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Aerosol Mass Spectrometry
Part 2: Thermal Desorption Techniques

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

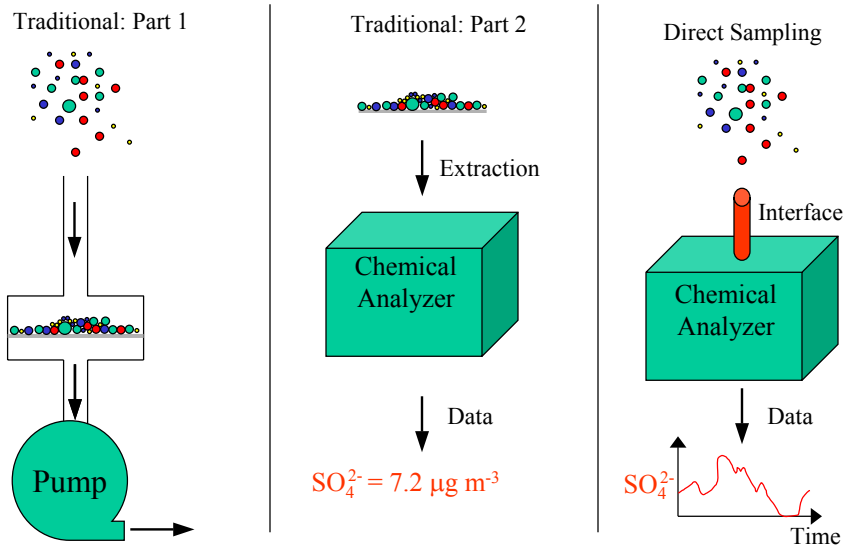
Outline

Introduction

1. Building Blocks
2. Instrument Designs
   - Main Properties
   - Quantification
   - Applications
3. The Future

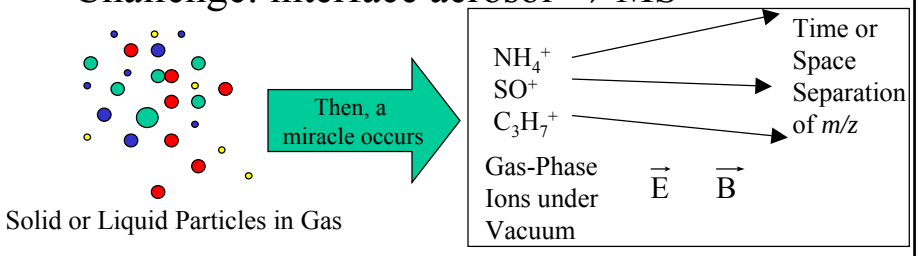
Note: focus on last 5-10 years – don't have time to cover early work
• see review papers at end or online reference lists

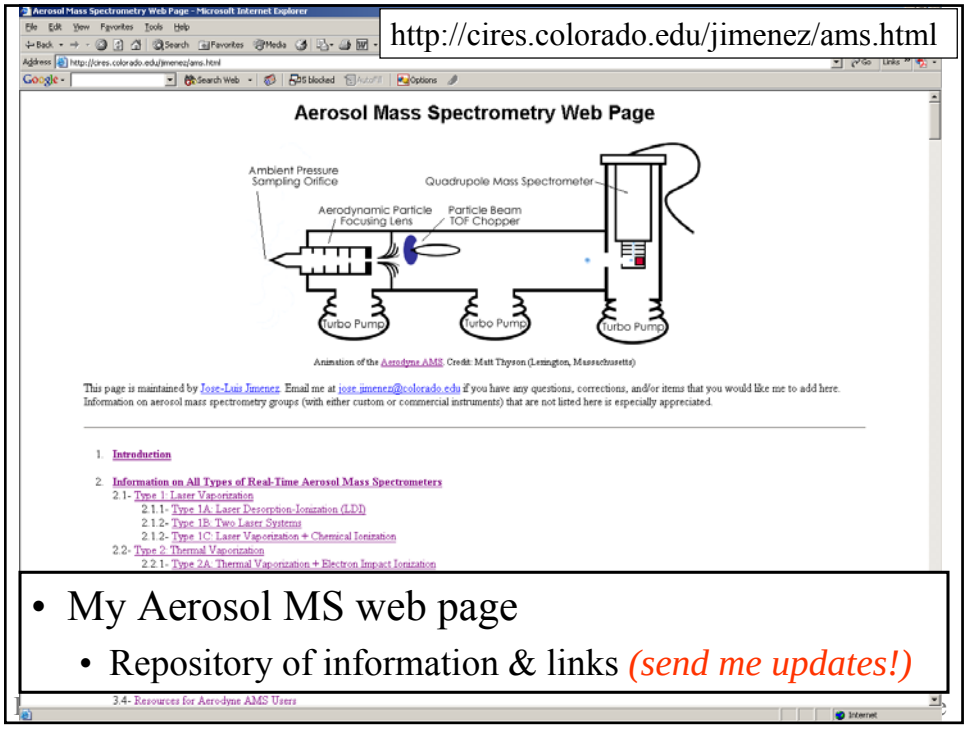
Aerosol Chemical Analysis



Why Aerosol Mass Spectrometry?

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

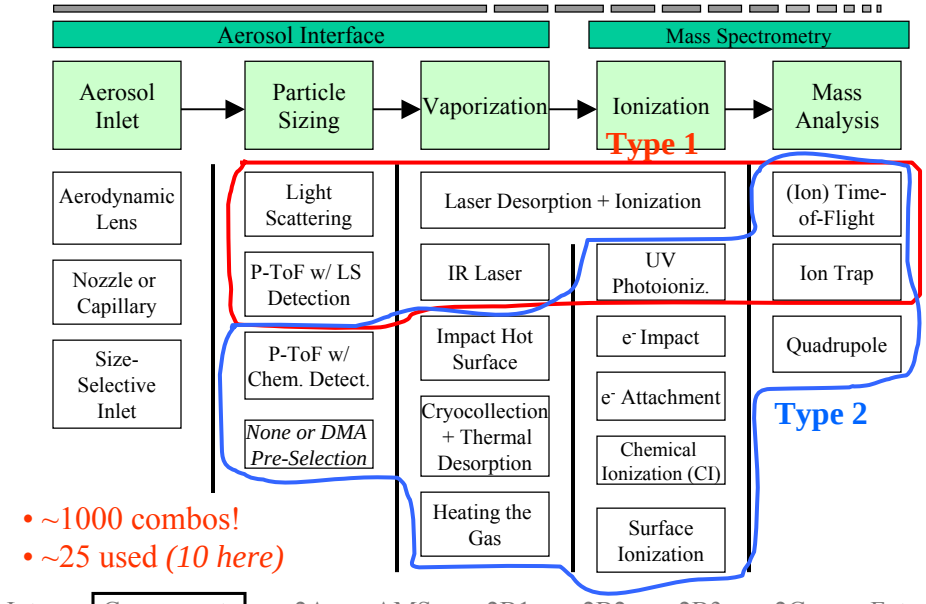




- My Aerosol MS web page
  - Repository of information & links *(send me updates!)*

Part 1: Instrumentation Building Blocks

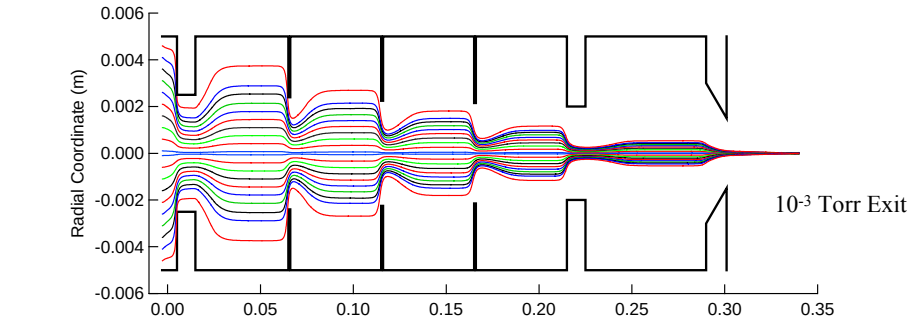
Conceptual Schematic of an Aerosol MS



Aerosol Inlets

- Particle Beam MS:
  - Introduce the particles into vacuum
  - Concentrate aerosols from gas-phase
    - ~10^{-8} particle/gas mass in ambient air
    - Reduce gas-phase interferences
  - Impart size-dependent velocity
    - Use to measure size by *particle* time-of-flight
- Other custom inlets

Aerodynamic Lenses



10^{-3} Torr Exit

2.4 Torr 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. (1995a). Aerosol Sci. Technol. 22:293–313.
• Liu, P., Ziemann, P. L., Kittelson, D. B., and McMurry, P.H. (1995b). Aerosol Sci. Technol. 22:314–324.
CFD Simulations:
• Zhang, X., Smith, K.A., Worsnop, D.R., Jimenez, J.L., Jayne, J.T., and Kolb, C.E. Aerosol Science and Technology, 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. Tech., 38: 619, 2004.

Aerosol Inlets: Aerodynamic Lenses

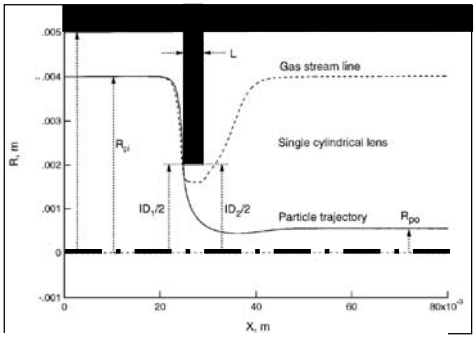


Figure 2. Schematic of a single thin cylindrical lens showing a gas streamline and the trajectory of a 500 nm particle. Q = 60 sec/min, L = 4 mm, $ID_1 = ID_2$ = 2 mm, OD = 10 mm, Re_0 = = 12.5, P_{up} = 280 Pa, R_{pi} = 4 mm, R_{po} = 0.5 mm.

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)

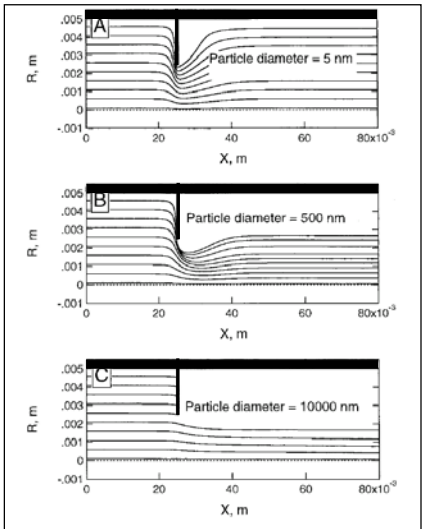


Figure 3. Particle trajectories through a single thin cylindrical lens (D_p = 5,500, 1000 nm). L = 0.5 mm, $ID_1 = ID_2$ = 5 mm, OD = 10 mm, Q = 60 scc/min, Re_0 = 12.5, and P_{up} = 280 Pa.

Size Distribution Quantification

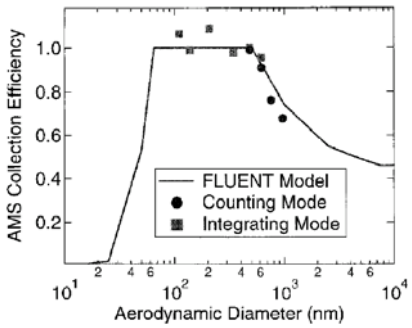


FIGURE 9. Summary of the AMS particle collection/detection efficiency as a function of aerodynamic diameter. Solid line is FLUENT model prediction. Circles are efficiencies determined by comparing AMS and CPC counting rates (data from Figure 8). Squares are collection efficiencies determined from the 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).

Aerodynamic
Lens Inlet

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.

Beam Width w/ Aerodynamic Lenses

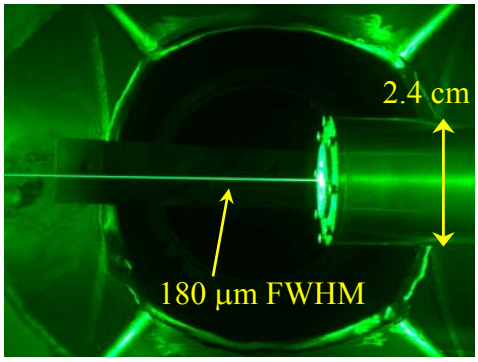


Figure courtesy of Guiseppe Petrucci, Univ. Vermont
http://www.uvm.edu/~gpetrucc/ams/particleinlet.htm

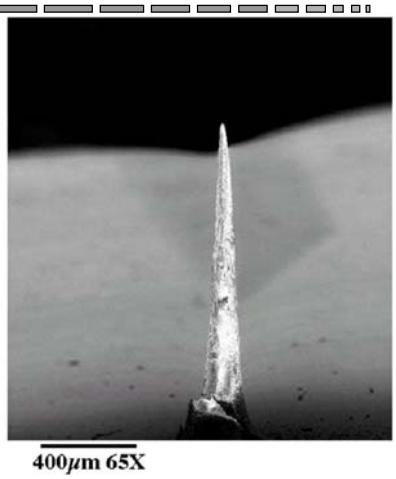
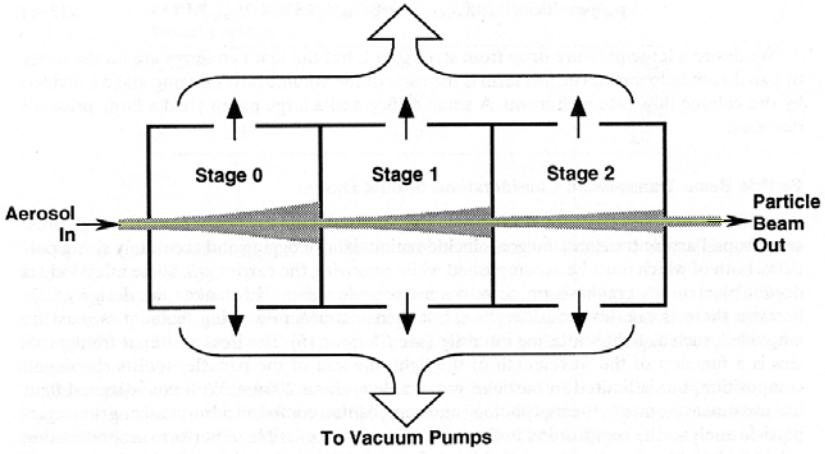


Fig. 6. SEM image of a silicon carbide 'tower' deposited by a focused nanoparticle beam [18].

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



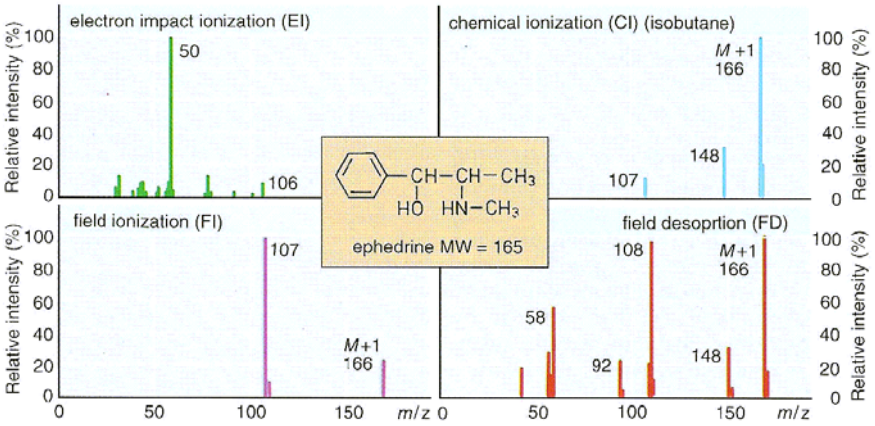
- E.g. in AMS: particles concentrated by 10^7 with respect to gas

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.

Ionization Objectives

- Produce ions from gas-phase neutral molecules
- Desirable properties
  - High efficiency (ions / molecule)
  - Number of ions linear with number of molecules
  - Universality *or* Selectivity
  - Fragmentation
    - Good and bad

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

EI Fragmentation vs. Molecular Structure

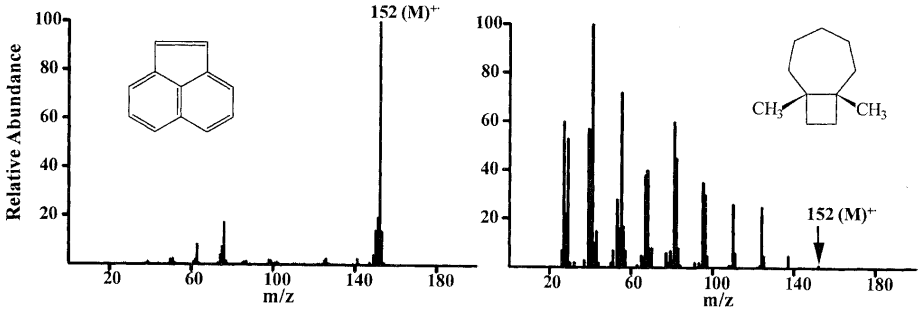


Figure 13-4 Contrasting degrees of fragmentation observed in the EI spectra of an aromatic and an alicyclic compound. The former resists dissociation and gives a molecular ion from which the molecular weight (152 Da) is measured. (From P.J. Ausloos, C. Clifton, O.V. Fateev, A.A. Levitsky, S.G. Lias, W.G. Mallard, A. Shamin, and S.E. Stein, NIST/EPA/NIH Mass Spectral Library—Version 1.5, National Institute of Standards and Technology, Gaithersburg, MD [1996].)

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

Breakdown Curve and Internal Energy Distribution

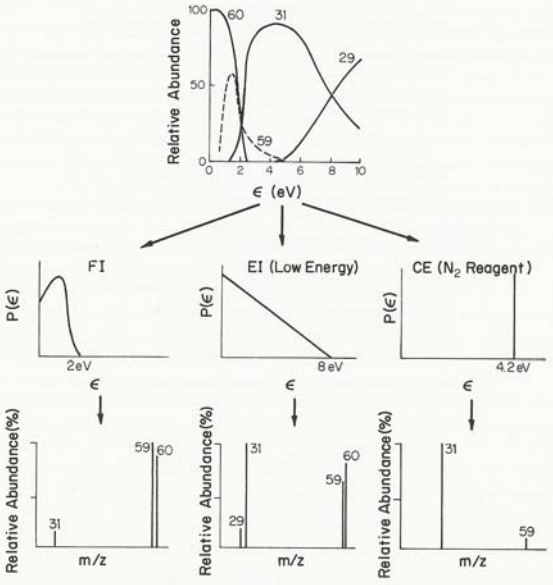


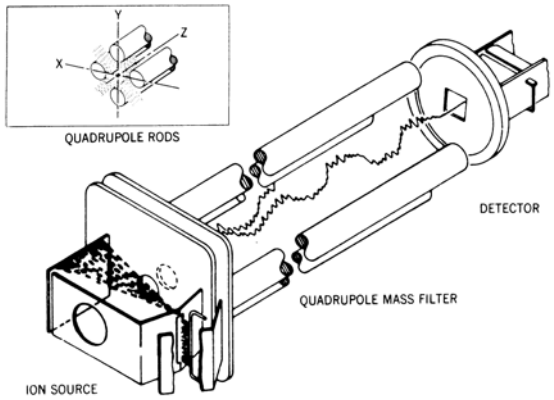
Figure 14-29 Convolution of the breakdown curve (top, an intrinsic property) with the internal energy distribution ($P[\varepsilon]$) resulting from different ionization techniques under particular experimental conditions to produce mass spectra of 1-propanol. FI indicates field ionization, a soft ionization method used for vapor phase samples.

