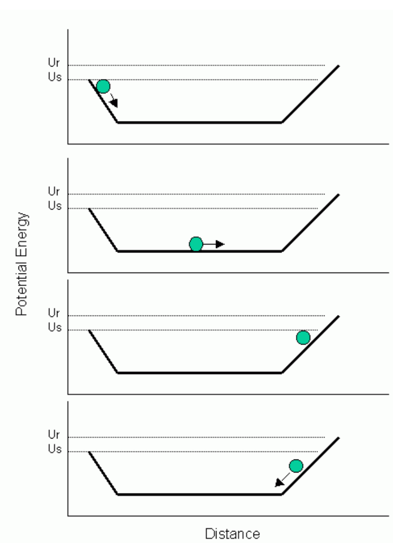
- Now we have made some ions
- Electrical / magnetic forces to sort ions according to *m/z*
- In most aerosol mass spectrometers
  - **(Ion) Time-of-Flight**
  - Quadrupole or Ion Trap
- Not generally used so far in Aerosol MS
  - Electric & magnetic sectors
  - Fourier Transform – Ion Cyclotron Resonance
  - Orbitrap
- More info on:
  - http://tinyurl.com/CHEM-5181 (my course)
  - http://en.wikipedia.org/wiki/Mass_spectrometry

Mass Spectrometer: (Ion)Time-of-Flight

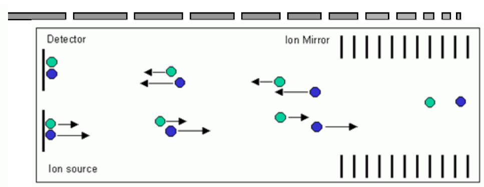
Animation courtesy of Deborah Gross Carleton College 19



Reflectron



From: http://www.chemistry.wustl.edu/~msf/damon/reflectrons.html



Reflectron consists of a series of electrodes, forming a linear field in direction opposite of initial acceleration.

Ions are slowed by this field, eventually turning around and accelerating back in direction of detector.

Penetration depth depends on U_s, which is function of U_0 and acceleration field, E.

Reflectron voltages are tuned to create a space focus at the plane of the detector.

Adapted from Joel Kimmel

An Inherent Dilemma

TOFMS is an ideal detector for pulsed ionization methods

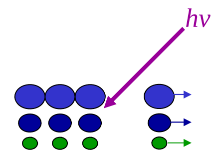
If ionization event is synchronized with time zero, high duty cycle is achieved

Because of pulsing, ions are wasted when TOFMS is applied to a continuous source

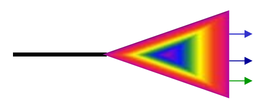
&

Increased efficiency comes at the expense of mass range and mass resolution

Still, figures of merit and cost make the technique desirable



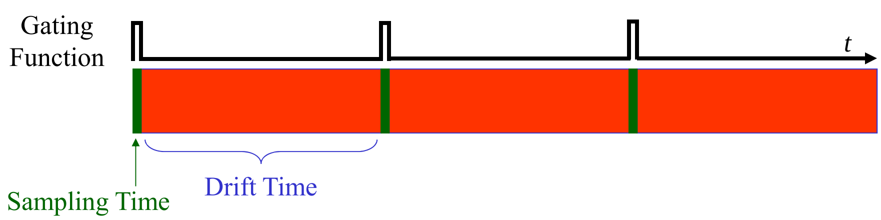
Laser Desorption: Static, solid sample probed with a pulsed laser



ESI: Sample is continuously flowing towards the mass analyzer

Adapted from Joel Kimmel

Performance Trade-offs: On Axis

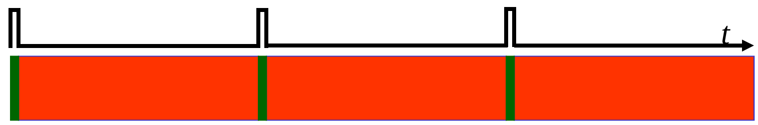


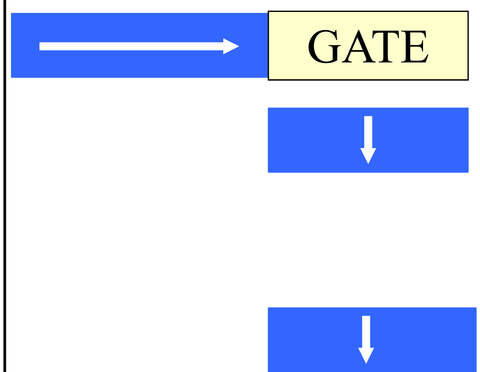
$$\textit{Duty Cycle} \approx \frac{\textit{Sampling Time}}{\textit{Sampling Time} + \textit{Drift Time}}$$

Δt proportional to sampling time

Mass Range proportional to drift time

Orthogonal Extraction

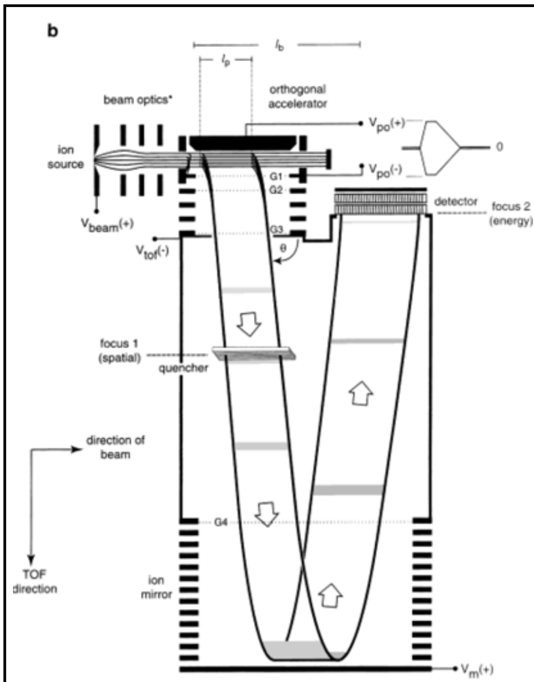




Ions are extraction in a direction orthogonal to source trajectory

Extraction event is still rapid (Δt), but extraction volume is determined by length of gate region.

oTOFMS



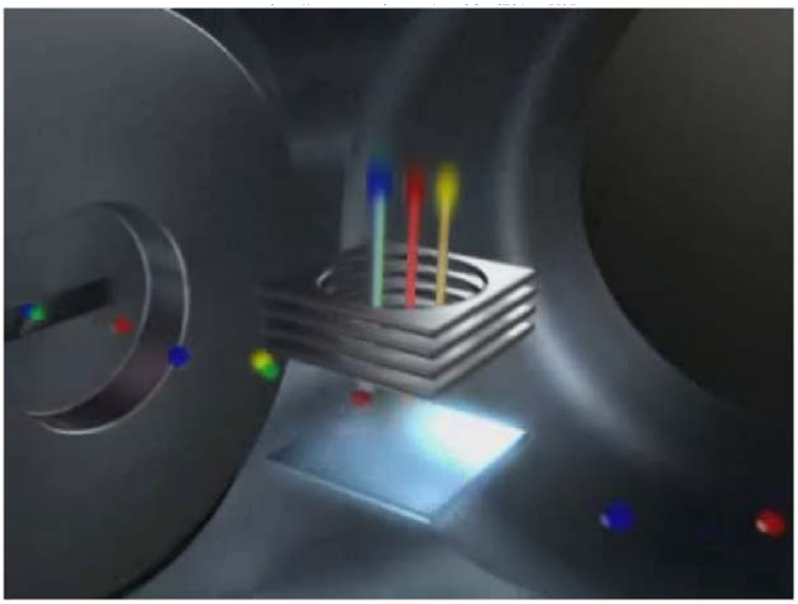
•Able to reduce average initial energy in ToF direction to 0 (resolution and accuracy).

