Aerosol Mass Spectrometer (AMS) Organic Data and Analysis

Qi Zhang
Atmospheric Science Research Center
State University of New York, Albany
qz@asrc.cestm.albany.edu
web: http://www.asrc.cestm.albany.edu/qz/
Phone: 518-437-8752 (o)

Updated from the tutorial I gave at the 6th AMS User’s Meeting
that took place in Juelich, Germany during August 25th – 28th, 2005

The concentration of a species in question is calculated by summing signals at its partial MS.

Deconvolve AMS Data: Mathematics

A measured AMS mass spectrum is the linear superposition of the mass spectra of components that contribute to AMS signals. (AMS data are quantitative, reproducible)

\[ \mathbf{m_s} = c_1 \cdot \mathbf{m_{s1}} + c_2 \cdot \mathbf{m_{s2}} + \ldots + c_s \cdot \mathbf{m_{ss}} + \epsilon \]

- \( \mathbf{m_s} \) = observed mass spec vector
- \( c_s \) = concentration of species \( s \)
- \( \epsilon \) = residual vector (analytical errors …)

Performance of 1st Deconvolution: AMS vs. Other Instruments

AMS OM vs. Carbon Analyzer OC
Deconvolve AMS Organic Data: Multivariate Analysis

- An AMS organic mass spectrum is the linear superposition of the mass spectra of individual organic species.

- AMS Mass Spectral Tracers (Pittsburgh)

- AMS Mass Spectral Tracers (CMU)

- Deconvolve AMS Organic Data: Algorithms

- AMS Organic Mass Spectrum

Obtain information on individual organic species / classes

1st step deconvolution works with 1 mass spectrum

This approach is not suitable for identifying organic components

- b/c thousands or more organic compounds in atmospheric aerosols

- Not able to definitively describe the relationships between peaks

- Can use multivariate analysis b/c the quantitative and additive nature of mass spec.
Reconstructed values explain >99% of the variance in measured. Indicate other (small) components.

Performance of the Technique:
measured vs. reconstruct organic mass conc.

Performance of the Technique:
measured vs. reconstruct average organic mass spectrum

Performance of the Technique:
measured vs. reconstruct organic matrix

Performance of the Technique:
Are extracted mass spectra chemically meaningful?

Mass concentrations and temporal variations of HOA & OOA in Pittsburgh

Components ≠ Individual Sources
Multiple sources may have similar MS

Extracted mass spectra

Measured mass spectra

Zhang et al., ES&T (2005)
Size distributions of HOA & OOA in Pittsburgh

Zhang et al., ACPD, 2005

Summary of HOA & OOA Deconvolution Technique

By performing a targeted (seeded) factor analysis that initializes with unique mass spectra tracers, we have obtained 2 components (HOA & OOA) are physically and chemically meaningful and together explain more than 99% of variance in measured organic values over 2 weeks in a major city.

References

Introduction to Instrument, Quantification Principles

AMS data contributed by UU, U. Manchester, Aarhus, SUNY-Albany, NIES (Japan), UNH, U Tokyo.

Call for Datasets: plan for writing an global OA paper

AMS data contributed by UU, U. Manchester, Aarhus, SUNY-Albany, NIES (Japan), UNH, U Tokyo.

Pittsburgh AMS Data Analysis

pdf available at http://cires.colorado.edu/jimenez/ams.html#Papers-AMS