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

Mass Spectrometer

- Use electrical and/or magnetic forces to separate ions according to *m/z*
- In most aerosol mass spectrometers
  - (Ion) Time-of-Flight
  - Quadrupole
  - Ion Trap
- Less common
  - Magnetic sector
- Not used so far in Aerosol MS
  - Fourier Transform – Ion Cyclotron Resonance
- More info on my MS course lecture notes:
  - http://www.colorado.edu/chemistry/chem5181

Mass Spectrometer: Quadrupole

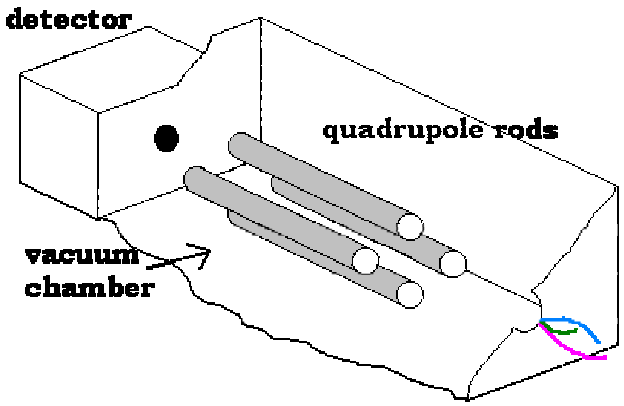


J. Throck Watson: Introduction to Mass Spectrometry. Lippincott-Raven, 1997.

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

Ion Motion inside a Quad



Mass Spectrometer: Ion Trap

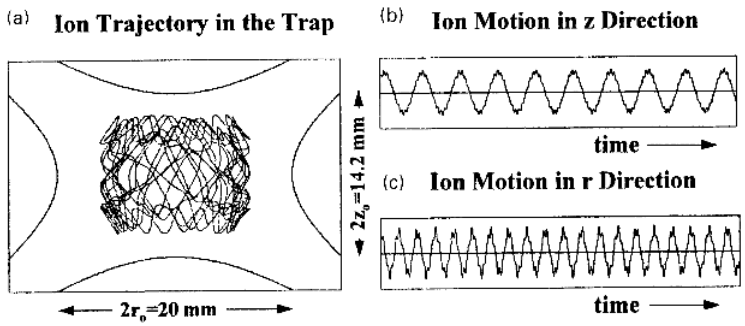
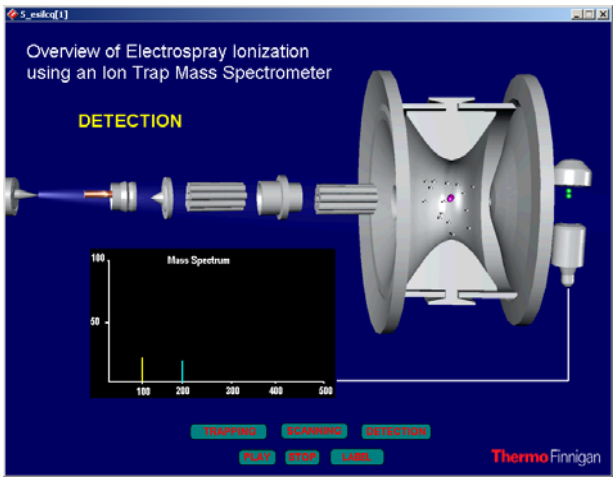


Figure 13-24 Simulation of motion of a single trapped ion in an ion trap: (a) shows the overall motion within the trap in cross section, (b) shows the time-dependent component of motion in the axial direction, and (c) shows the radial-direction component.

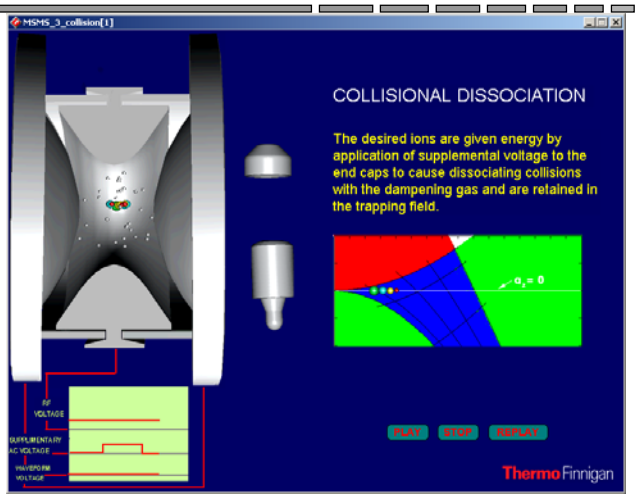
J.B. Lambert, H.F. Shurvell, D.A. Lightner, R. G. Cooks, Organic Structural Spectroscopy. Prentice-Hall, 2002.

Ion Trap Movie



- These and more available at:
  - http://www.colorado.edu/chemistry/chem5181

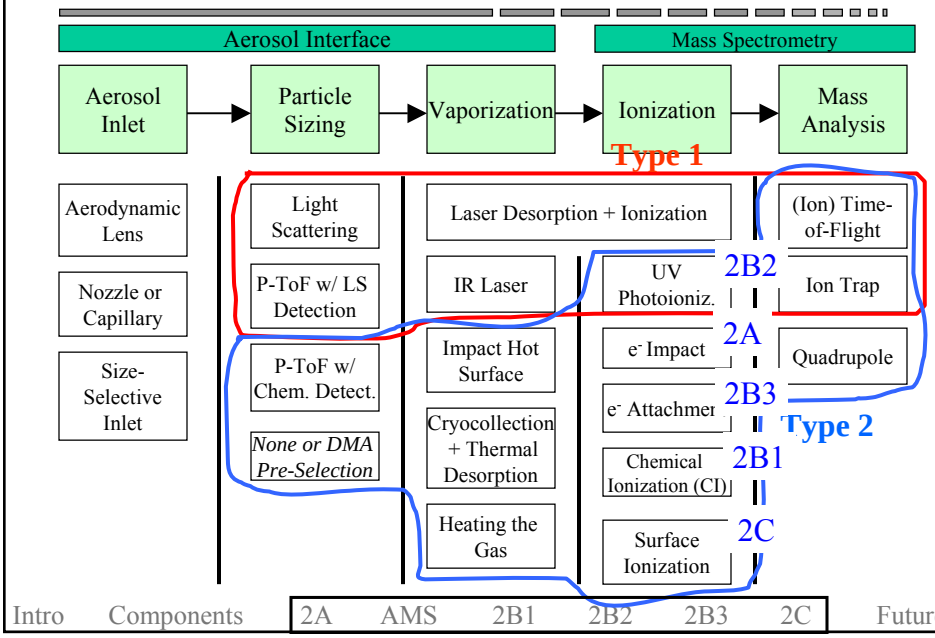
MS/MS with an Ion Trap



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

Part 2: Instrument Implementations

Conceptual Schematic of an Aerosol MS



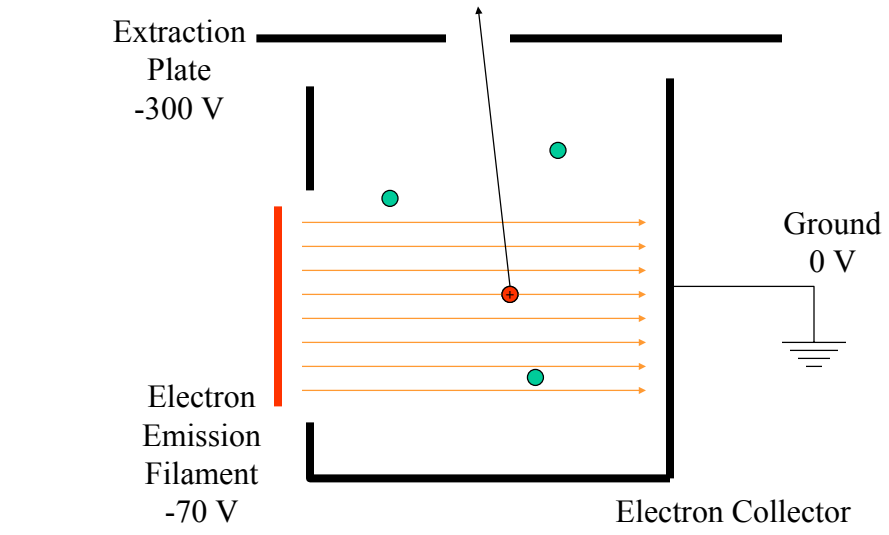
Types of Implementations

- **Type 1: Laser Vaporization**
  - 1A: Laser-Desorption Ionization (25 groups, TSI)
  - 1B: Laser Vaporization + Soft Ionization (e.g. Baer)
- **Type 2: Thermal Vaporization +**
  - 2A: Electron Impact Ionization
    - Aerodyne, Ziemann, Schreiner, Goldstein
  - 2B: Soft Ionization
    - 2B1: Chemical (Hoffmann, Wennberg, J. Smith, G. Smith)
    - 2B2: VUV (Baer, Johnston)
    - 2B3: Electron Attachment (Petrucci)
  - 2C: Surface Ionization
    - Petersson

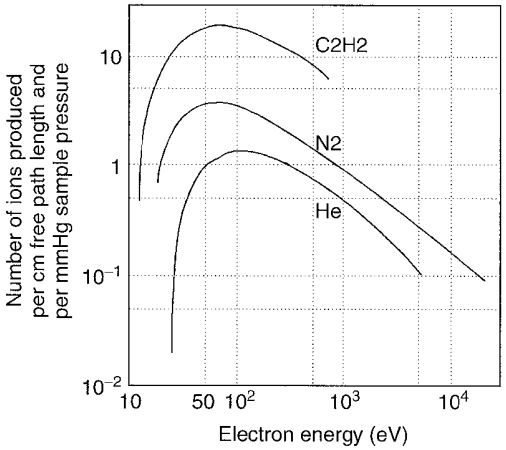
Type 2A:
TD + Electron Impact

- Aerosol Mass Spectrometer (AMS): Aerodyne + 30 groups, Worsnop, Jayne, *et al.*
- Aerosol Composition Mass Spectrometer (ACMS): Max Planck, Schreiner *et al.*
- Thermal Desorption Particle Beam Mass Spectrometer (TDPBMS): UC Riverside, Ziemann *et al.*
- Thermal Desorption Aerosol GC/MS-FID (TAG): UC Berkeley, Goldstein *et al.*

Electron Ionization Source Scheme



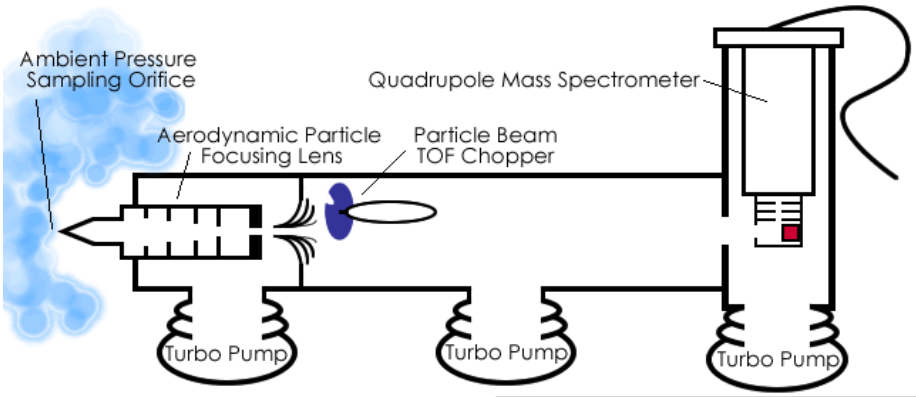
Ionization Efficiency vs. Electron Energy



Edmon de Hoffmann and Vincent Stroobant. Mass Spectrometry: Principles and Applications. John Wiley & Sons, 2002.

Figure 1.2
Number of ions produced as a function of the electron energy. A wide maximum appears at around 70 eV

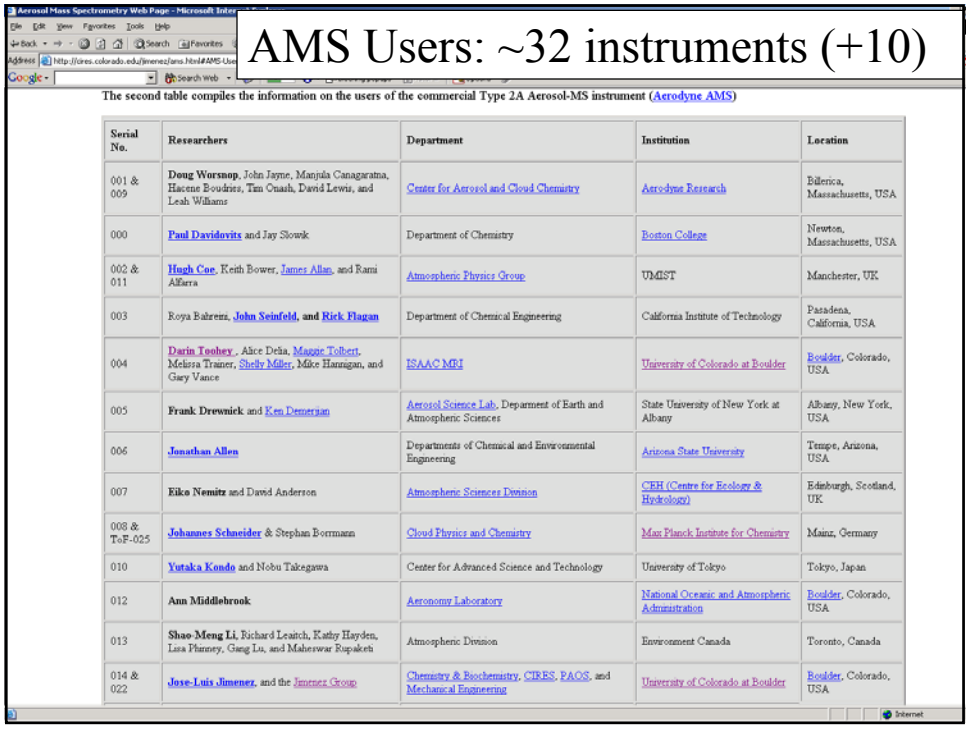
Type 2A: Aerodyne AMS



Jayne et al., Aerosol Science and Technology 33:1-2(49-70), 2000.
Jimenez et al., Journal of Geophysical Research, 108(D7), 8425, 2003.

Aerodynamic Lens	Light Scattering	Laser Desorption + Ionization		(Ion) Time-of-Flight
Nozzle or Capillary	P-ToF w/ LS Detection	IR Laser	UV Photoioniz.	Ion Trap
Size-Selective Inlet	P-ToF w/ Chem. Detect.	Impact Hot Surface	e- Impact	Quadrupole
	None or DMA Pre-Selection	Cryocollection + Thermal Desorption	e- Attachment	
			Chemical Ionization (CI)	
		Heating the Gas	Surface Ionization	

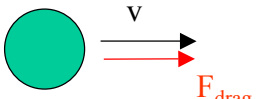
AMS Users: ~32 instruments (+10)



The second table compiles the information on the users of the commercial Type 2A Aerosol-MS instrument (Aerodyne AMS)

Serial No.	Researchers	Department	Institution	Location
001 & 009	**Doug Worsnop**, John Jayne, Manjula Canagaratna, Hacene Boudries, Tim Onash, David Lewis, and Leah Williams	Center for Aerosol and Cloud Chemistry	Aerodyne Research	Billerica, Massachusetts, USA
000	**Paul Davidovits** and Jay Slowik	Department of Chemistry	Boston College	Newton, Massachusetts, USA
002 & 011	**Hugh Coe**, Keith Bower, James Allan, and Rami Alfarra	Atmospheric Physics Group	UMIST	Manchester, UK
003	Roya Bahreini, **John Seinfeld**, and **Rick Flagan**	Department of Chemical Engineering	California Institute of Technology	Pasadena, California, USA
004	**Darin Toohey**, Alice Delia, Maggie Tolbert, Melissa Trainer, Shelly Miller, Mike Hannigan, and Gary Vance	ISAAC MRI	University of Colorado at Boulder	Boulder, Colorado, USA
005	**Frank Drewnick** and Ken Demerjian	Aerosol Science Lab, Deparment of Earth and Atmospheric Sciences	State University of New York at Albany	Albany, New York, USA
006	**Jonathan Allen**	Departments of Chemical and Environmental Engineering	Arizona State University	Tempe, Arizona, USA
007	**Eiko Nemitz** and David Anderson	Atmospheric Sciences Division	CEH (Centre for Ecology & Hydrology)	Edinburgh, Scotland, UK
008 & ToF-025	**Johannes Schneider** & Stephan Borrmann	Cloud Physics and Chemistry	Max Planck Institute for Chemistry	Mainz, Germany
010	**Yutaka Kondo** and Nobu Takegawa	Center for Advanced Science and Technology	University of Tokyo	Tokyo, Japan
012	**Ann Middlebrook**	Aeronomy Laboratory	National Oceanic and Atmospheric Administration	Boulder, Colorado, USA
013	**Shao-Meng Li**, Richard Leaitch, Kathy Hayden, Lisa Phinney, Gang Lu, and Maheswar Rupaketi	Atmospheric Division	Environment Canada	Toronto, Canada
014 & 022	**Jose-Luis Jimenez**, and the Jimenez Group	Chemistry & Biochemistry, CIRES, FAOS, and Mechanical Engineering	University of Colorado at Boulder	Boulder, Colorado, USA

Aerodynamic Forces on a Particle



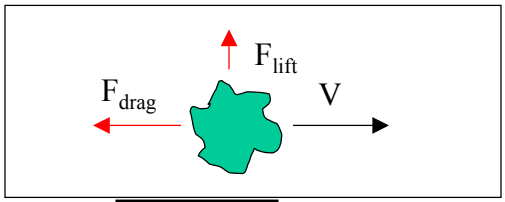
v: relative velocity between the gas and the particle

$F_{drag} \alpha d^2 v$

$F_{drag} = m a$

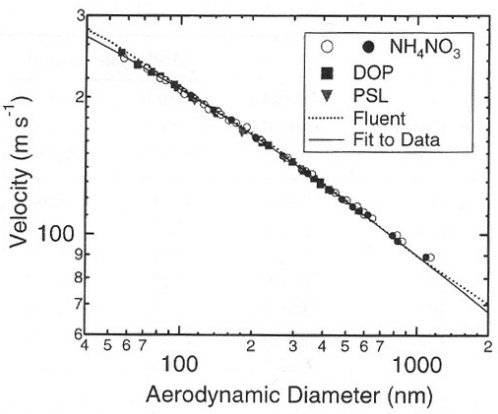
$m \alpha d^3$

$a \alpha d^{-1}$



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

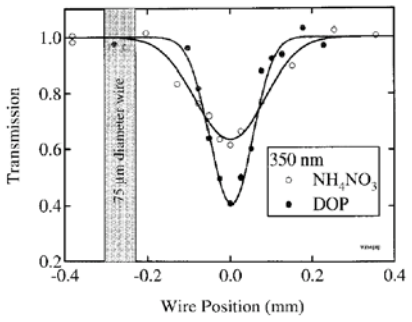


FIGURE 11. Particle beam width measurement for spherical DOP and nonspherical NH_4NO_3 particles. Beam widths are determined by passing a 75 μm diameter wire across the particle beam path and calculating particle transmission from the ratio of the single particle count rates measured by the mass spectrometer 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_4NO_3.