•Independent control of beam energy and drift energy, allows maximum duty cycle.

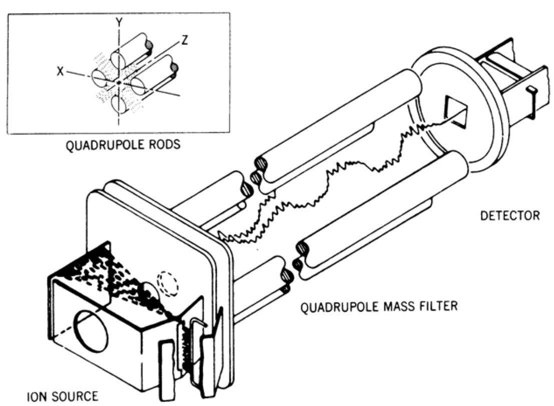
•Want tightly collimated beam in extraction region

See: Guilhaus, *et al. Mass Spec Rev*, 2000, 65-107

TOFMS Animation from Agilent:



Mass Spectrometer: Quadrupole

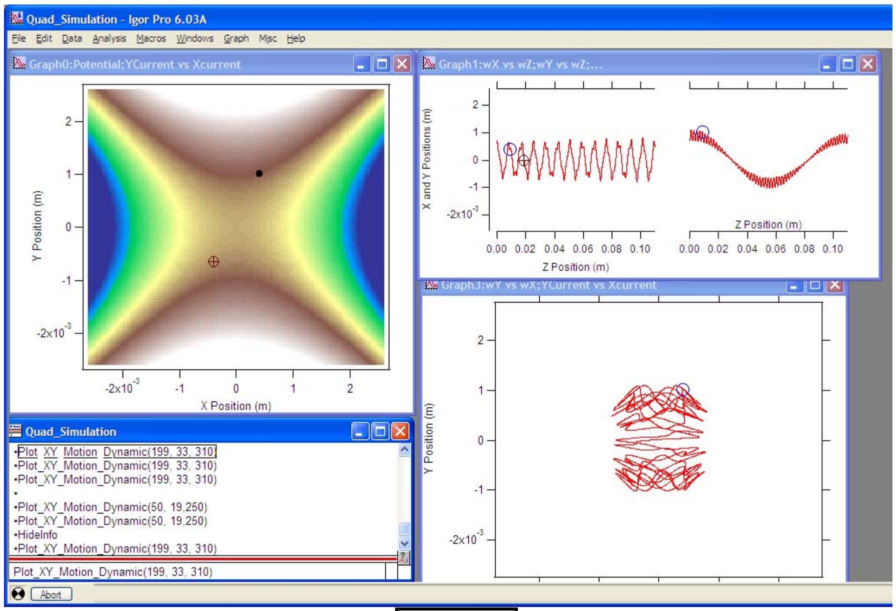


J. Throck Watson: Introduction to Mass Spectrometry. Lippincott-Raven, 1997.

FIG. 4.7. Schematic diagram of quadrupole mass spectrometer illustrating irregular flight path of ions from the ion source through the central space between the quadrupole rods to the detector. (Courtesy of Finnigan Corporation.)

- Advantage: simple, rugged, lightweight
- Disadvantage: only one *m/z* at a time

Quad Simulation



Mass Spectrometer: Ion Trap

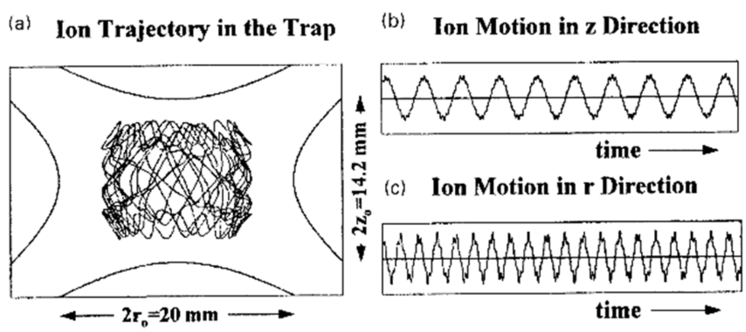
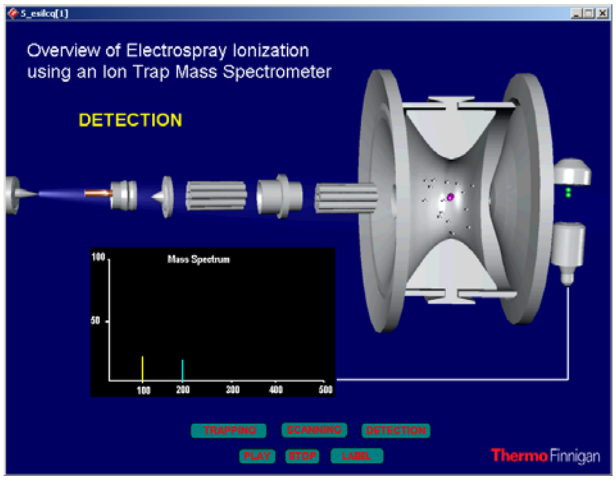


Figure 13-24 Simulation of motion of a single trapped ion in an ion trap: (a) shows the overall motion within the trap in cross section, (b) shows the time-dependent component of motion in the axial direction, and (c) shows the radial-direction component.

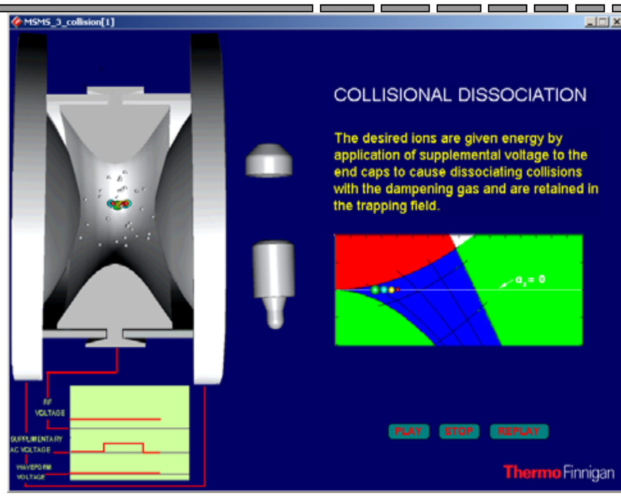
J.B. Lambert, H.F. Shurvell, D.A. Lightner, R. G. Cooks, Organic Structural Spectroscopy. Prentice-Hall, 2002.

Ion Trap Movie



- These and more available at:
  - http://tinyurl.com/CHEM-5181

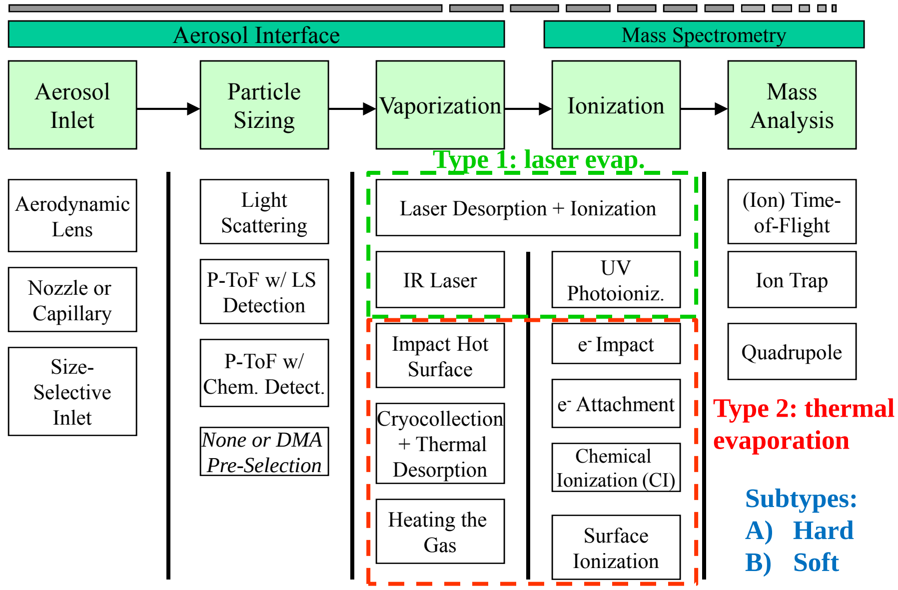
MS/MS with an Ion Trap



- MS/MS: isolate an ion, break it into pieces
  - Obtain its "mass spectrum"

Part 2: Instrument Implementations

Conceptual Schematic of an Aerosol MS



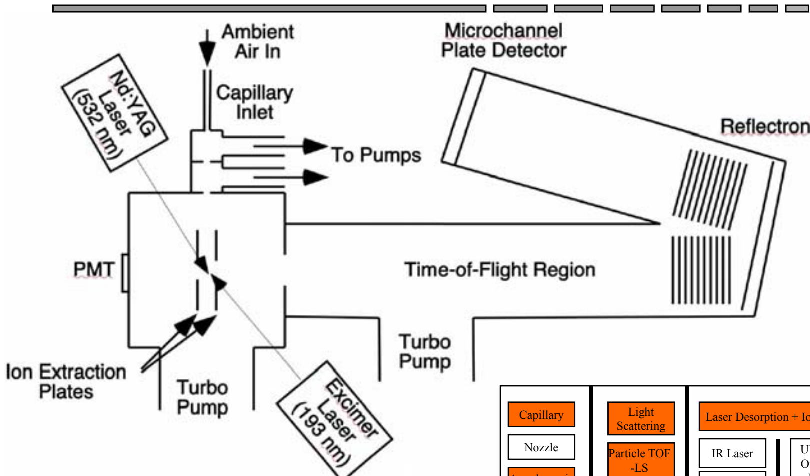
Type 1A:
Laser Vaporization + Ionization

- Particle Analysis by Mass Spectrometry (PALMS): Dan Murphy et al., NOAA-Boulder (co-developed by M. Johnston)
- Aerosol Time-of-Flight Mass Spectrometer (ATOFMS): Kim Prather et al., U. California (R/SD)
- Single-Particle Laser Ablation Mass Spectrometer (SPLAT): Alla Zelenyuk, Dan Imre et al., US DOE PNNL

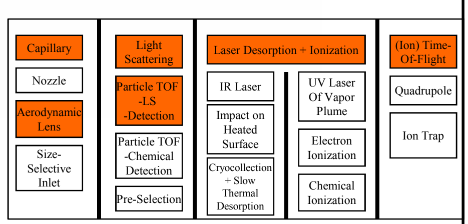
Some Key Publications

- D.M. Murphy. The design of single-particle mass spectrometers. *Mass Spec. Rev.*, 26, 150– 165, 2007.
- D. M. Murphy, D. J. Cziczo, K. D. Froyd, et al., Single-particle mass spectrometry of tropospheric aerosol particles, J. Geophys. Res., 111, D23S32, doi:10.1029/2006JD007340, 2006.
- K.A. Pratt, J.E. Mayer, J.C. Holecek, R.C. Moffet, R.O. Sanchez, T.P. Rebotier, P. Thomas , H. Furutani, M. Gonin, K. Fuhrer, Y.X. Su, S. Guazzotti, K.A. Prather. Development and Characterization of an Aircraft Aerosol Time-of-Flight Mass Spectrometer. *Anal. Chem.*, 81, 1792-1800, 2009.
- A. Zelenyuk, and D. Imre. Beyond single particle mass spectrometry: multidimensional characterisation of individual aerosol particles, *International Reviews in Physical Chemistry*, 28:2,309 -358, 2009.

Type 1A: PALMS (Murphy *et al.*)

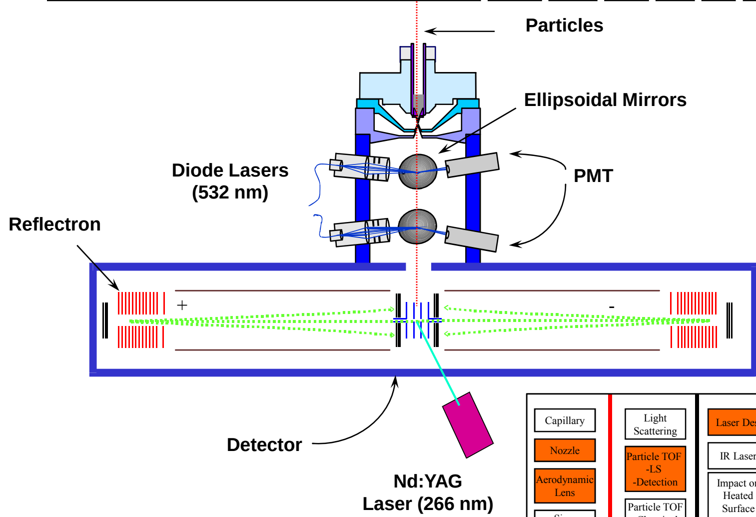


Middlebrook, A., Murphy, D.M., et al. An intercomparison of Particle Mass Spectrometers During the 1999 Atlanta Supersite Project. Journal of Geophysical Research-Atmospheres, 108(D7), 8424, doi:10.1029/2001JD000660, 2003.



Intro Inlets & Sizing TOFMS Other MS LDI AMS CIMS Conc.