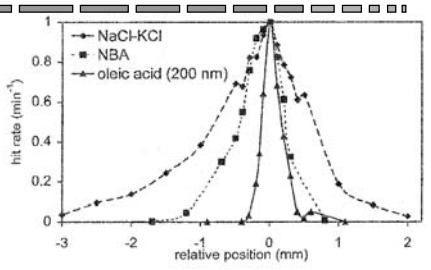


Figure 2. Particle beam profile measurements for NaCl-KCl, NBA, and oleic acid aerosols. NaCl-KCl and NBA aerosols are polydisperse with the average diameter of the detected particles approximately 85 nm. The oleic acid aerosol is monodisperse with a diameter of 200 nm.

(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.

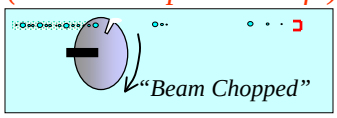
• David B. Kane, Berk Oktem, and Murray V. Johnston. Nanoparticle Detection by Aerosol Mass Spectrometry. Aerosol Science and Technology 34: 520–527 (2001)

AMS: Information Obtained

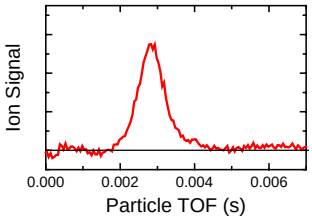
Dual Operating Modes

Size Distribution

(limited composition info)

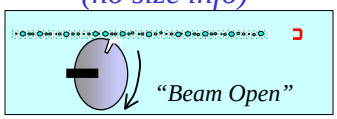


Spectrometer Setting is Fixed (small subset of 0-300 amu)

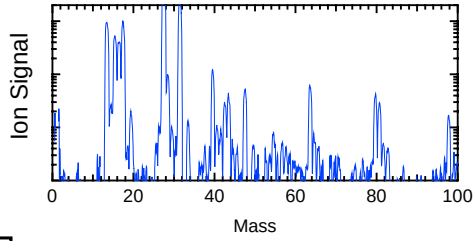


Average Composition

(no size info)



Spectrometer is Scanned (0-300 amu)



Katrib et al.

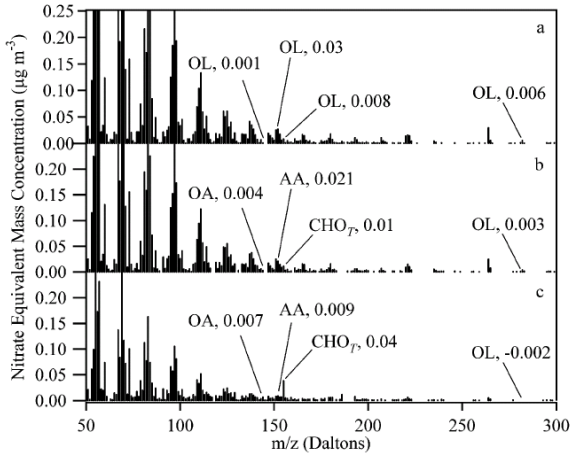


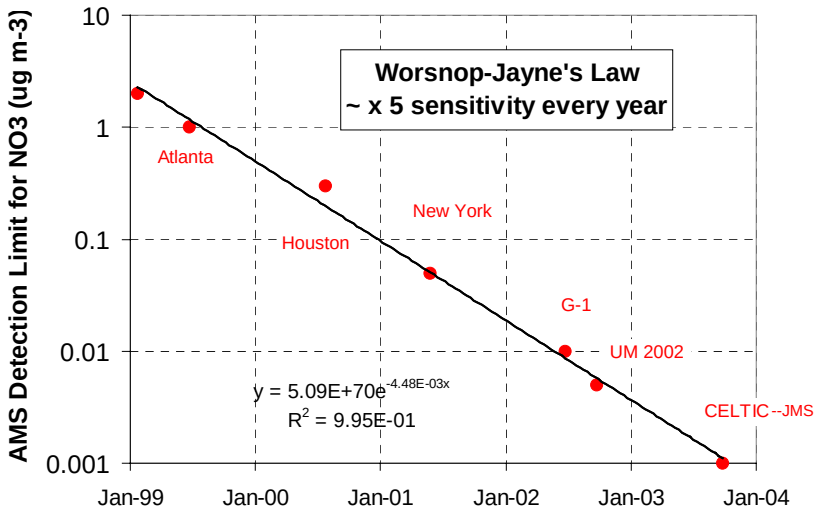
Figure 5. (a) Mass spectrum of pure oleic acid particles. (b) Mass spectrum after ozone exposure of 1.98×10^{-5} atm·s. (c) Mass spectrum after ozone exposure of 6.6×10^{-5} atm·s. Identified peaks are 152 amu for AA, 144 amu for OA, 155 amu for CHO_7, and 282 amu for OL. The numbers next to each label are the *y*-axis values at the specific *m/z* value. Conditions: 11 nm coating on PSL core.

AMS in Lab Studies

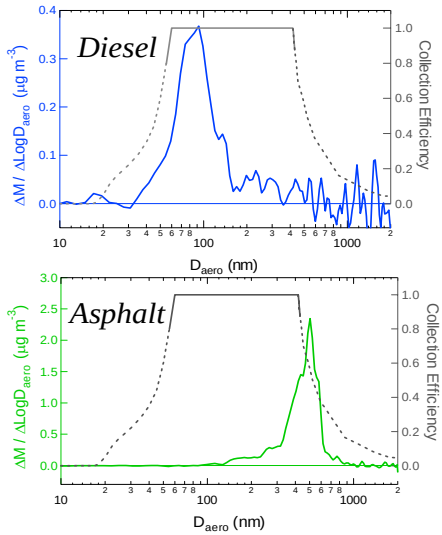
- Reaction of oleic acid particles with O_3

Products and Mechanisms of Ozone Reactions with Oleic Acid for Aerosol Particles Having Core-Shell Morphologies
Y. Katrib et al. J. Phys. Chem. A 2004, 108, 6686-6695.

Improvement in AMS Sensitivity



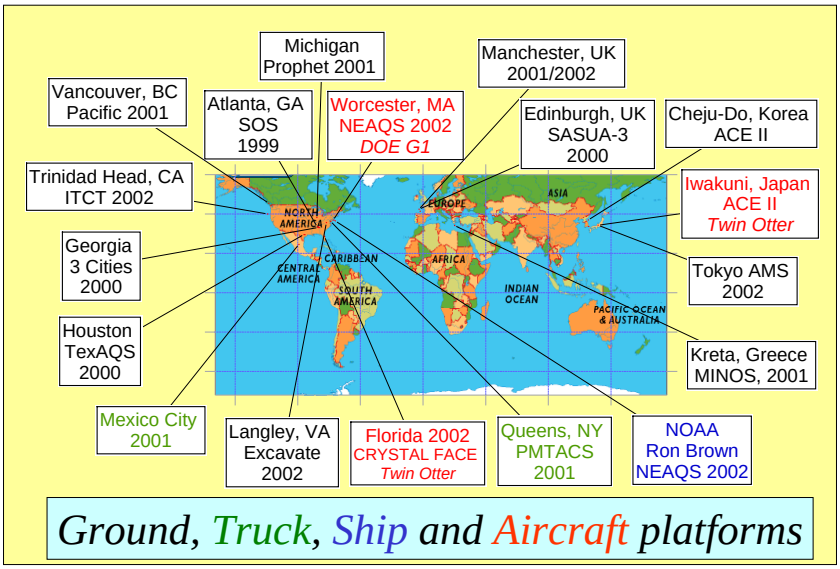
AMS: 4-Second Data Rate



Courtesy of Aerodyne Research.

Emission factors can be determined while chasing individual vehicles on road

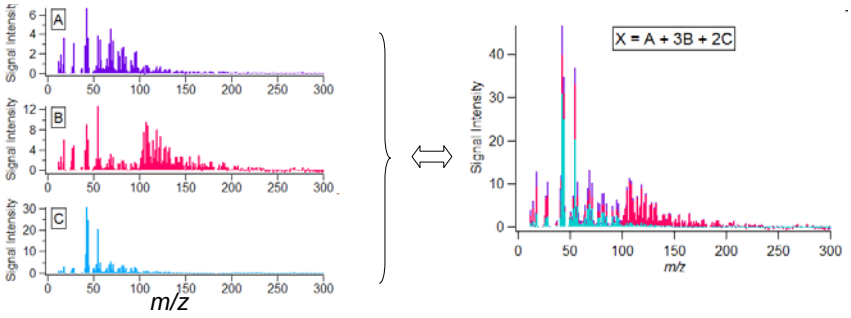
AMS: Ambient Sampling



Ground, Truck, Ship and Aircraft platforms

Deconvolve AMS Data: Mathematics

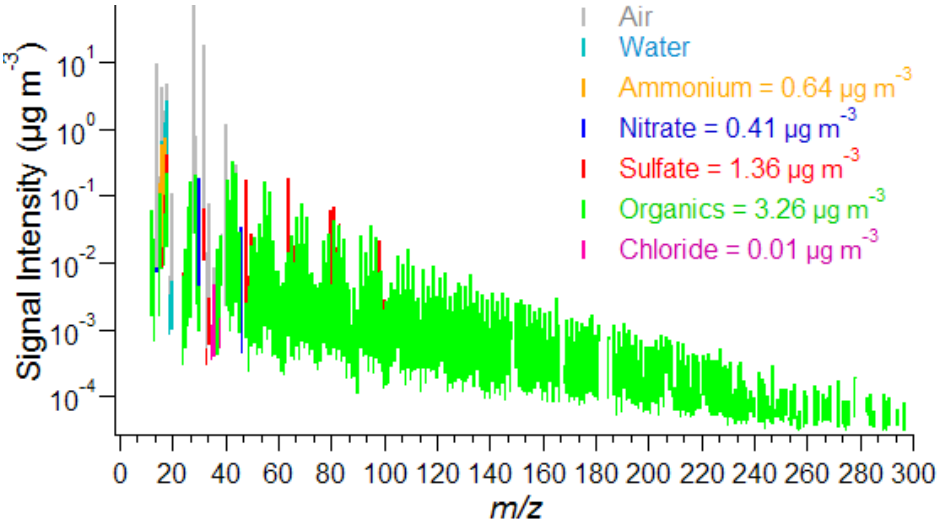
A measured AMS mass spectrum is essentially the linear superposition of the distinctive mass spectra of components in the analyte:



$$\mathbf{ms}_t = c_1 \cdot \mathbf{ms}_1 + c_2 \cdot \mathbf{ms}_2 + \ldots + c_n \cdot \mathbf{ms}_n + \varepsilon_i$$

- $\mathbf{ms}_t$ – observed mass spec vector
- $\mathbf{ms}_n$ – mass spec vector of component n
- c_n – concentration of component n
- ε_i – residual vector

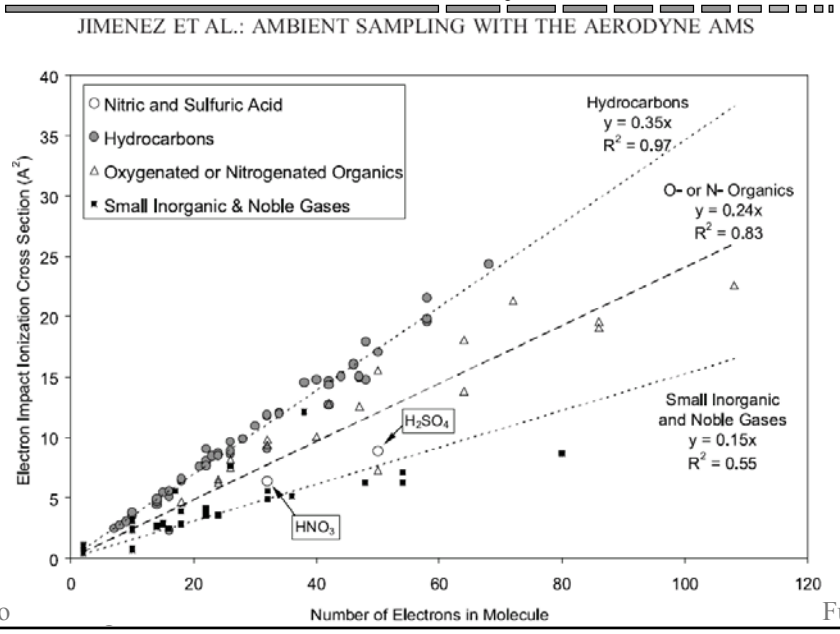
AMS Ambient Mass Spectrum



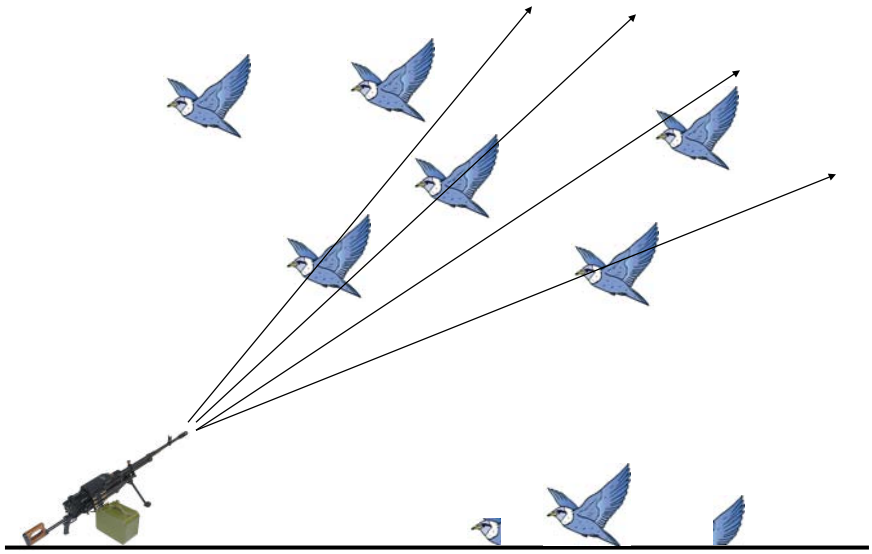
Why does this work? See:

- Jimenez et al. J. Geophys. Res., 108(D7), 8425, 2003.
- Allan et al., Journal of Aerosol Science, 35: 909, 2004.

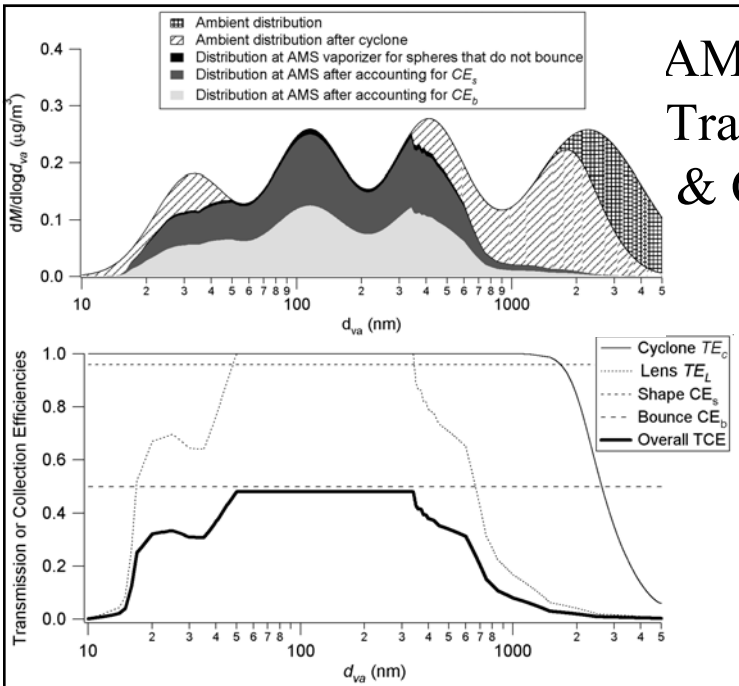
Ionization Efficiency α Electrons



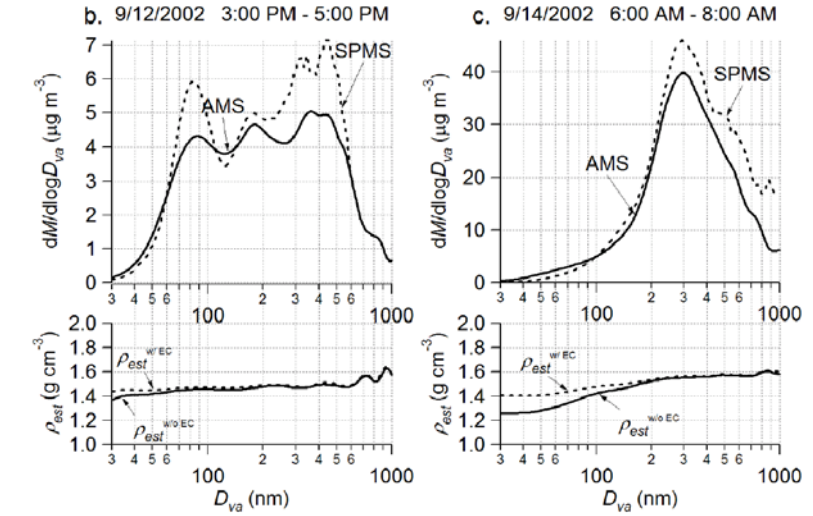
AMS Organic Quantification



AMS Particle Transmission & Collection



AMS vs. SMPS in Pittsburgh



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. Journal of Geophysical Research - Atmospheres (Special issue on EPA Supersites), in press, August 2004. http://cires.colorado.edu/jimenez/Papers/Pittsburgh_Overview.pdf

Status of Quantification w/ AMS I

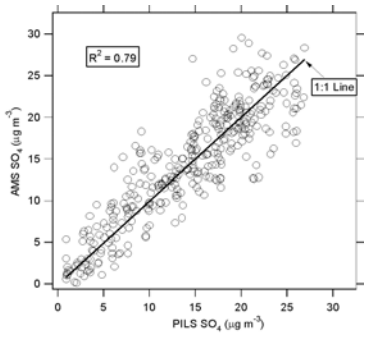
- Collection efficiency due to shape: CE_s
  - Negligible except for very irregular particles (soot)
- Collection efficiency due to bounce: CE_b
  - Dominant cause of uncertainty at present
  - Likely greatly reduced in future
- Tranmission efficiency of lens (TE_L)
  - AMS is currently a PM_1 instrument
    - "Not fair" to compare $PM_{2.5}$ vs PM_1
  - Lens for $PM_{2.5}$ being tested

Status of Quantification w/ AMS II

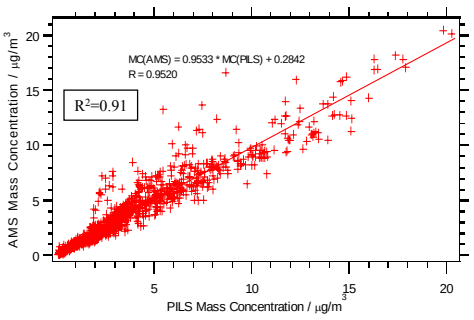
- So how quantitative is it?
  - For more volatile particles in the lab, ~10%
    - Recently submitted paper claims even better
  - For ambient particles
    - By itself: +/- 40%
    - Together with other quantitative instruments (PILS, SMPS…): +/- 15%
    - Scatter in field comparisons is sometimes due to *the other* instrument
- Will it get better?
  - Yes, Aerodyne and many groups working on these issues
  - Bounce issue definitively identified summer'04, may or may not be hard to eliminate

(2A) AMS: SO_4 Mass Conc.