Type 1A: ATOFMS (Prather *et al.*)



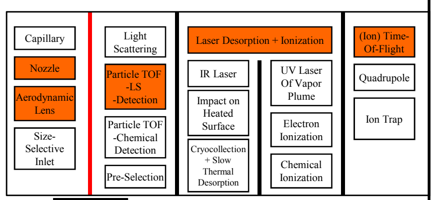
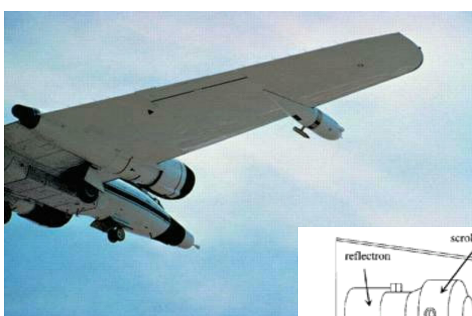


Figure courtesy of Prof. Kim Prather

Type 1A: PALMS on Nose of WB-57



- Very short inlet to minimize perturbation of particles (e.g. evaporation)
- Pilot has on/off switch

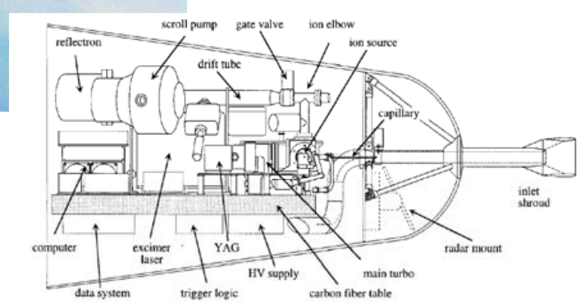
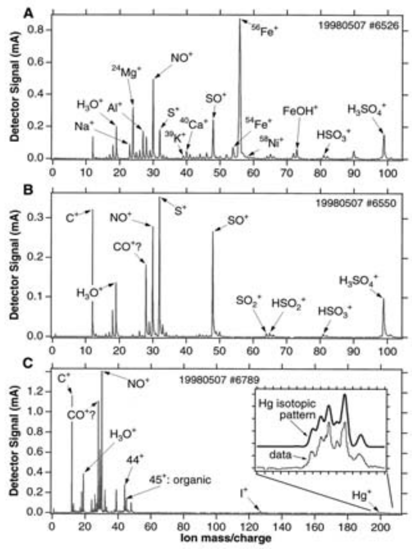


FIGURE 3. Schematic layout of the PALMS instrument components. For scale, the carbon fiber table is 122 cm (48") long.

David S. Thomson, Mike E. Schein, and Daniel M. Murphy. Particle Analysis by Laser Mass Spectrometry: WB-57F Instrument Overview. Aerosol Science and Technology 33:153-169 2000.

Type 1A: PALMS: Stratospheric Aerosols

Murphy et al. (1998) Science, 282, 1664

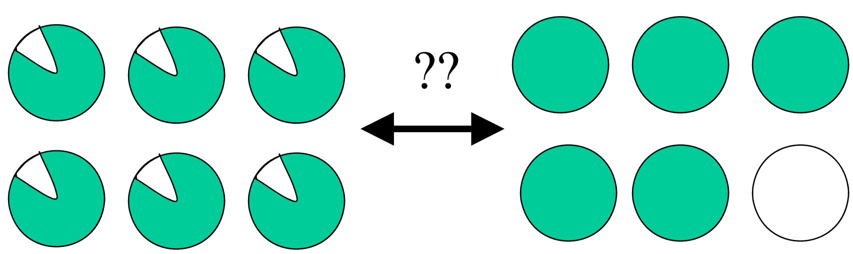


- Several common types of positive ion spectra in the stratosphere.
- The most common type contained iron, magnesium, and other metals as well as sulfate (A). About half of the stratospheric spectra had a large Fe peak.
- Between 20 and 40% of the spectra obtained more than 2 km above the tropopause showed little Fe, Hg, K, or other metals (B).
- Some organic material and NO^+ was almost always present.
- Some particles contained mercury (C), usually with a distinctive pattern of other peaks including a large C^+ peak and a peak at m/z = 127 that is presumed to be I^+.
- These spectra were obtained within minutes of each other in an otherwise fairly homogeneous air mass at 19 km

Ensemble vs. Single Particle Analysis

For example: 17% of the mass is organics, 83% is sulfate

"Internally Mixed" "Externally Mixed"



- Single Particle instruments DIRECTLY detect the mixing state
  - Superior for e.g. ice nucleation studies (also refractory)
  - Ensemble averaging instruments only provide indirect info. on mixing state
- SP also superior for low number density situations

Type 1A: Nano Aerosol MS (NAMS)

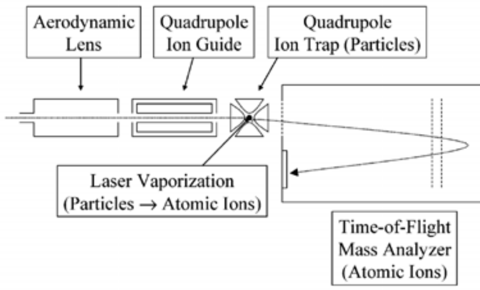


Figure 1. Basic design of the nanoaerosol mass spectrometer.

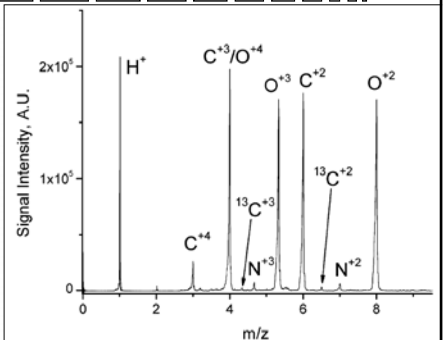


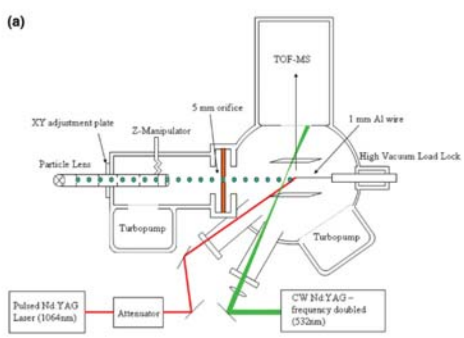
Figure 2. Low *m/z* region of the mass spectrum of ~10-nm-diameter sucrose particles, average of 50 individual spectra.

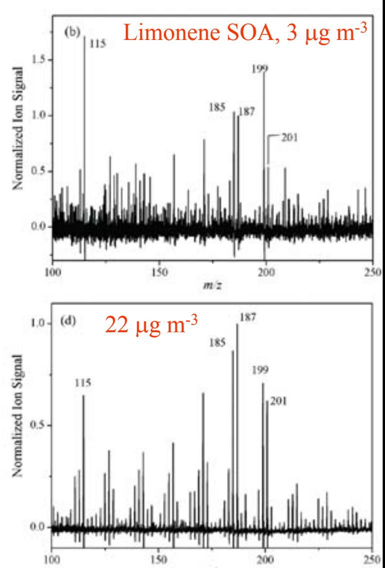
- Extremely high laser intensity
- Turn all atoms in the particle into multiply charged ions (high sens.)
- Determine elemental composition of nanoparticles

• S. Wang, C.A. Zordan, and M.V. Johnston. Chemical Characterization of Individual, Airborne Sub-10-nm Particles and Molecules. *Anal. Chem.* 2006, 78, 1750-1754

• NAMS follows up on earlier work from Reents and Ge, *Aerosol Sci. Technol.* 33, 122, 2000.

Type 1B: Near IR-LDI-MS





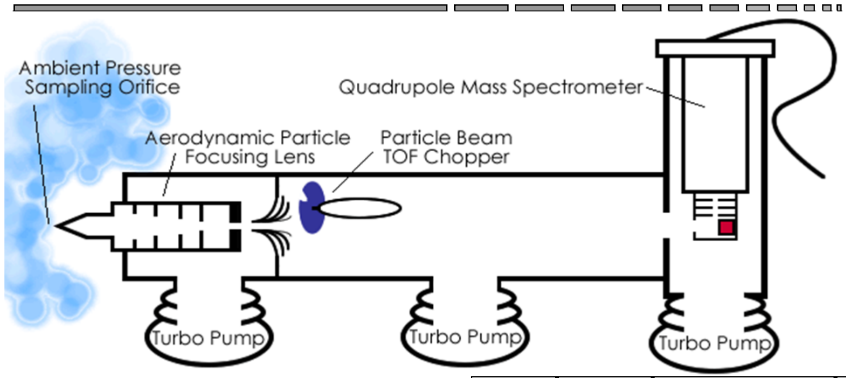
- High signal w/ low fragmentation

S. Geddes, B. Nichols, S. Flemer, J. Eisenhauer, J. Zahardis, and G.A. Petrucci. Near-Infrared Laser Desorption/Ionization Aerosol Mass Spectrometry for Investigating Primary and Secondary Organic Aerosols under Low Loading Conditions. *Anal. Chem.*, ASAP paper, doi: 10.1021/ac1013354.

Type 2A:
TD + Electron Impact

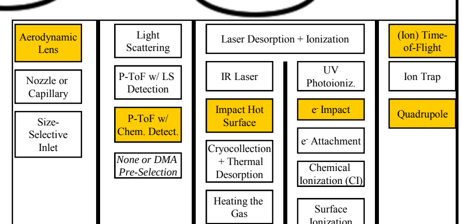
- Aerosol Mass Spectrometer (AMS): Aerodyne + 70 groups, Worsnop, Jayne, *et al.*
- Thermal Desorption Particle Beam MS (TDPBMS): UC Riverside, Ziemann *et al.*
- Thermal Desorption Aerosol GC/MS (TAG): UC Berkeley, Goldstein *et al.*

Type 2A: Aerodyne AMS

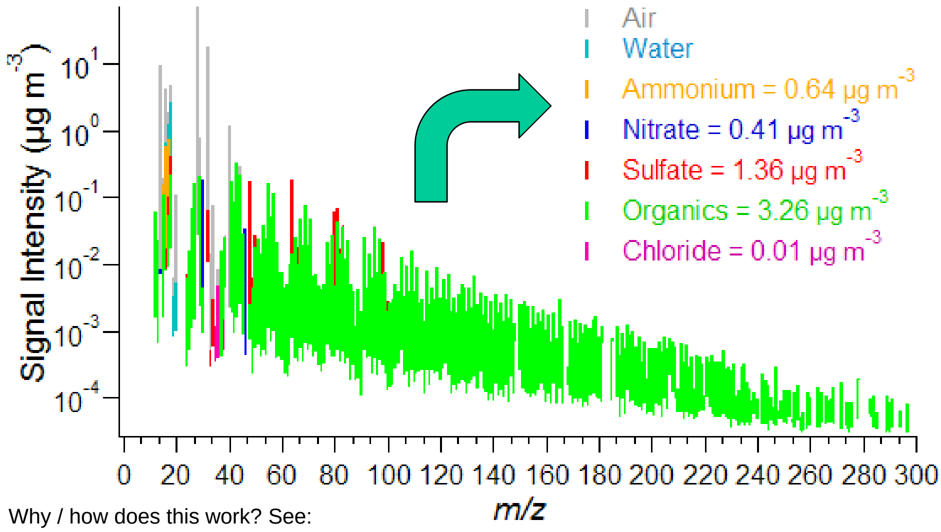


Key instrument papers

- Jayne et al., *Aerosol Sci. Technol.* 33, 49-70, 2000.
- Jimenez et al., *J. Geophys. Res.-Atmos.*, 108, 8425, 2003.
- Drewnick et al., *Aerosol Sci. Technol.*, 39, 637-658, 2005.
- DeCarlo et al., *Anal. Chem.*, 78, 8281-8289, 2006.
- Canagaratna et al. *Mass Spec. Rev.*, 26, 185-222, 2007.



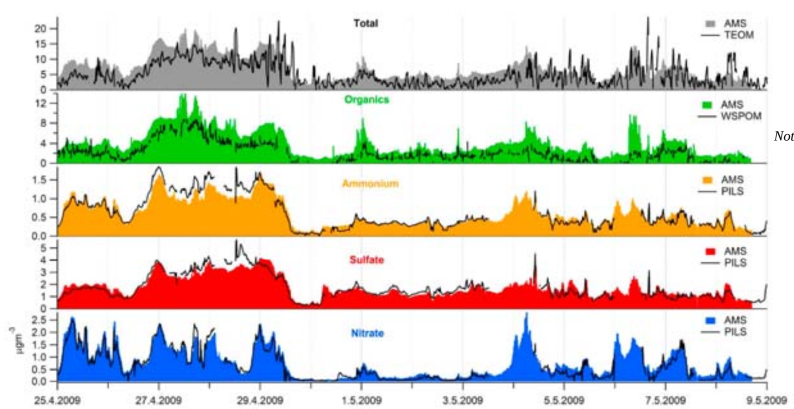
AMS: Ambient Mass Spectrum



Why / how does this work? See:

- Jimenez et al. *J. Geophys. Res.*, 108, 8425, 2003.
- Allan et al., *J. Aerosol Sci.*, 35, 909, 2004.
- Canagaratna et al., *Mass. Spec. Rev*., 26, 185-222, 2007

AMS vs. Other Instruments: Helsinki

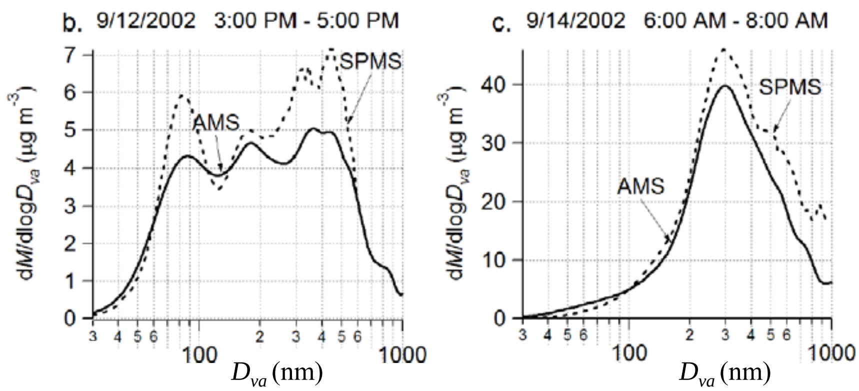


Note OA > WSOA

Fig. 2. Concentrations of major ions and WSPOM (using conversion factor 1.6 to convert WSOC to WSPOM) measured by PILS-TOC-IC and AMS from 25 April to 8 May 2009. PILS-TOC-IC (ions, WSPOM) and TEOM (total mass) results are marked with the black line. AMS results are marked with colors (blue = nitrate, red = sulfate, yellow = ammonium, green = total organics, grey = total mass i.e. sum of ions and organics).