Atlanta 1999
Jimenez et al. (2003)

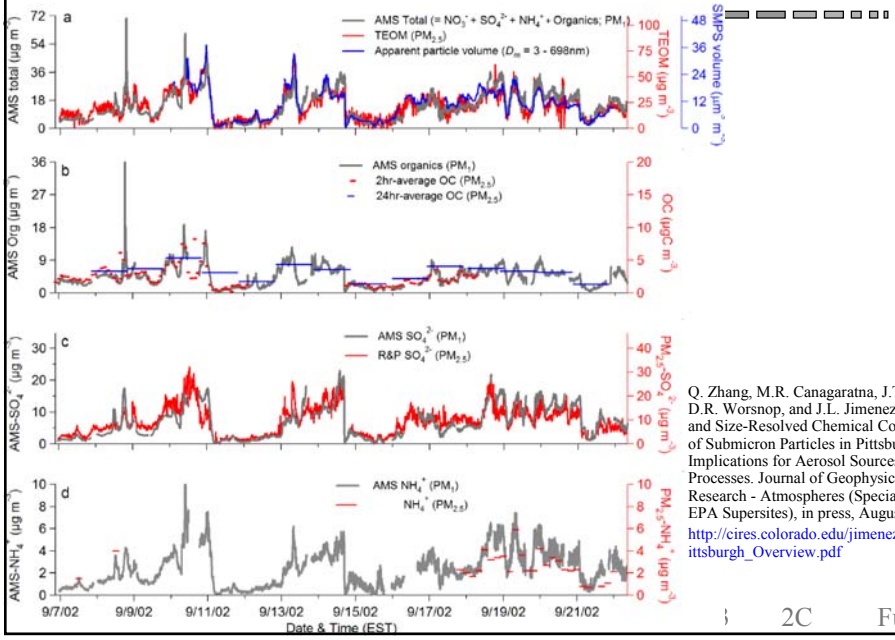


New York City 2001
Drewnick et al. (2004)



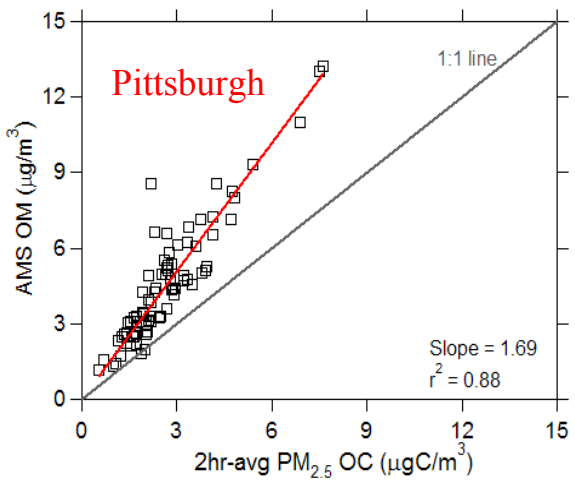
- CE_b ~50%

AMS vs. Other Instruments: Pittsburgh



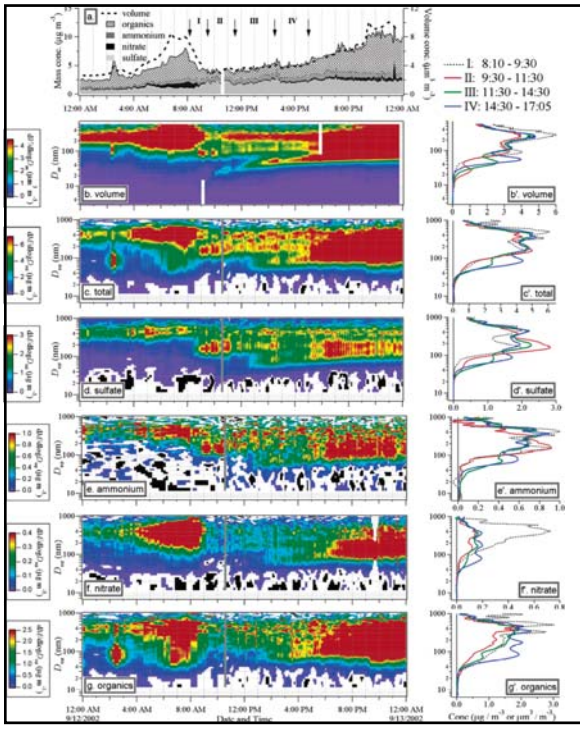
Q. Zhang, M.R. Canagaratna, J.T. Jayne, D.R. Worsnop, and J.L. Jimenez. Time and Size-Resolved Chemical Composition of Submicron Particles in Pittsburgh – Implications for Aerosol Sources and Processes. Journal of Geophysical Research - Atmospheres (Special issue on EPA Supersites), in press, August 2004
http://cires.colorado.edu/jimenez/Papers/Pittsburgh_Overview.pdf

AMS Organics vs. Sunset Lab OC



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. Journal of Geophysical Research - Atmospheres (Special issue on EPA Supersites), in press, August 2004
http://cires.colorado.edu/jimenez/Papers/Pittsburgh_Overview.pdf

- Good agreement, Average OM : OC ≈ 1.7 in Pittsburgh
- Similar at other locations (Houston, Tokyo, New England)



AMS @ Pittsburgh Supersite

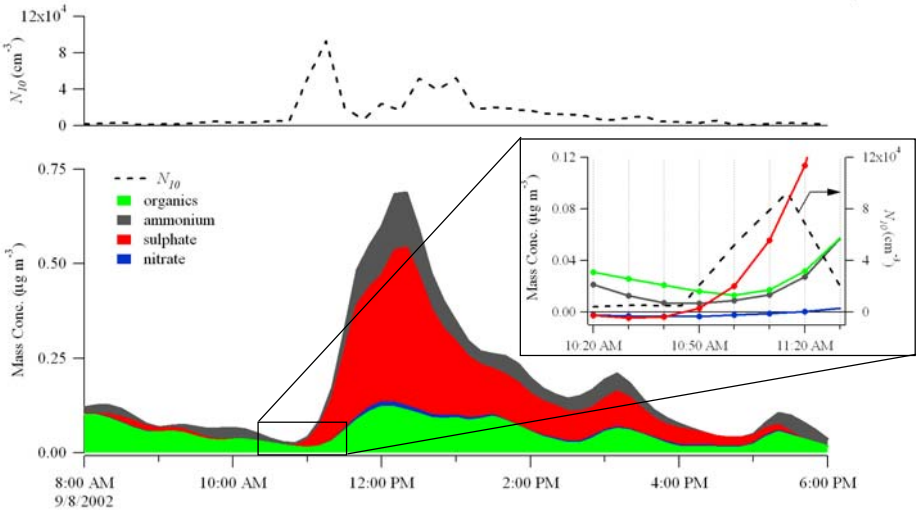
- Enormous detail on size-resolved composition

1C2 Zhang et al.

2B4 DeCarlo et al.

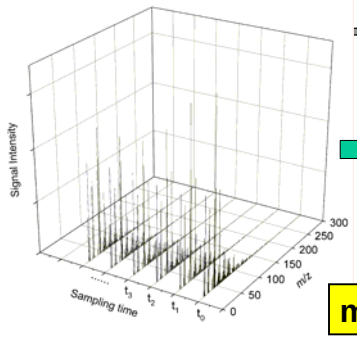
Q. Zhang, C.O. Stanier, M.C. Canagaratna, J.T. Jayne, D.R. Worsnop, S.N. Pandis, and J.L. Jimenez. Insights into the Chemistry of Nucleation Bursts and New Particle Growth Events in Pittsburgh Based on Aerosol Mass Spectrometry. Environmental Science and Technology, 38: 4797-4809, 2004. http://cires.colorado.edu/jimenez/Papers/es035417u_Published.pdf

Composition of Growing New Particles



Q. Zhang, C.O. Stanier, M.C. Canagaratna, J.T. Jayne, D.R. Worsnop, S.N. Pandis, and J.L. Jimenez. Insights into the Chemistry of Nucleation Bursts and New Particle Growth Events in Pittsburgh Based on Aerosol Mass Spectrometry. Environmental Science and Technology, 38: 4797-4809, 2004. http://cires.colorado.edu/jimenez/Papers/es035417u_Published.pdf

Deconvolve AMS Organic Data: Mathematics



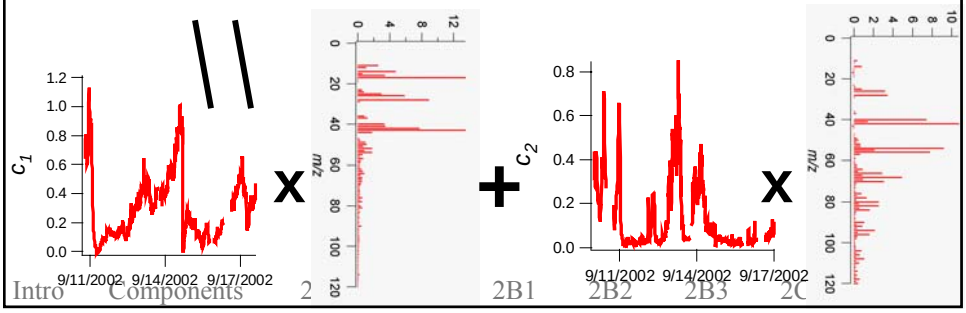
$$\begin{bmatrix} m_{1,1} & m_{2,1} & \cdots & m_{300,1} \\ m_{1,2} & m_{2,2} & \cdots & m_{300,2} \\ \cdots & \cdots & \cdots & \cdots \\ m_{1,t} & m_{2,t} & \cdots & m_{300,t} \end{bmatrix}$$

t

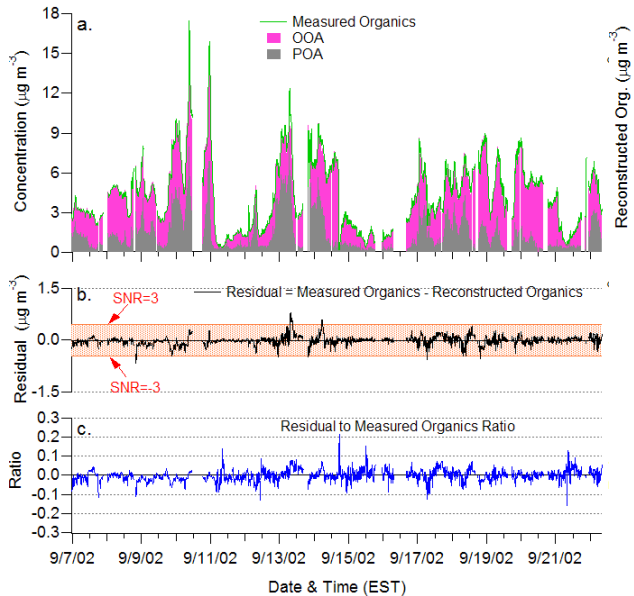
Row: mass spec
Column: t series

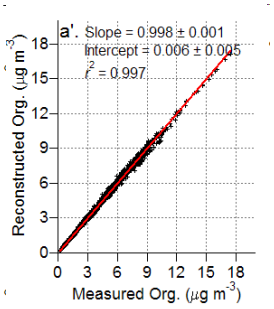
Pittsburgh:
N_t = 3200
Mexico City
N_t = 9100

$$ms_t = c_1 \cdot ms_1 + c_2 \cdot ms_2 + c_3 \cdot ms_3 + \varepsilon_i$$



Pittsburgh POA and OOA Quantification





1C2 Zhang et al.

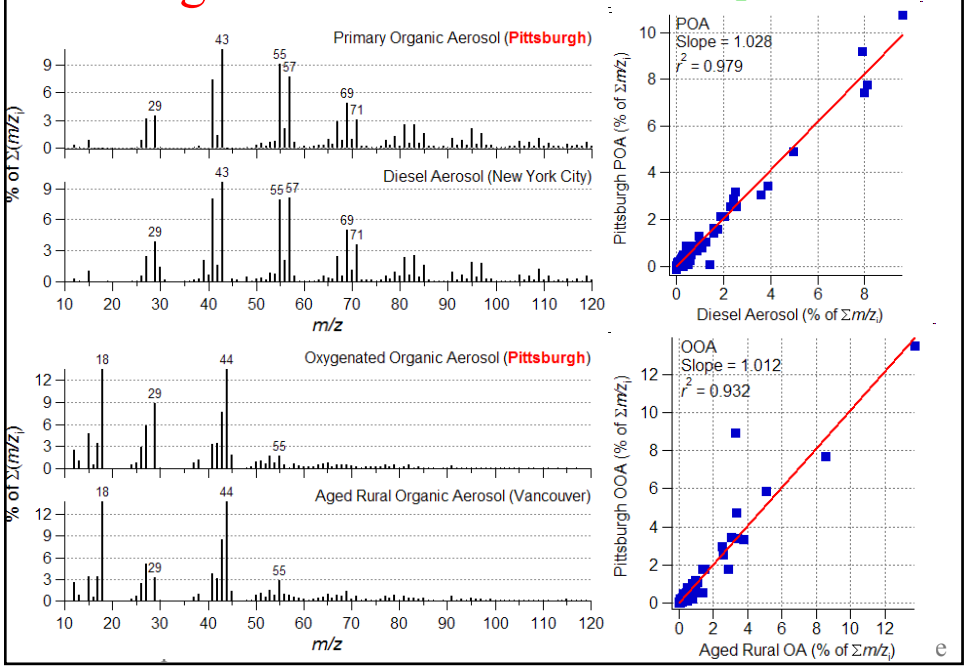
4D1 Jimenez et al.

8PA6 Weimer et al.

11B4 Jimenez et al.

Pittsburgh

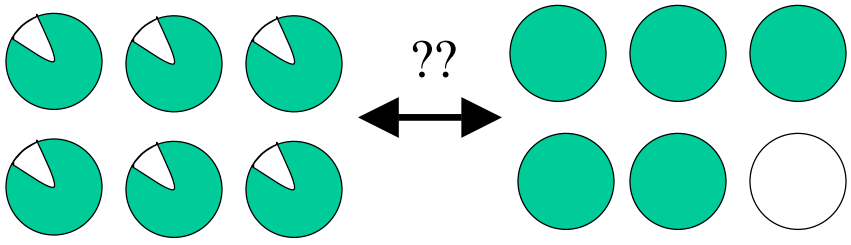
POA and OOA Mass Spectra



Ensemble vs. Single Particle Analysis

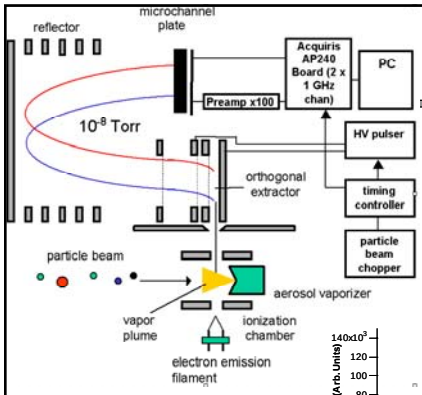
For example: 17% of the mass is organics, 83% is sulfate

"Internally Mixed" "Externally Mixed"

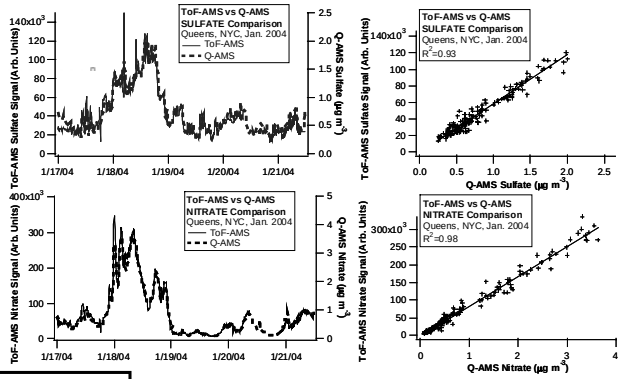


- Single Particle Instruments DIRECTLY detect the mixing state
- Ensemble Averaging Instruments can only answer the mixing question indirectly, and with lower precision

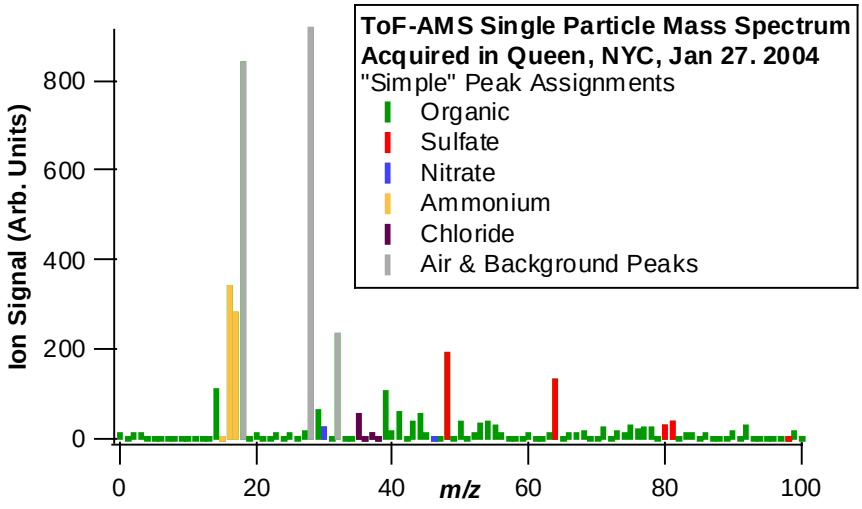
Time-of-Flight AMS



Aerodynamic Lens	Light Scattering	Laser Desorption + Ionization		(Ion) Time-of-Flight
Nozzle or Capillary	P-ToF w/ LS Detection	IR Laser	UV Photoioniz.	Ion Trap
Size-Selective Inlet	P-ToF w/ Chem. Detect.	Impact Hot Surface	e- Impact	Quadrupole
	None or DMA Pre-Selection	Cryocollection + Thermal Desorption	e- Attachment	
		Heating the Gas	Chemical Ionization (CI)	
			Surface Ionization	



Single Particles with ToF-AMS

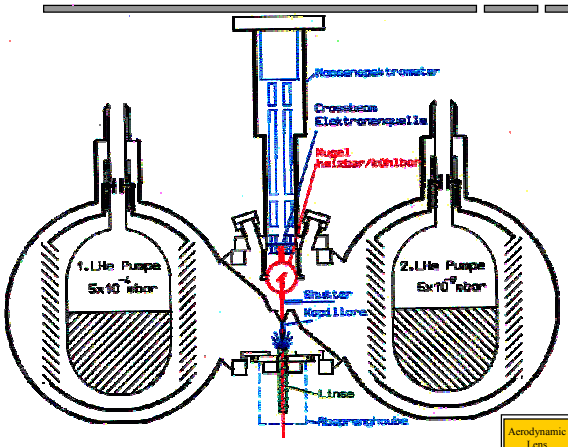


- Statistics: Particle coincidence can be neglected at typical ambient conc.

AMS References and Links

- 13 talks and 22 posters at AAAR'04
- http://cires.colorado.edu/jimenez/ams.html#Papers-AMS *(41 papers to date)*
- Introduction to Instrument, Quantification Principles
  - Jayne et al., *Aerosol Sci. Technol*., 33, 49-70, 2000. *(#1)*
  - Jimenez et al. *J. Geophys. Res. – Atmos.*, 108(D7), 8425, 2003. *(#2)*
  - Allan et al. *J. Geophys. Res. – Atmos.*, 108(D3), 4090, 2003. (*Part 1*). *(#8)*
  - Allan et al. *J. Aerosol Sci.*, 35: 909–922, 2004. *(#23)*
- Ambient sampling & quantification
  - Drewnick et al., *Aerosol Sci. Technol*., 38(S1):92–103, 2004. *(#12)*
  - Zhang et al., *Env. Sci. Technol.*, 38: 4797-4809, 2004. *(#26)*
  - Hogrefe et al. *J. Air Waste Manag. Assoc.*, 54:1040–1060. *(#40)*
  - Zhang et al. *J. Geophys. Res. – Atmos.*, in press, August 2004. *(#28)*
- Size Measurement
  - Jimenez et al. *J. Geophys. Res. – Atmos*, 108(D10), 4318, 2003. (+ Corr.). *(#7)*
  - DeCarlo et al., *Aerosol Sci. Technol*., submitted July 2004. *(#33)*
- Organic Analysis
  - Alfarra et al., *Atm. Env.*, in press, January 2004. *(#17)*
  - Zhang et al. *Env. Sci. Technol.*, submitted Sep. 2004. *(#41)*
  - Katrib et al., *J. Phys. Chem.* A, 108, 6686, 2004. *(#30)*

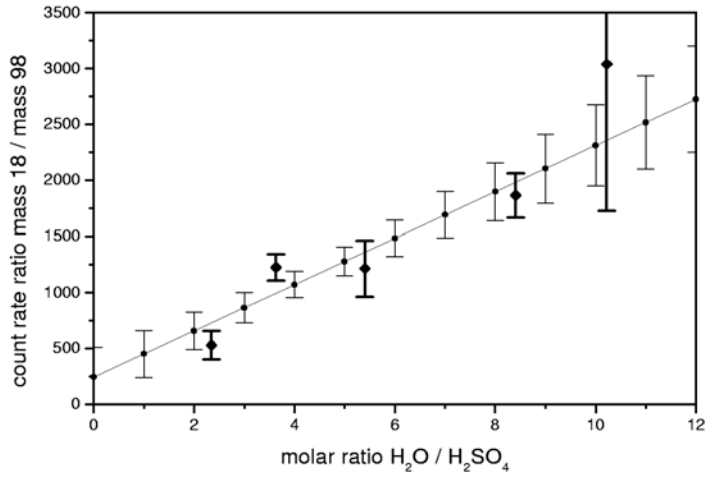
Type 2A: ACMS (Schreiner *et al.*)



Courtesy of Jochen Schreiner
Max Plank Institute fur KernPhysik
http://www.mpi-hd.mpg.de/mauersberger/schreiner/index.htm

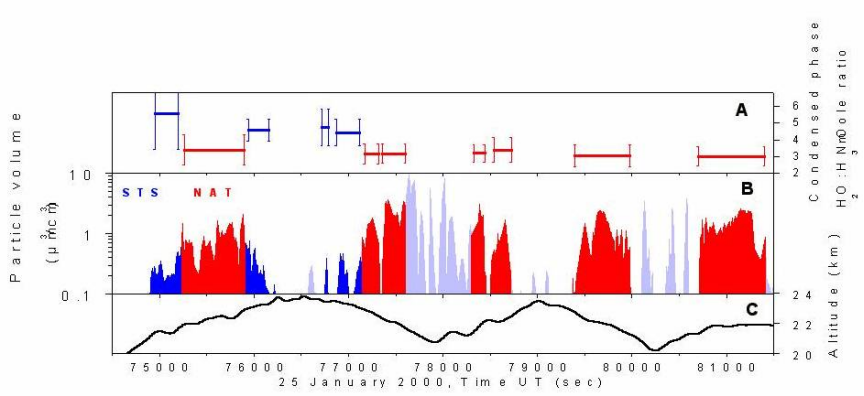
Aerodynamic Lens	Light Scattering	Laser Desorption + Ionization		(Ion) Time-of-Flight
Nozzle or Capillary	P-ToF w/ LS Detection	IR Laser	UV Photoioniz.	Ion Trap
Size-Selective Inlet	P-ToF w/ Chem. Detect.	Impact Hot Surface	e⁻ Impact	Quadrupole
	None or DMA Pre-Selection	Cryocollection + Thermal Desorption	e⁻ Attachment	
		Heating the Gas	Chemical Ionization (CI)	
			Surface Ionization	

ACMS Quantification



http://www.mpi-hd.mpg.de/mauersberger/schreiner/index.htm

ACMS: Polar Strat. Cloud Analysis



- Very careful measurement on H_2O/HNO_3 in PSCs

http://www.mpi-hd.mpg.de/mauersberger/schreiner/Flug2000.htm

ACMS References and Links

• Schreiner J, Voigt C, Zink P, et al. A mass spectrometer system for analysis of polar stratospheric aerosols. REVIEW OF SCIENTIFIC INSTRUMENTS 73 (2): 446-452 Part 1 FEB 2002.

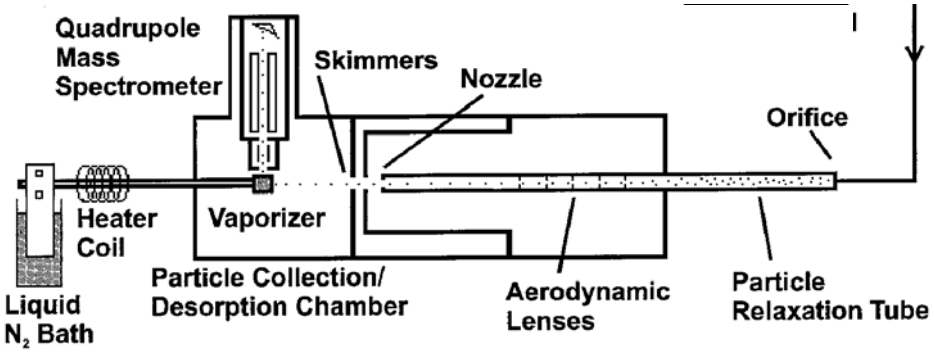
• Chemical analysis of polar stratospheric cloud particles. Schreiner J, Voigt C, Kohlmann A, Amold F, Mauersberger K, Larsen N. SCIENCE 283 (5404): 968-970 FEB 12 1999.

• Voigt C., J. Schreiner, A. Kohlmann, P. Zink, *K. Mauersberger, N. Larsen, T.Deshler, C. Kröger, J. Rosen, A. Adriani, F. Cairo, G. Di Donfrancesco, M. Viterbini, J. Ovarlez, H. Ovarlez, C. David, A. Dörnbrack, Nitric acid trihydrate (NAT) in polar stratospheric cloud particles , Science 290, 1756 (2000)

• http://www.mpi-hd.mpg.de/mauersberger/schreiner/index.htm

• *Not at AAAR, not sure if still active*

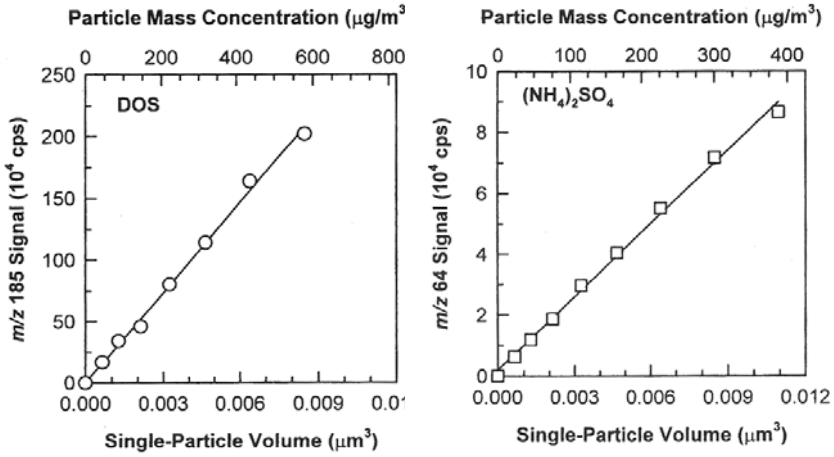
Type 2A: TDPBMS (Ziemann *et al.*)



Herbert J. Tobias and Paul J. Ziemann. Compound Identification in Organic Aerosols Using Temperature-Programmed Thermal Desorption Particle Beam Mass Spectrometry. Anal. Chem.1999, 71, 3428-3435.

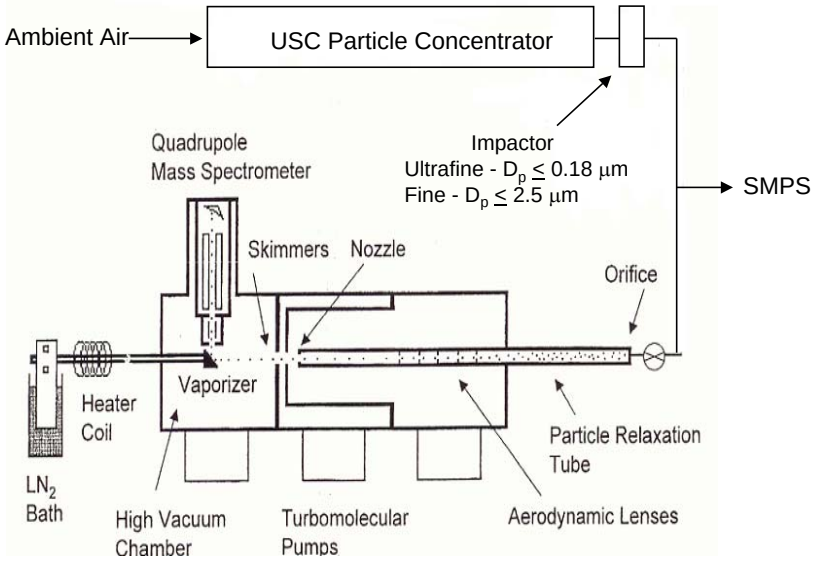
Aerodynamic Lens	Light Scattering	Laser Desorption + Ionization		(Ion) Time-of-Flight
Nozzle or Capillary	P-ToF w/ LS Detection	IR Laser	UV Photoioniz.	Ion Trap
Size-Selective Inlet	P-ToF w/ Chem. Detect.	Impact Hot Surface	e⁻ Impact	Quadrupole
	None or DMA Pre-Selection	Cryocollection + Thermal Desorption	e⁻ Attachment	
		Heating the Gas	Chemical Ionization (CI)	
			Surface Ionization	

TDPBMS: Quantification

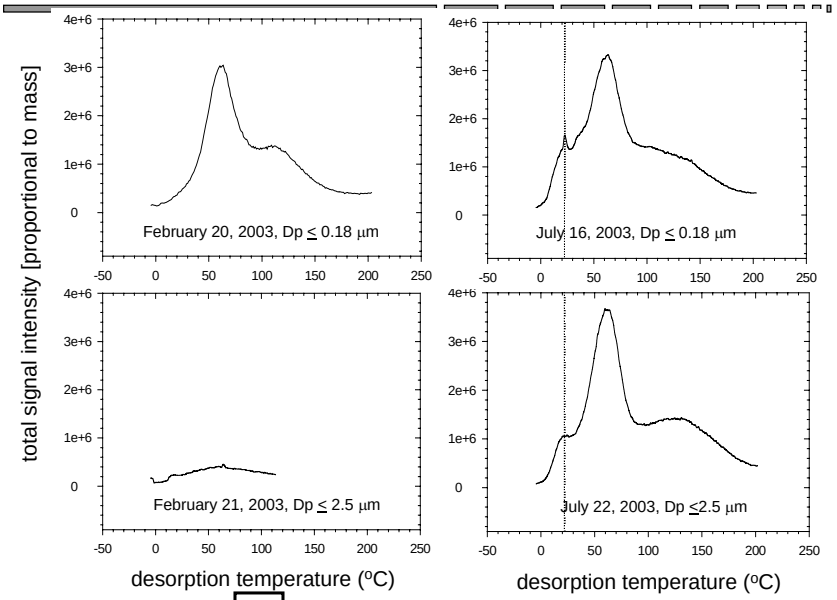


Herbert J. Tobias, Peter M. Kooiman, Kenneth S. Docherty, and Paul J. Ziemann. Real-Time Chemical Analysis of Aerosols Using a Thermal Desorption Particle Beam Mass Spectrometer. Aerosol Science & Technology, 33:1-2, 170 (2000).

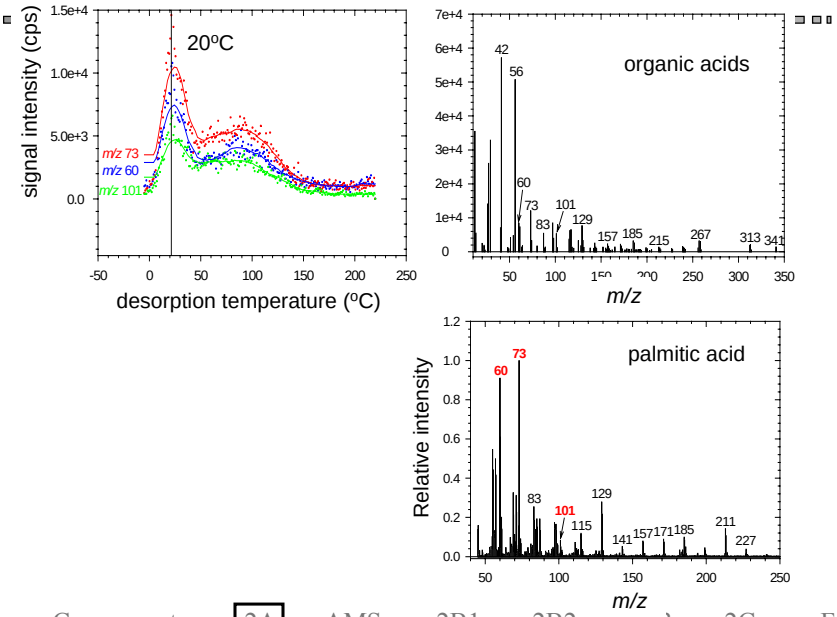
TDPBMS + Particle Concentrator: Ambient



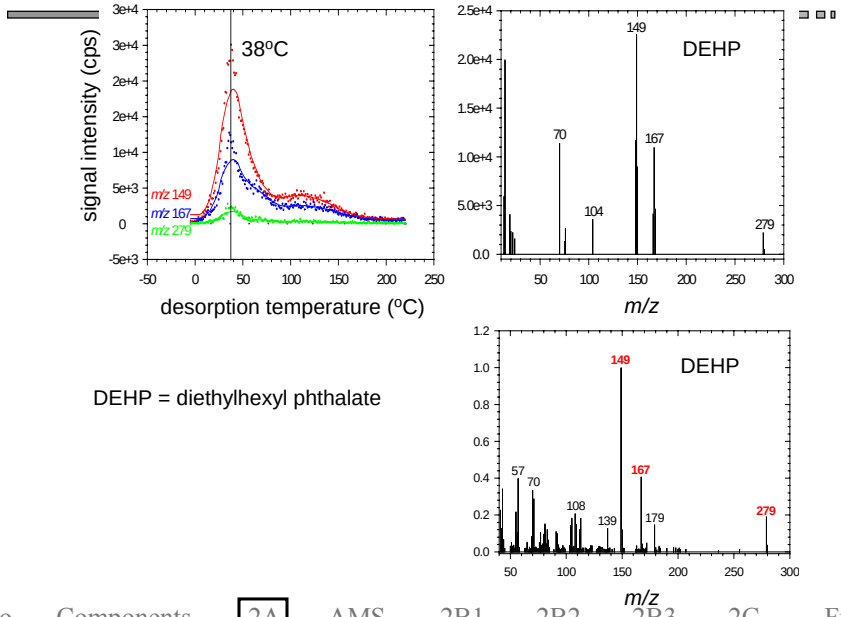
Desorption Profiles for Volatile Mass: Winter and Summer Ultrafine Particles in Riverside, CA