Timonen, H., M. Aurela, S. Carbone, K. Saarnio, S. Saarikoski, T. Makela, M. Kulmala, V.-M. Kerminen, D.R. Worsnop, and R. Hillamo. High Time-resolution Chemical Characterization of the Water-soluble Fraction of Ambient Aerosols with PILS-TOC-IC and AMS. *Atmospheric Measurement Techniques*, 3, 1063-1074, 2010.

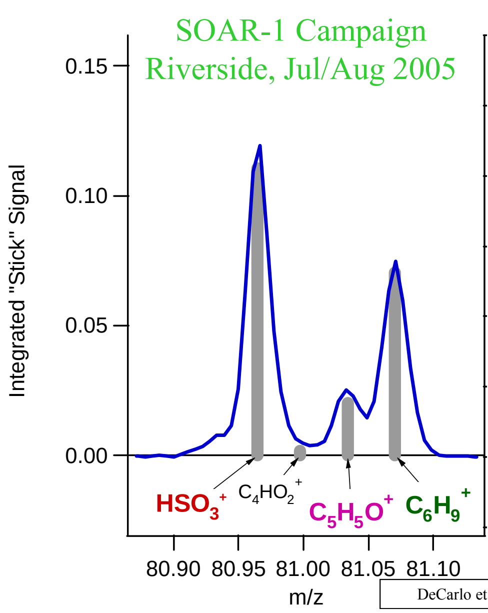
AMS: Comparison with SMPS

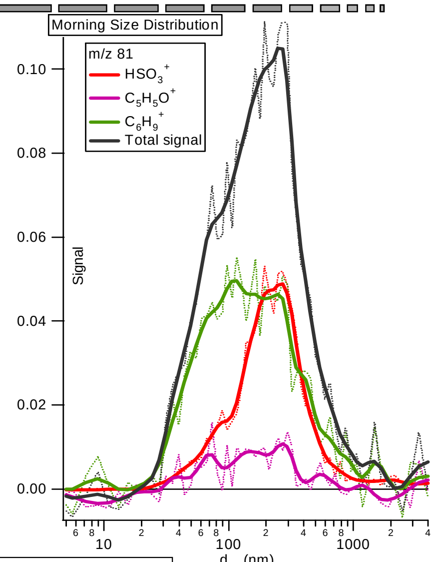


- Typical level of agreement between AMS and SMPS
- Real differences: effect of shape, refractory particles, size transmission…

Q. Zhang, M.R. Canagaratna, J.T. Jayne, D.R. Worsnop, and J.L. Jimenez. Time and Size-Resolved Chemical Composition of Submicron Particles in Pittsburgh – Implications for Aerosol Sources and Processes. *J. Geophys. Res.*, 110, D07S09, doi:10.1029/2004JD004649, 2005.
http://cires.colorado.edu/jimenez/Papers/Pittsburgh_Overview.pdf

First High Resolution Aerosol Field Data

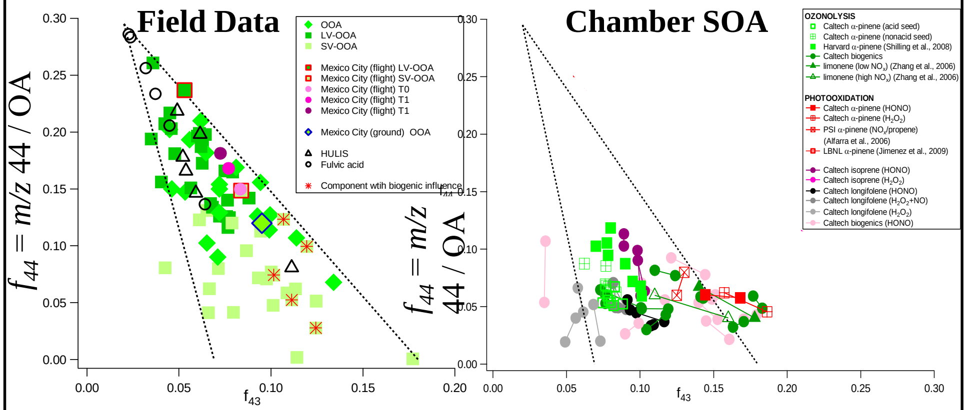




DeCarlo et al., *Anal. Chem.* 2006

Intro Inlets & Sizing TOFMS Other MS LDI AMS CIMS Conc.

AMS *m/z* markers: Field vs. Lab Comparisons

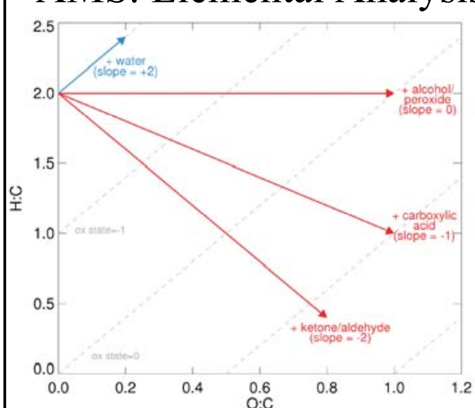


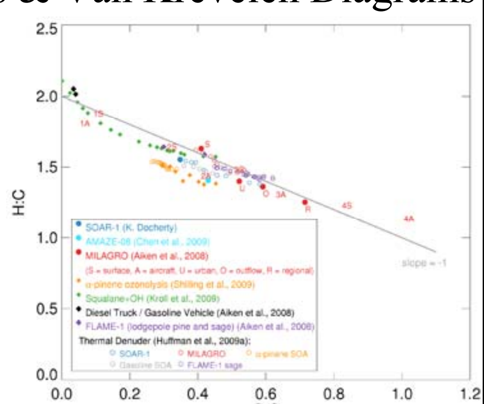
f_{43} = *m/z* 43 / OA $\quad$ f_{43} = *m/z* 43 / OA

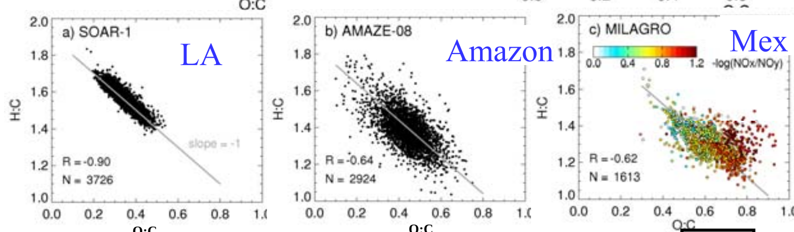
- Not enough OH exposure?
  - < 6 x 10^7 molec cm^{-3} hr (chamber) vs 5 x 10^8 (atmosphere)