TPTD Profile and Mass Spectrum of 20ºC Component

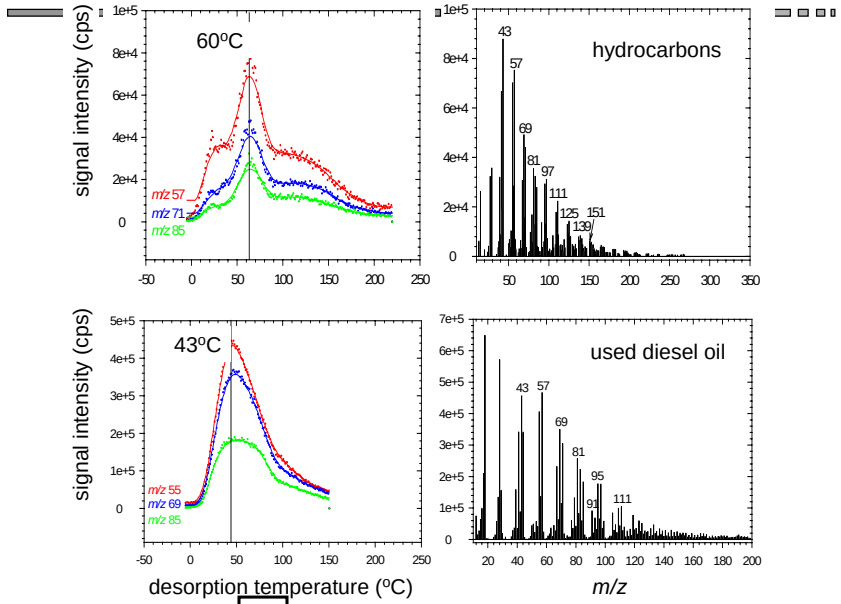


TPTD Profile and Mass Spectrum of 38ºC Component

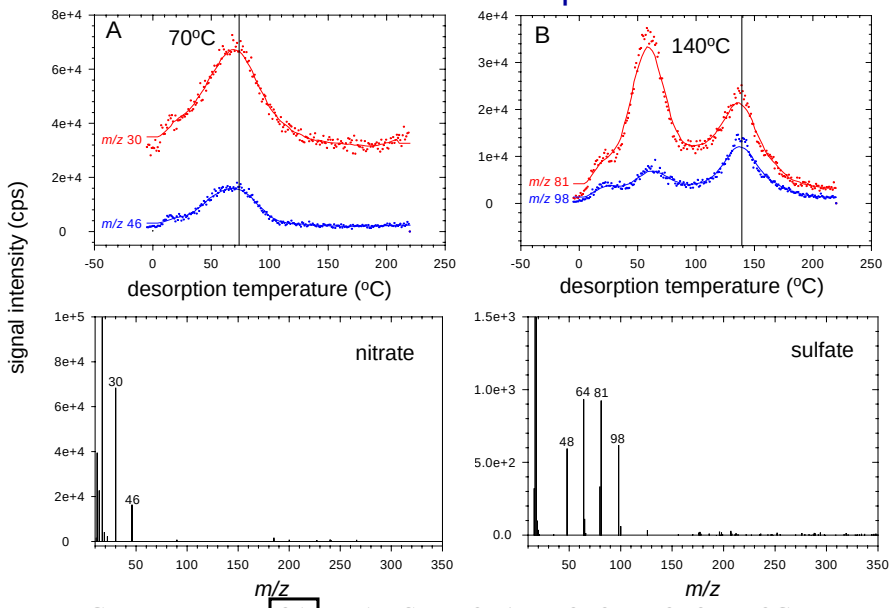


DEHP = diethylhexyl phthalate

TPTD Profile and Mass Spectrum of 60ºC Component



TPTD Profiles and Mass Spectra of 70º and 140ºC Components



TDPBMS References and Links

• **Talk 1C4:** VAPOR PRESSURES OF CARBOXYLIC ACIDS IN SOLID AND LIQUID MATRICES MEASURED USING A THERMAL DESORPTION PARTICLE BEAM MASS SPECTROMETER SULEKHA CHATTOPADHYAY, Paul Ziemann.

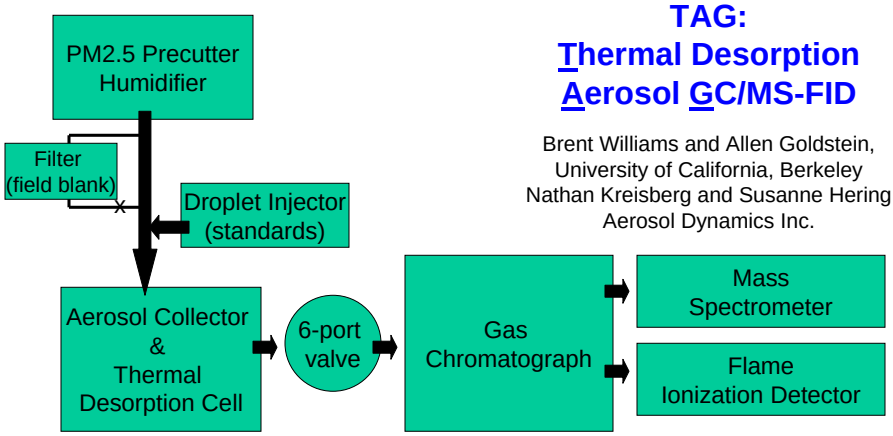
• **Talk 2C4:** CHEMISTRY OF SECONDARY ORGANIC AEROSOL FORMATION FROM THE REACTIONS OF LINEAR ALKENES WITH OH RADICALS KENNETH DOCHERTY, Paul Ziemann

• **Talk 9B2:** PRODUCTS AND MECHANISM OF THE HETEROGENEOUS REACTION OF NITRATE RADICALS WITH OLEIC ACID PARTICLES Kenneth Docherty, Huiming Gong, PAUL ZIEMANN

•Herbert J. Tobias and Paul J. Ziemann. Compound Identification in Organic Aerosols Using Temperature-Programmed Thermal Desorption Particle Beam Mass Spectrometry. Anal. Chem.1999, 71, 3428-3435.

•Herbert J. Tobias, Peter M. Kooiman, Kenneth S. Docherty, and Paul J. Ziemann. Real-Time Chemical Analysis of Aerosols Using a Thermal Desorption Particle Beam Mass Spectrometer. Aerosol Science & Technology, 33:1-2, 170 (2000).

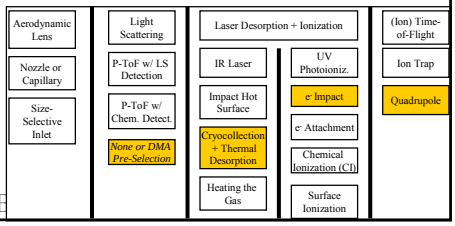
• http://envisci.ucr.edu/Faculty/pziemann/default.htm



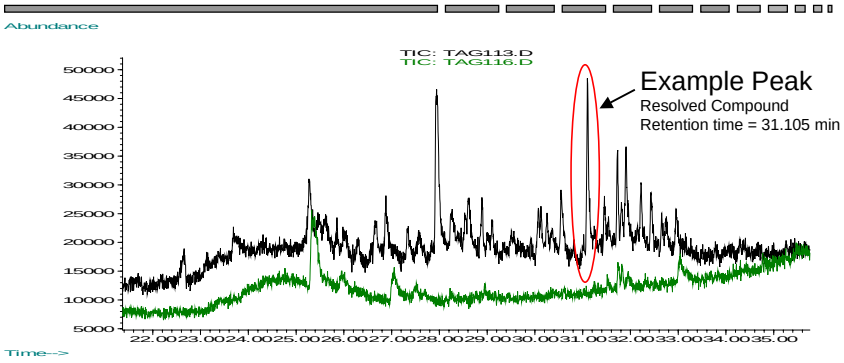
TAG:
Thermal Desorption
Aerosol GC/MS-FID

Brent Williams and Allen Goldstein,
University of California, Berkeley
Nathan Kreisberg and Susanne Hering
Aerosol Dynamics Inc.

Semi-continuous, in-situ measurement: One-hour time resolution



TAG: Ambient Data



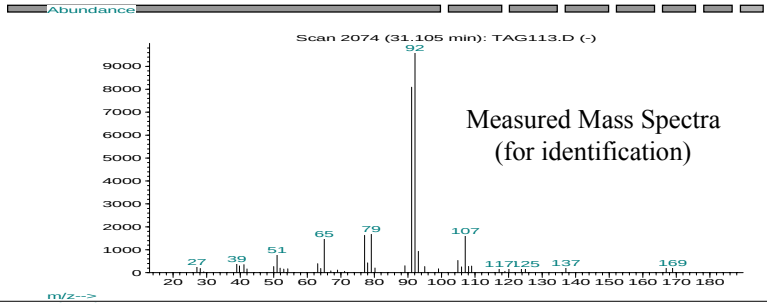
Chebogue Point, Nova Scotia. July 8, 2004

Ambient sample. **(sample collected 16:00-16:29 GMT)**
Filtered ambient sample. **(sample collected 19:00-19:29 GMT)**

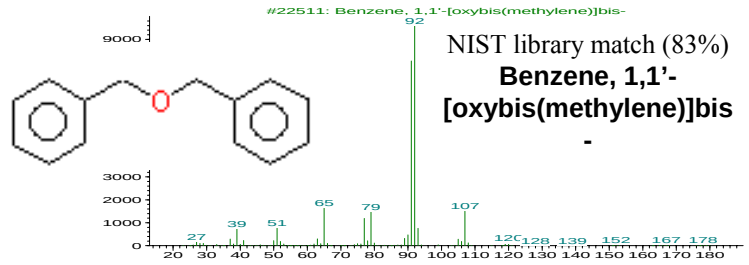
Desorption: 50-300^{0}C
GC oven temp. range shown here: ~ 85^{0}C to ~ 208^{0}C

Total Organic Aerosol = Resolved Compounds + Unresolved Compounds + Non-Eluting Compounds

TAG: Ambient Data



Measured Mass Spectra
(for identification)



NIST library match (83%)
Benzene, 1,1'-[oxybis(methylene)]bis-

TAG References and Links

• **Talk 5D4:** SPECIATED ORGANIC COMPOSITION OF ATMOSPHERIC AEROSOLS: A NEW, IN-SITU INSTRUMENT. BRENT J. WILLIAMS, Allen H. Goldstein, Nathan M. Kreisberg, Susanne V. Hering

• Very new, no publications yet

• *At least two other groups pursuing very similar approaches*

Type 2B1:
TD + Chemical Ionization

- Atmospheric Pressure Chemical Ionization Mass Spectrometer (APCI-MS): U. Mainz, Hoffmann *et al*
- Aerosol Chemical Ionization Mass Spectrometer (A-CIMS): U. Georgia, G. Smith *et al.*
- Selected-Ion Chemical Ionization Mass Spectrometer (SI-CIMS): Caltech, Wennberg *et al.*
- Thermal Desorption Chemical Ionization Mass Spectrometer (TDCIMS): NCAR, J. Smith *et al.*

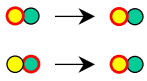
Ion-Molecule Reactions

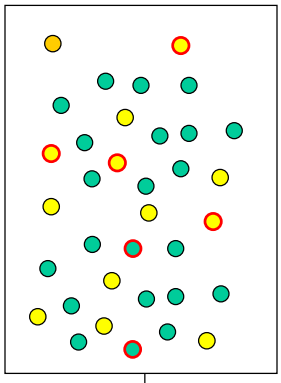
Limit 1: High local Pressure => many collisions

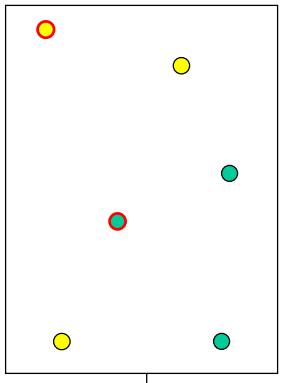
Limit 2: Very Low Local Pressure: no collisions

Neutrals	Ions
A	A^+
B	B^+

$IP_A > IP_B$







Extensive Chemical Ionization

No CI

Efficiency of Ion-Molecule Reactions

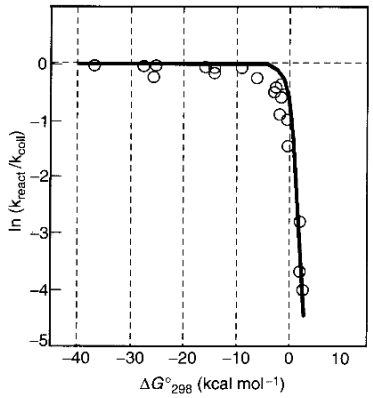


Figure 1.38
The natural logarithm of the number of reactions per collision ratio indicates that the proton transfer is almost 100% efficient when the process is exergonic. When it becomes endergonic, the efficiency drops sharply. (Reproduced (modified) from Ref. 77 with permission)

- Approx. every collision leads to a proton transfer, if $\Delta G^0 < 0$

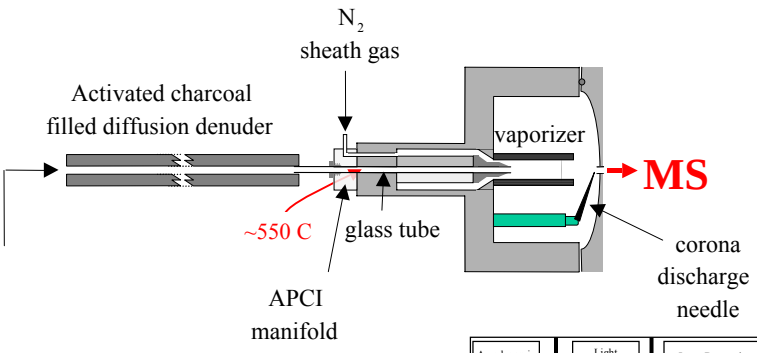
Edmon de Hoffmann and Vincent Stroobant. Mass Spectrometry: Principles and Applications. John Wiley & Sons, 2002.

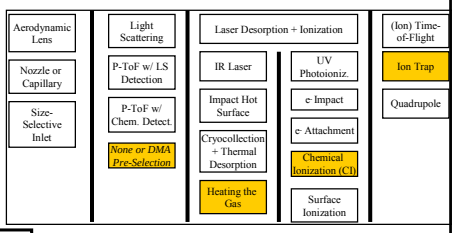
Ionization: Chemical

- Charge exchange: $M + Ar^+ \rightarrow M^{+\cdot} + Ar$
- Proton transfer: $M + CH_5^+ \rightarrow (M+H)^+ + CH_4$
- Adduct formation: $M + TiCl_2^+ \rightarrow (M+TiCl_2)^+$

- Need Collisions!
  - $\lambda < 0.1$ mm ($P > 0.6$ mbar)
  - Sometimes at 1 atm (APCI)

Type 2B1: APCI-MS (*Thorsten Hoffman*)



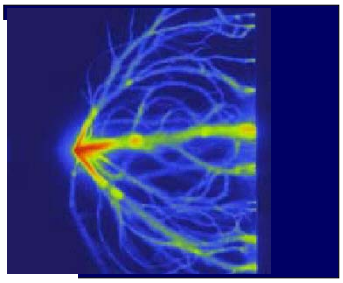


Courtesy of Thorsten Hoffmann, Institute of Spectrochemistry, Dortmund, Germany

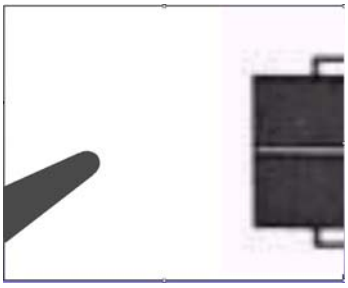
Optimisation of APCI *(corona discharge)*

Factors influencing the sensitivity

- **source design**
  - point-to-plate distance
  - sheath and auxillary gas flows
- **discharge current**
- **temperature**
- **CI-Gases**
- **analytes** (e.g. proton affinity)

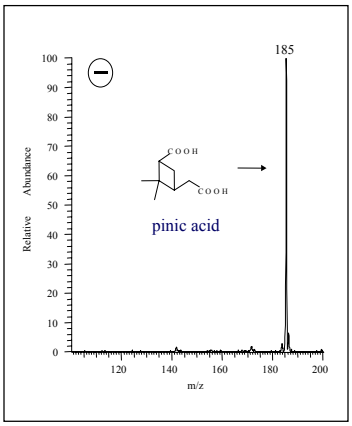


Point-to-Plate discharge



AP-CIMS: Low Fragmentation

Formation of negative Ions:



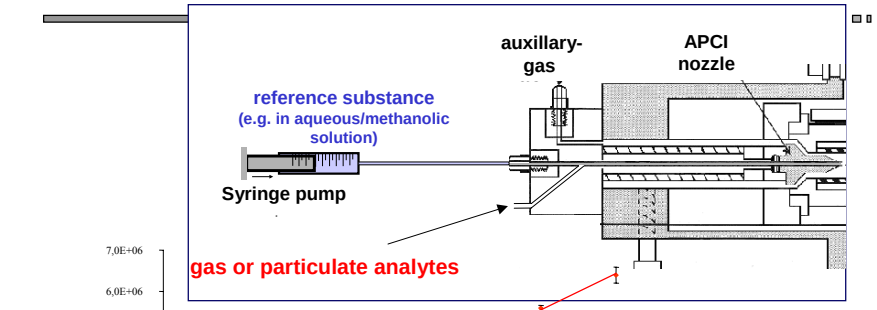
$O_2 + e^- \rightarrow O_2^{-\cdot}$

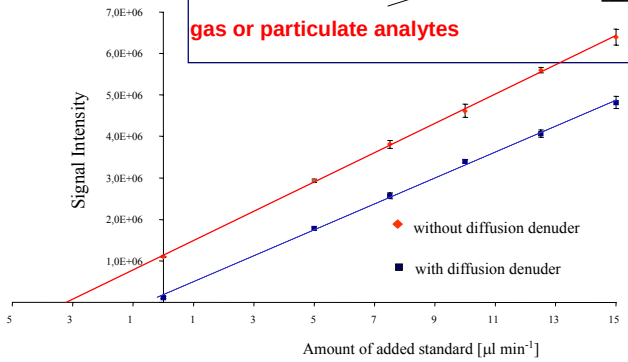
$O_2^{-\cdot} + n\ H_2O \rightarrow O_2^{-\cdot} \cdot (H_2O)_n$

Deprotonation:

$O_2^{-\cdot} \cdot (H_2O)_n + M \rightarrow [M\text{-}H]^- + HO_2 + n\ H_2O$

APCIMS: Quantification using standard addition

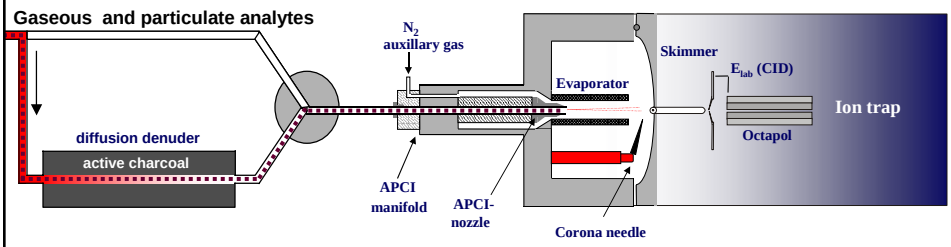




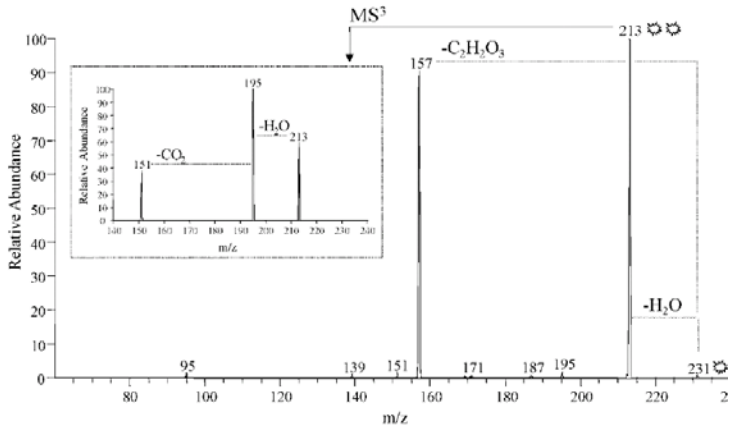
Results of pinonaldehyde quantification with and without diffusion denuder

Warscheid und Hoffmann, **(2003)**, *Anal. Chem.*

Sample introduction into the APCI-source



MS/MS of Smog Chamber with AP-CIMS



•Warscheid B, Hoffmann T. Direct analysis of highly oxidised organic aerosol constituents by on-line ion trap mass spectrometry in the negative-ion mode. RAPID COMMUNICATIONS IN MASS SPECTROMETRY 16 (6): 496-504 2002.