Ng, Canagaratna, Zhang, Jimenez, et al., Atmos. Chem. Phys. 10, 4625-4641

AMS: Elemental Analysis & Van Krevelen Diagrams

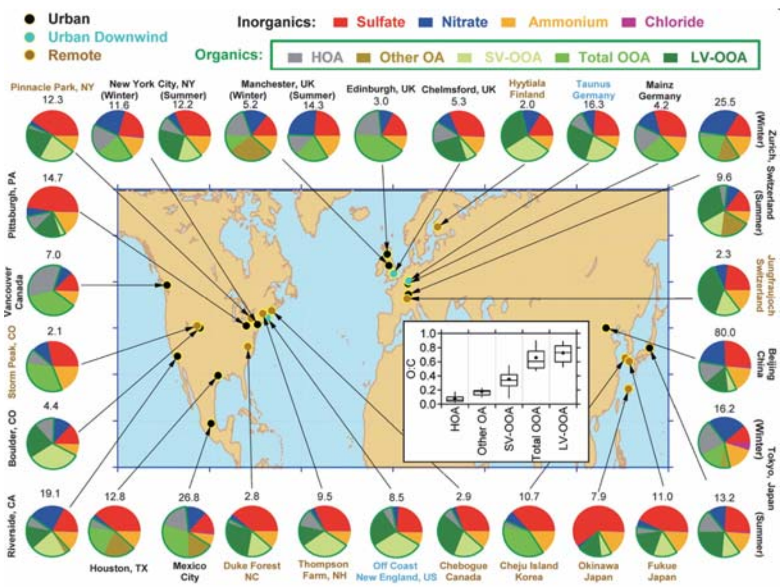






C.L. Heald, et al. A simplified description of organic aerosol composition and implications for atmospheric aging. *Geophys. Re. Lett.*, 37, L08803, 2010.

AMS: Non-Refractory Composition Worldwide



Jimenez, Canagaratna, Donahue, et al., Science 326, 1525 (2009)

Type 2B:
TD + Soft Ionization

- Aerodyne MOVI-CIMS: UW, R. Yatavelli & J. Thornton
- Aerosol Chemical Ionization MS (A-CIMS): U. Georgia, G. Smith *et al.*
- Thermal Desorption Chemical Ionization MS (TDCIMS): NCAR, J. Smith *et al.*

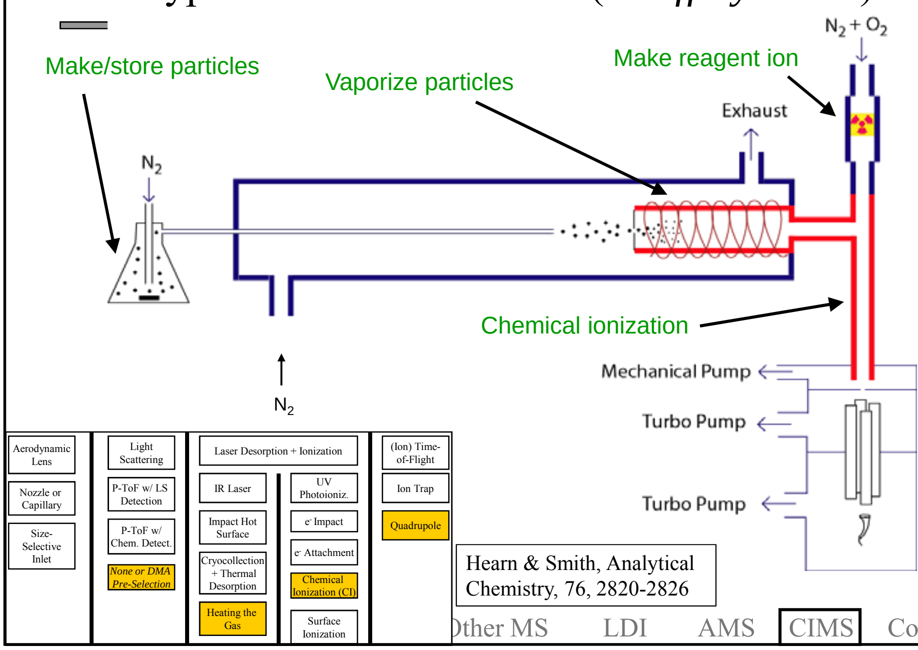
• R.L.N.Yatavelli, F. Lopez-Hilfiker, J.D. Wargo, J.R. Kimmel, M.J. Cubison, T.H. Bertram, J.L. Jimenez, M. Gonin, D.R. Worsnop, J.A. Thornton. A Chemical Ionization High-Resolution Time-of-Flight Mass Spectrometer Coupled to a Micro Orifice Volatilization Impactor (MOVI-HRToF-CIMS) for Analysis of Gas and Particle-Phase Organic Species. *Aerosol Sci. Technol.*, 46, 1313–1327, 2012.
• A New Chemical Ionization Mass Spectrometry Method for the Online Analysis of Organic Aerosols. John D. Hearn and Geoffrey D. Smith, *Anal. Chem.*, 76, 2820-2826, 2004.
• Thermal Desorption Chemical Ionization Mass Spectrometer for Ultrafine Particle Chemical Composition, D. Voisin et al., *Aerosol Sci. Technol.*, 37, 471-475, 2003.

Ionization: Chemical

- Electron transfer: $M + I^- \rightarrow M^- + I$
- Proton transfer: $M + H_3O^+ \rightarrow (M{+}H)^+ + H_2O$
- Adduct formation: $M + CF_3O^- \rightarrow (M{+}\,CF_3O)^-$

- Need Collisions!
  - λ < 0.1 mm (P > 1 mbar)
  - Sometimes at 1 atm (APCI)

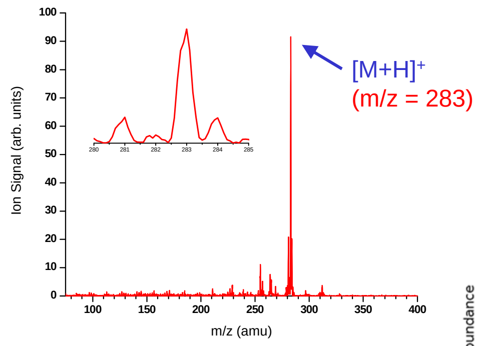
Type 2B1: Aerosol CIMS (*Geoffrey Smith*)

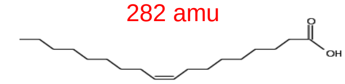


Hearn & Smith, Analytical Chemistry, 76, 2820-2826

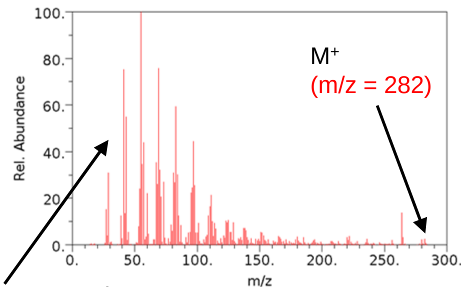
Low Fragmentation with Chemical Ionization

Chemical Ionization using $H^+(H_2O)_2$





Electron Impact (EI) Ionization



Low degree of fragmentation aids in:

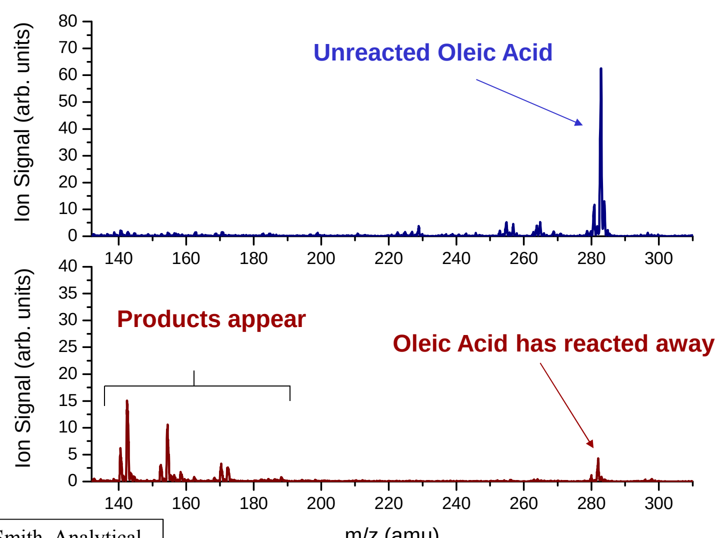
- identification
- quantification

Large degree of fragmentation

From: NIST Chemistry WebBook

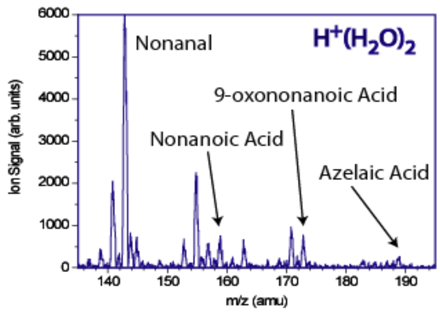
Hearn & Smith, Analytical Chemistry, 76, 2820-2826

Mass Spectra of Reacted Particles

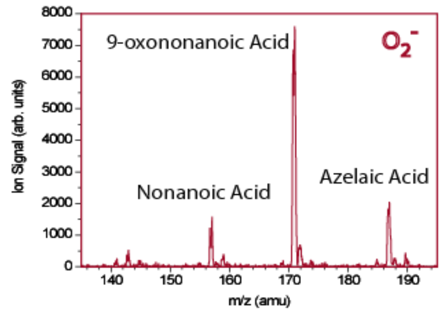


Hearn & Smith, Analytical Chemistry, 76, 2820-2826

Use of different CI reagent ions



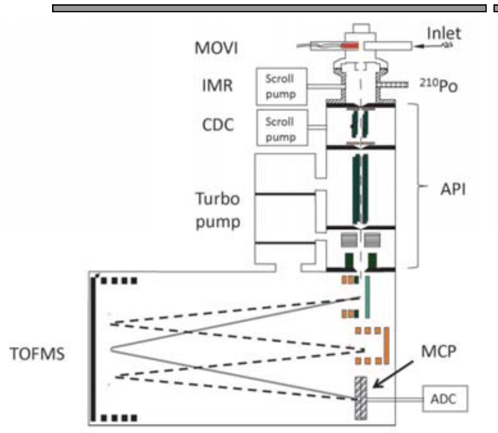
Proton transfer



Negative CI with O_2^-

Hearn & Smith, "Kinetics and Product Studies for Ozonolysis Reactions of Organic Particles Using Aerosol CIMS, *J. Phys. Chem. A*, 108, 10019-10029 (2004).

UW/Aerodyne MOVI-CIMS



- R.L.N. Yatavelli, F. Lopez-Hilfiker, J.D. Wargo, J.R. Kimmel, M.J. Cubison, T.H. Bertram, J.L. Jimenez, M. Gonin, D.R. Worsnop, J.A. Thornton. A Chemical Ionization High-Resolution Time-of-Flight Mass Spectrometer Coupled to a Micro Orifice Volatilization Impactor (MOVI-HRToF-CIMS) for Analysis of Gas and Particle-Phase Organic Species. *Aerosol Sci. Technol.*, 46, 1313–1327, 2012.
- R.L.N. Yatavelli, and J.A. Thornton. Particulate Organic Matter Detection Using a Micro-Orifice Volatilization Impactor Coupled to a Chemical Ionization Mass Spectrometer (MOVI-CIMS). *Aerosol Sci. Technol.*, 44:61–74, 2010.

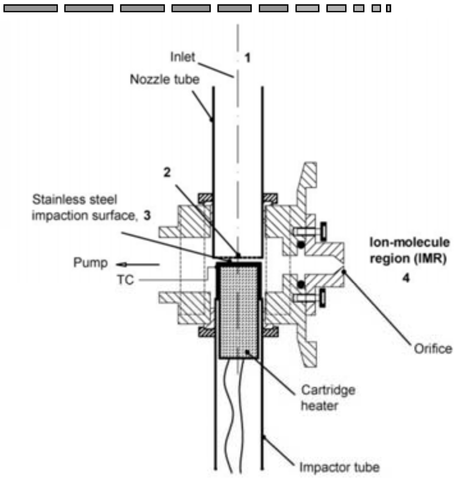


FIG. 1. Schematic of the improved micro-orifice volatilization impactor. Numbers 1–4 correspond to different pressure regions with region 3 at 863 mbar and region 4 at 90 mbar.

My Take on Near Future of Aerosol MS

- Components
  - Inlets: aerodynamic lenses dominate, slowly going supermicron
  - Practical soft ionization finally coming online
    - Results are extremely complex, more degrees of freedom
  - EI and LDI will remain important
- Uses of Aerosol MS
  - *Research* tool
    - Commonplace, e.g. at least one in each field study site / airplane…
    - Advanced users/developers vs. basic users
  - Rapidly expanding into advanced monitoring (ACSM)
  - Specialization on what different techniques do well, e.g.:
    - LDI for ice nucleation, low number density situations, mixing state
    - AMS and soft ionization for organic aerosols
    - NAMS and TDCIMS for nanoparticles
- New techniques will continue to be developed

  - Specialized for problems that the commercial instruments don’t do well

Some Additional References

- Special issues on mass spectrometry of aerosols
  - *Aerosol Science and Technology*, 33(1-2), July/Aug. 2000.
  - *International Journal of Mass Spectrometry*, 258(1-3), Dec. 2006
- Other review papers, first two good historical reviews:
  - David T. Suess and Kimberly A. Prather (1999). Mass Spectrometry of Aerosols. *Chem. Rev.* 99, 3007-3035.
  - Noble, C. A., and Prather, K. A. (2000). “Real-time single particle mass spectrometry: A historical review of a quarter century of the chemical analysis of aerosols.” *Mass Spec. Rev.*, 19, 248-274.
  - Wexler, A. S., and Johnston, M. V. (2001). “Real-time single-particle analysis.” Aerosol Measurement: Principles, Techniques, and Applications, P. A. Baron and K. Willeke, eds., Wiley-Interscience, New York, 365-386.
  - Nash, D.G., Baer, T., Johnston, M.V. Aerosol mass spectrometry: An introductory review. *Int. J. Mass Spec.* 258, 2-12, 2006.
- All AMS papers: http://cires.colorado.edu/jimenez/ams.html
- List of Single Particle MS papers: http://mae.ucdavis.edu/wexler/spa_refs.html