Figure 3. MS^2 and MS^3 fragment spectra of $[M - H]^-$ ions (m/z 231) of the tentatively identified $C_{10}H_{16}O_6$ carboxylic acid product (LO6) derived from the gas-phase reaction of limonene with ozone.

AP-CIMS References and Links

- **Not at AAAR 2004**

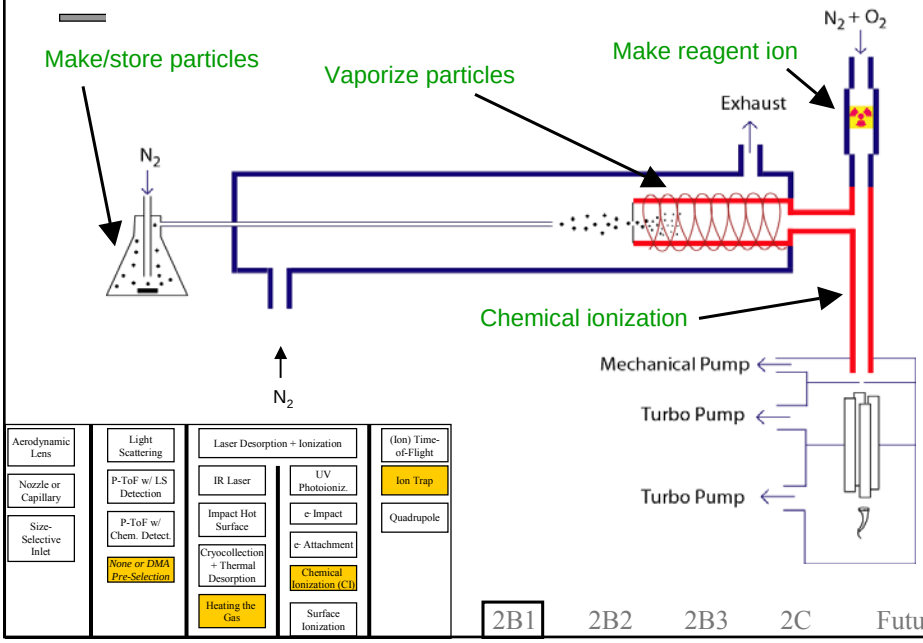
- Warscheid B, Kuckelmann U, Hoffmann T. Direct quantitative analysis of organic compounds in the gas and particle phase using a modified atmospheric pressure chemical ionization source in combination with ion trap mass spectrometry. ANALYTICAL CHEMISTRY 75 (6): 1410-1417 MAR 15 2003.

- Hoffmann T, Bandur R, Hoffmann S, et al. On-line characterization of gaseous and particulate organic analytes using atmospheric pressure chemical ionization mass spectrometry. SPECTROCHIMICA ACTA PART B-ATOMIC SPECTROSCOPY 57 (10): 1635-1647 OCT 15 2002.

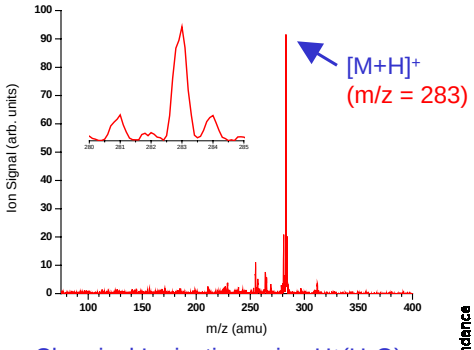
- Warscheid B, Hoffmann T. Direct analysis of highly oxidised organic aerosol constituents by on-line ion trap mass spectrometry in the negative-ion mode. RAPID COMMUNICATIONS IN MASS SPECTROMETRY 16 (6): 496-504 2002.

- Warscheid B, Hoffmann T. Structural elucidation of monoterpene oxidation products by ion trap fragmentation using on-line atmospheric pressure chemical ionisation mass spectrometry in the negative ion mode. RAPID COMMUNICATIONS IN MASS SPECTROMETRY 15 (23): 2259-2272 2001

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



Low Fragmentation with Chemical Ionization

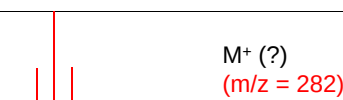


Chemical Ionization using $H^+(H_2O)_2$

Low degree of fragmentation aids in:

- identification
- quantification

Oleic acid
282 amu

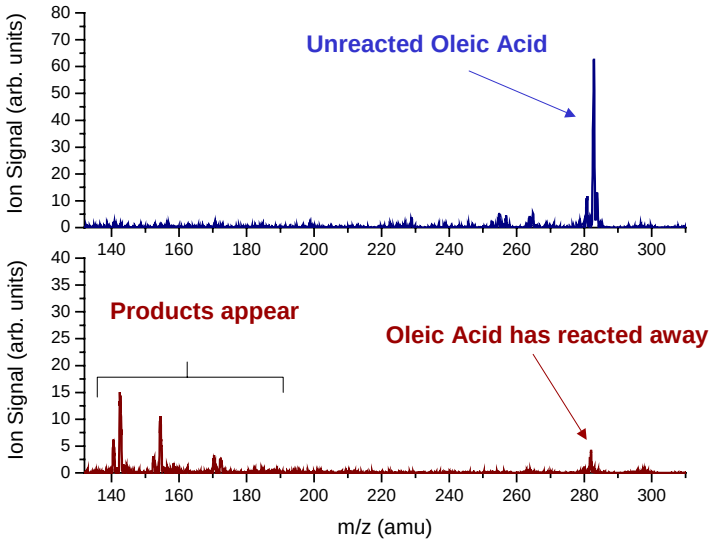


Electron Impact (EI) Ionization

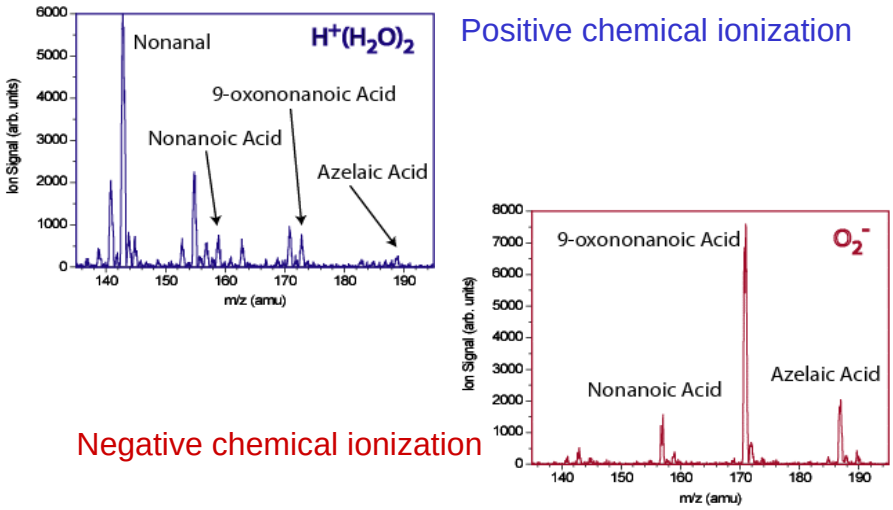
Large degree of fragmentation

From: NIST Chemistry WebBook

Mass Spectra of Reacted Particles



Product Identification

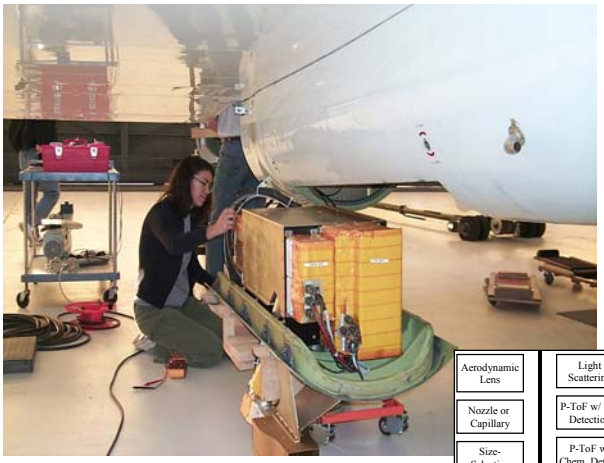


from: Hearn & Smith, *JPC A*, in press

A-CIMS References and Links

- **Poster 7PB4**: THE ROLE OF PARTICLE SUBSTRATE EFFECTS IN DETERMINING THE REACTIVITY OF ORGANIC AEROSOLS GEOFFREY D. SMITH, John D. Hearn.
- "Kinetics and Product Studies for Ozonolysis Reactions of Organic Particles Using Aerosol CIMS." John D. Hearn and Geoffrey D. Smith, J. Phys. Chem. A, accepted for publication.
- "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.
- http://www.chem.uga.edu/gsmith

Type 2B1: SI-CIMS (Wennberg *et al.*)



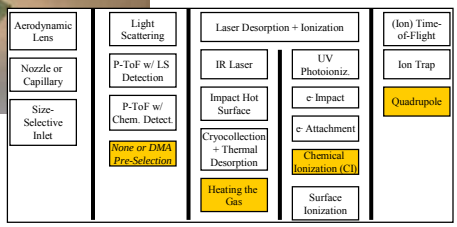
Dr. Karena McKinney of Caltech preparing the SI-CIMS on the ER-2

Courtesy of Paul Wennberg, Caltech
http://www.gps.caltech.edu/~wennberg/cims.html

- Conceptually similar to A-CIMS
- Flown in Stratosphere in ER-2 aircraft

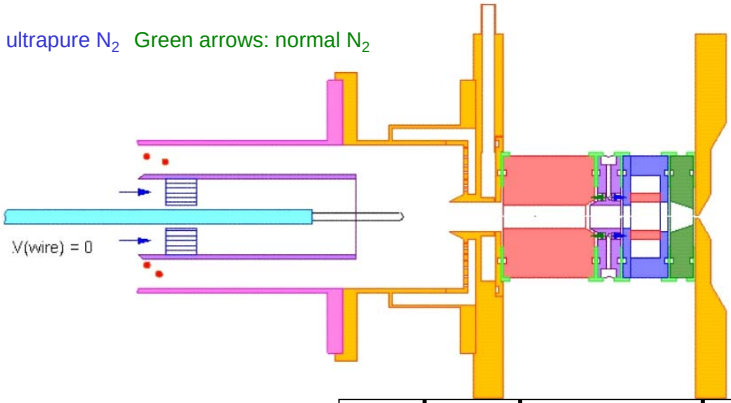
- **Not at AAAR 2004**

The detection of large HNO3-containing particles in the winter arctic stratosphere, Fahey et al., Science, 291, 1026-1031, 2001.



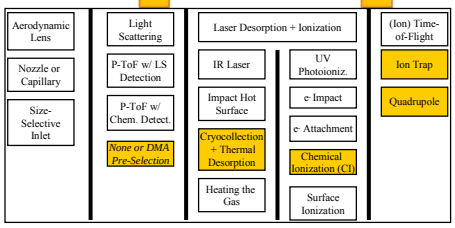
Type 2B1: TDCIMS: Gas Flow in Source

Blue arrows: ultrapure N_2 Green arrows: normal N_2



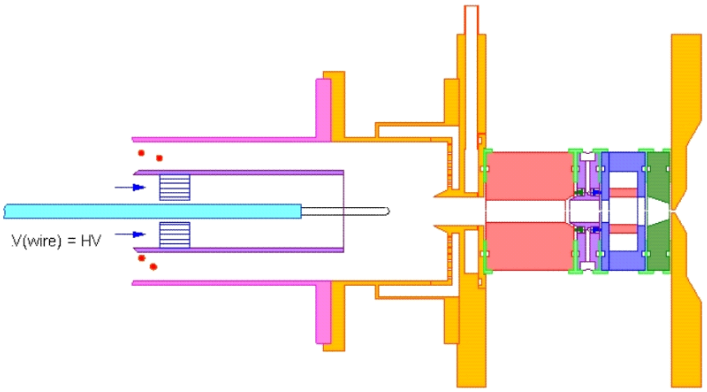
Courtesy of Jim Smith, NCAR
http://www.acd.ucar.edu/~jimsmith/POP

- Ultra pure N_2 sheath flow isolates wire from sampled particles and gas
- Some contamination of the wire from gases is inevitable, so we periodically collect "background spectra" with no particles being collected (as above).



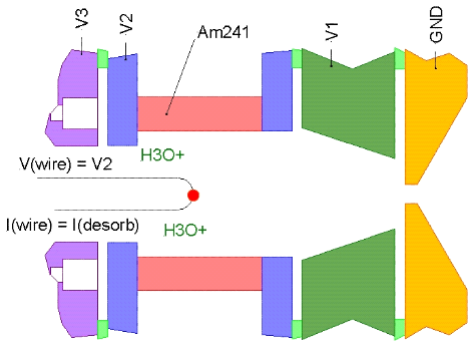
TDCIMS: Step 1 – Particle Collection

Courtesy of Jim Smith, NCAR
http://www.acd.ucar.edu/~jimsmith/POP



- Sample air with charged particles enters electrostatic precipitator
- Collection filament is biased at a ca. 4 Kvolts with respect to chamber walls.
- Particles cross flow streamlines to collect on metal filament
- After a few minutes, wire is inserted into ion source for sample analysis

TDCIMS: Step 2 – Sample Desorption and Analysis



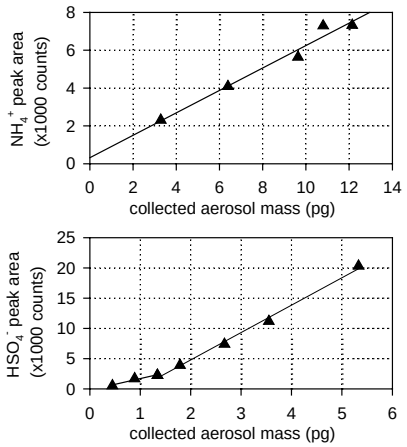
- Wire momentarily heated at temperatures up to 300 °C to desorb sample
- Neutral compounds are ionized using chemical ionization, e.g.: $H_3O^+ + NH_3 \rightarrow NH_4^+ + H_2O$
- Reagent ions are created by α particles emitted from the source, generating mostly H_3O^+, O_2^- and CO_3^-
- Ionized analyte injected into a quadrupole mass spectrometer for analysis

Courtesy of Jim Smith, NCAR
http://www.acd.ucar.edu/~jimsmith/POP

TD-CIMS: Quantification

Calibration with 14 nm (for NH_4^+) and 10 nm (for HSO_4^-) ammonium sulfate aerosol

Instrument response as a function of collected mass



Voisin et al., Aerosol Sci. Technol., 37(6): 471-475, 2003.

TDCIMS: Ambient Sampling

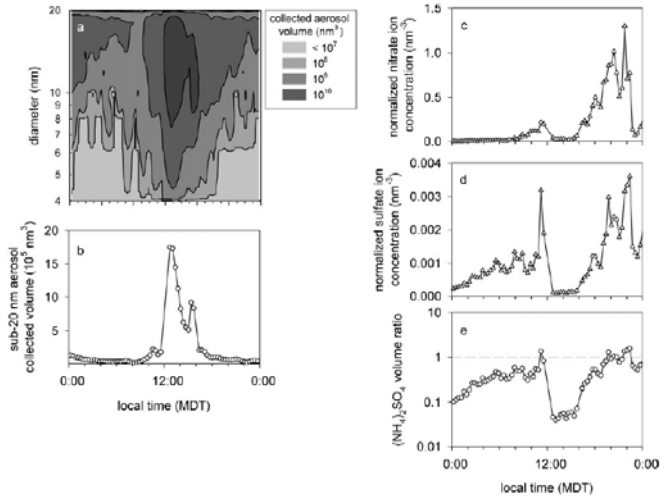


Figure 9. Aerosol sub-20 nm chemical composition on October 19, 2002, as measured by negative ion TDCIMS. (a) Collected aerosol volume as a function of aerosol diameter and local time, (b) total collected sub-20 nm diameter aerosol volume, (b) total collected sub-20 nm diameter aerosol volume, (c) aerosol nitrate volume-normalized concentration, (d) aerosol sulfate volume-normalized concentration, and (e) $(NH_4)_2SO_4$ aerosol volume fraction based on measured bisulfate concentration (see Equation (5)).

Atmospheric Measurements of Sub-20 nm Diameter Particle Chemical Composition by Thermal Desorption Chemical Ionization Mass Spectrometry, J. N. Smith, K. F. Moore, P. H. McMurry, and F. L. Eisele, Aerosol Sci. Technol., 2004, 38: 100-110.

TDCIMS References and Links

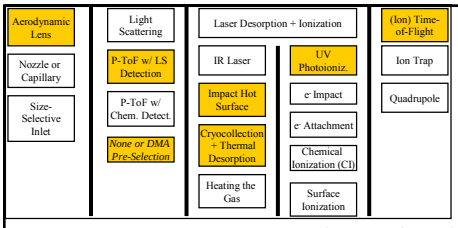
• **Poster 1PE1:** MEASUREMENT OF THE SIZE DISTRIBUTION AND CHEMICAL COMPOSITION OF RURAL ATMOSPHERIC NANOPARTICLES. MATTHEW J. DUNN, Katharine Moore, Fred L. Eisele, James N. Smith, National Center for Atmospheric Research

•**Talk 9E4:** SIZE-DEPENDENT CHEMICAL COMPOSITION OF SUB-20 NANOMETER ATMOSPHERIC AEROSOL. KATHARINE F. MOORE, James N. Smith, Matt Dunn, Fred L. Eisele, Peter H. McMurry, Melissa Fink, Mark R. Stolzenburg,

• Atmospheric Measurements of Sub-20 nm Diameter Particle Chemical Composition by Thermal Desorption Chemical Ionization Mass Spectrometry, J. N. Smith, K. F. Moore, P. H. McMurry, and F. L. Eisele, Aerosol Sci. Technol., 2004, 38: 100-110.

• Thermal Desorption Chemical Ionization Mass Spectrometer for Ultrafine Particle Chemical Composition, D. Voisin, J. N. Smith, H. Sakurai, P. H. McMurry, and F. L. Eisele, Aerosol Sci. Technol., 2003, 37(6): 471-475.

• http://www.acd.ucar.edu/~jimsmith/POP



Type 2B2: TD + VUV Ionization

• UNC-Chapel Hill, Baer, Miller *et al.* **Not at AAAR'04**

Thermal vaporization-vacuum ultraviolet laser ionization time-of-flight mass spectrometry of single aerosol particles Sykes DC, Woods E, Smith GD, **Baer T**, **Miller RE**. ANALYTICAL CHEMISTRY 74 (9): 2048-2052 MAY 1 2002

• Photoionization Aerosol Mass Spectrometry (PIAMS): U. Delaware, Johnston *et al.*

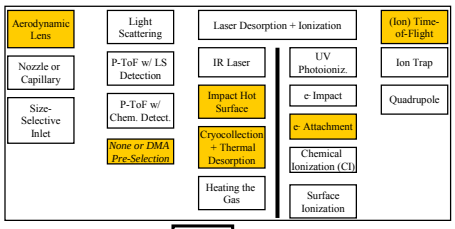
On-line analysis of organic components in fine and ultrafine particles by photoionization aerosol mass spectrometry Oktem B, Tolocka MP, Johnston MV. ANALYTICAL CHEMISTRY 76 (2): 253-261 JAN 15 2004

11B1 - OZONOLYSIS OF ORGANIC AEROSOLS: KINETICS AND FORMATION OF HIGH MOLECULAR WEIGHT PRODUCTS. *MICHAEL TOLOCKA, Matthew Dreyfus, Julie Lloyd and Murray Johnston*

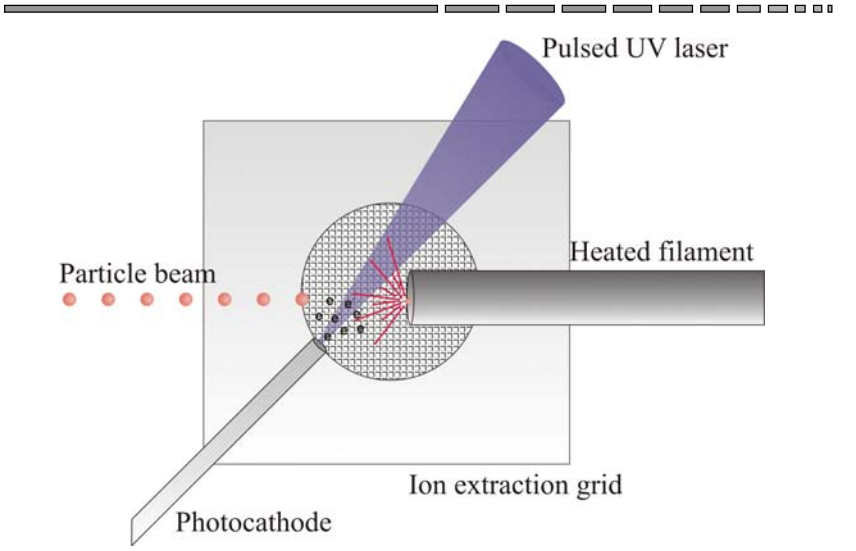
Won't cover here since already discussed in Part 1

Type 2B3:
TD + Electron Attachment

- Photoelectron Resonance Capture Ionization Aerosol Mass Spectrometer (PERCI-AMS): U. Vermont, G. Petrucci *et al.*
  - aka *electron attachment*

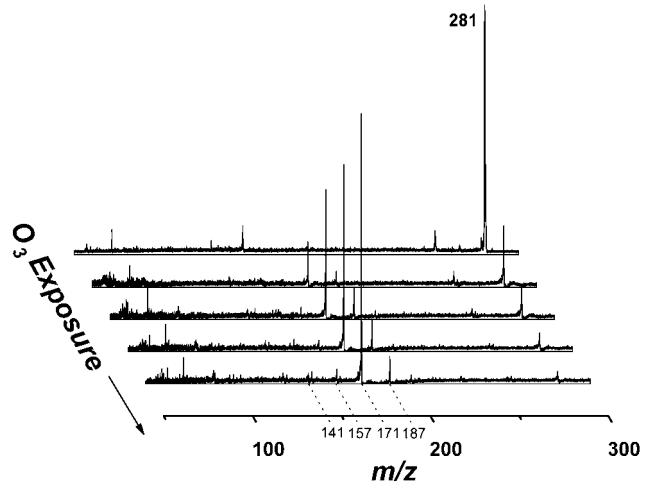


PERCI-AMS



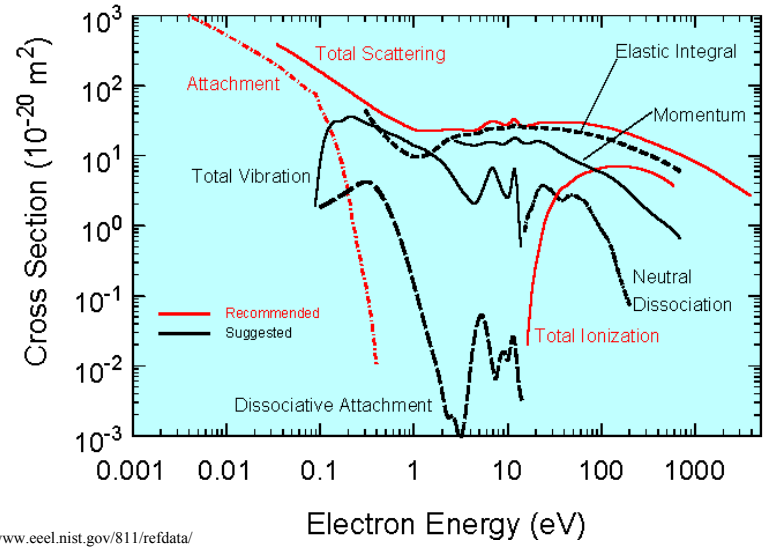
http://www.uvm.edu/~gpetrucc/ams/PERCI.htm

PERCI-AMS: Oleic Acid + O_3 Reaction



- Very little fragmentation

Electron Interaction Cross Sections (SF_6)



http://www.eeel.nist.gov/811/refdata/

Electron Interaction Cross Sections (CF_4)

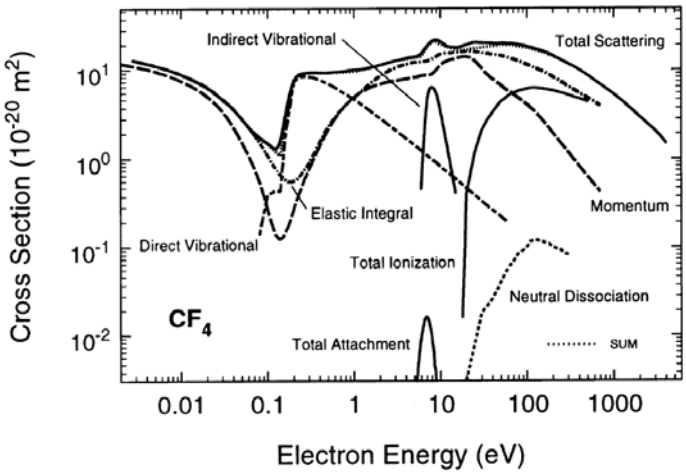


Figure 1: Electron-interaction cross sections for CF_4 [1]

http://physics.nist.gov/Divisions/Div842/Icamdata/PDF/1Databases/christo.pdf
http://www.eeel.nist.gov/811/refdata/

PERCI-AMS Summary

+ Soft ionization method (decreased molecular fragmentation)
+ Tunable electron energies α to $h\nu$ and photocathode work function, ϕ
+ Improved selectivity (resonance process)
+ Improved sensitivity

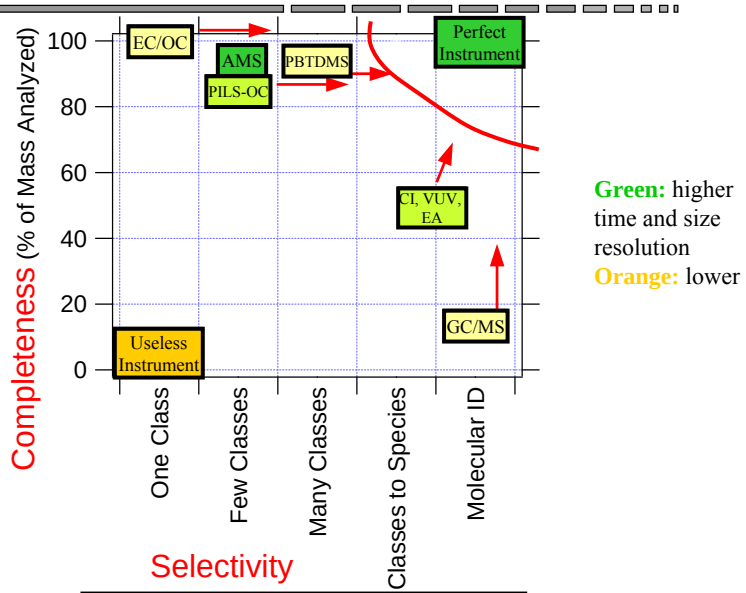
- Difficult to generate large fluxes of low energy electrons
- Difficult to accurately control electron energies and minimize energy bandwidth (space charge)

http://www.uvm.edu/~gpetrucc/ASMS2003_Poster_ThPJ1_162_Petrucci.pdf

PERCI-AMS References

- **Poster LB 21** - INVESTIGATION OF OZONOLYSIS OF OLEIC ACID PARTICLES BY PERCI-MS. Zahardis, LaFranchi, PETRUCCI
- LaFranchi, B. W.; Zahardis, J.; Petrucci, G. A., Photoelectron resonance capture ionization mass spectrometry: A soft ionization source for mass spectrometry of particle-phase organic compounds. Rapid Communications in Mass Spectrometry 2004, in press.
- LaFranchi, B. W.; Petrucci, G. A., Photoelectron resonance capture ionization (PERCI): a novel technique for the soft-ionization of organic compounds. Journal of the American Society for Mass Spectrometry 2004, 15, (3), 424-430.
- http://www.uvm.edu/~gpetrucc/ams/PERCI.htm

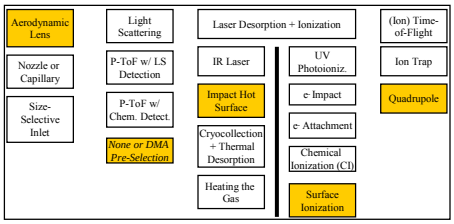
Organic Analysis in Context



Green: higher time and size resolution
Orange: lower

Type 2C:
(TD) + Surface Ionization

- Surface-Ionization Particle Beam Mass Spectrometer (SI-PBMS): Goteborg Univ., Pettersson *et al.*



SI-PBMS: Instrument Design

Aerosol Science and Technology, 38:655–663, 2004

ISSN: 0278-6826 print / 1521-7388 online
DOI: 10.1080/02786820490485944

Chemical Analysis of Individual Alkali-Containing Aerosol Particles: Design and Performance of a Surface Ionization Particle Beam Mass Spectrometer

Maria Svane, Magnus Hagström, and Jan B. C. Pettersson
Department of Chemistry, Atmospheric Science, Göteborg University, Göteborg, Sweden

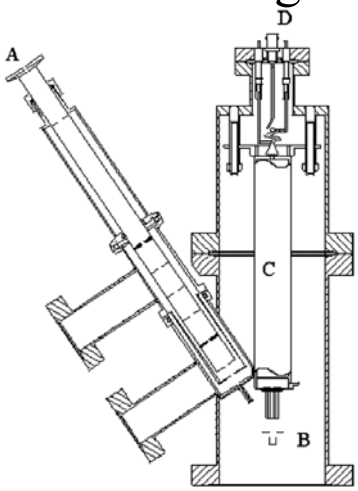
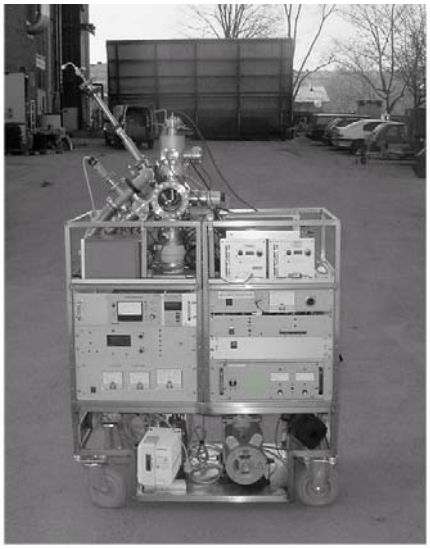


Figure 1. Cross-section view of the vacuum system of the PBMS. A, the particle inlet containing the aerodynamic lens system; B, the ionizing platinum surface and a focusing electrode; C, QMS; D, electron multiplier and electronic feedthroughs.

SI-PBMS: Tranportable Instrument



AMS

Figure 2. The mobile PBMS outside Göteborg University, Sweden.

SI-PBMS: Test w/ Pure NaCl

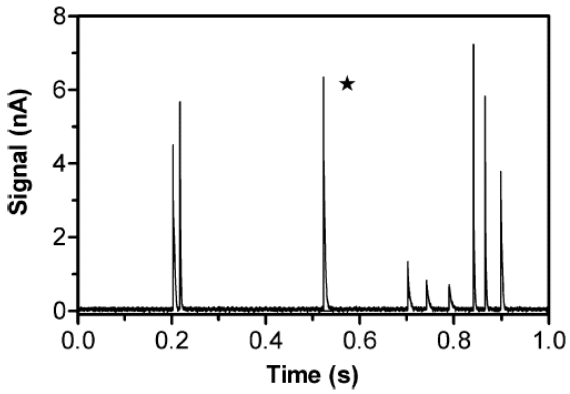


Figure 3. Example of the recorded output signal using a laboratory-generated NaCl aerosol. Individual alkali salt particles give rise to clearly time-resolved peaks. The peak indicated with (⋆) corresponds to a particle with a calculated diameter of 240 nm.

SI-PBMS Quantification

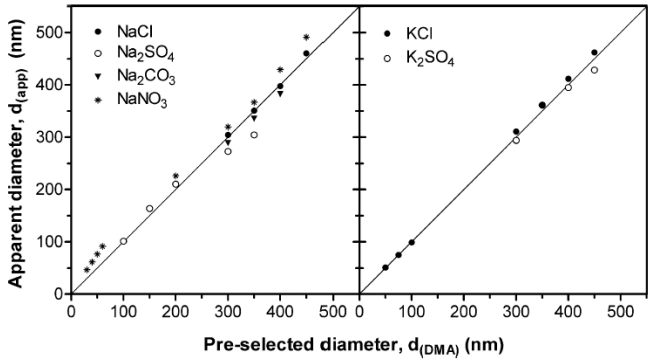


Figure 6. The measured apparent particle diameter (d_{app}) is plotted against the particle diameter preselected with a DMA for different sodium and potassium salts, respectively. The straight line in each graph represents $d_{app} = d_{DMA}$.

From Svane et al., 2004

SI-PBMS References and Links

- Not presenting at AAAR'04

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Department of Chemistry, Atmospheric Science, Göteborg University, Göteborg, Sweden

Part 3:
The Future

My Take on Near Future of TD Aerosol MS

- Techniques will keep evolving for another decade
- Components
  - Inlets: improved and "tuned" aerodynamic lenses
  - Further development of Soft ionizations
  - EI will remain very important
- Uses of Aerosol MS
  - *Research* tool
    - Commonplace, e.g. at least one in each field study site / airplane…
  - Ongoing work to adapt to routine monitoring
- Commercial instruments used by non-specialists
  - Thanks to software & hardware improvements
  - Like evolution of DMA in the last 10-20 years
  - Price will still be limiting factor
  - A few more commercial options (e.g. soft ionization)
- Custom-built instruments
  - specialized for problems that the commercial instruments don't do well

Some References

- http://cires.colorado.edu/jimenez/ams.html
  - Lists of references in there
- Special issue on mass spectrometry of aerosols: Aerosol Science and Technology, 33(1-2), July/Aug. 2000.
- Review papers, more focused on Laser Ablation, also good coverage of early TD work:
  - 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.
  - 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 Spectrometry Reviews, 19(4), 248-274.
  - David T. Suess and Kimberly A. Prather (1999). Mass Spectrometry of Aerosols. Chem. Rev. 99, 3007-3035.

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- Paul Wennberg
- Jim Smith
- Joe Petrucci
- Ann Middlebrook
- Qi Zhang
- John Jayne
- Doug Worsnop
- Manjula Canagaratna
- James Allan
- Frank Drewnick
- AMS Users
- *My mass spec. students & my group at Colorado*