Thermodenuder-AMS, and Organic Component Analysis, and CCN Closure with AMS Data

Peter DeCarlo, Alex Huffman, Qi Zhang, James Allan, Mike Cubison, Eben Cross, Doug Worsnop, Paul Ziemann, Athanasios Nenes, Anne Jefferson, Betsy Andrews, John Ogren, and Jose-Luis Jimenez

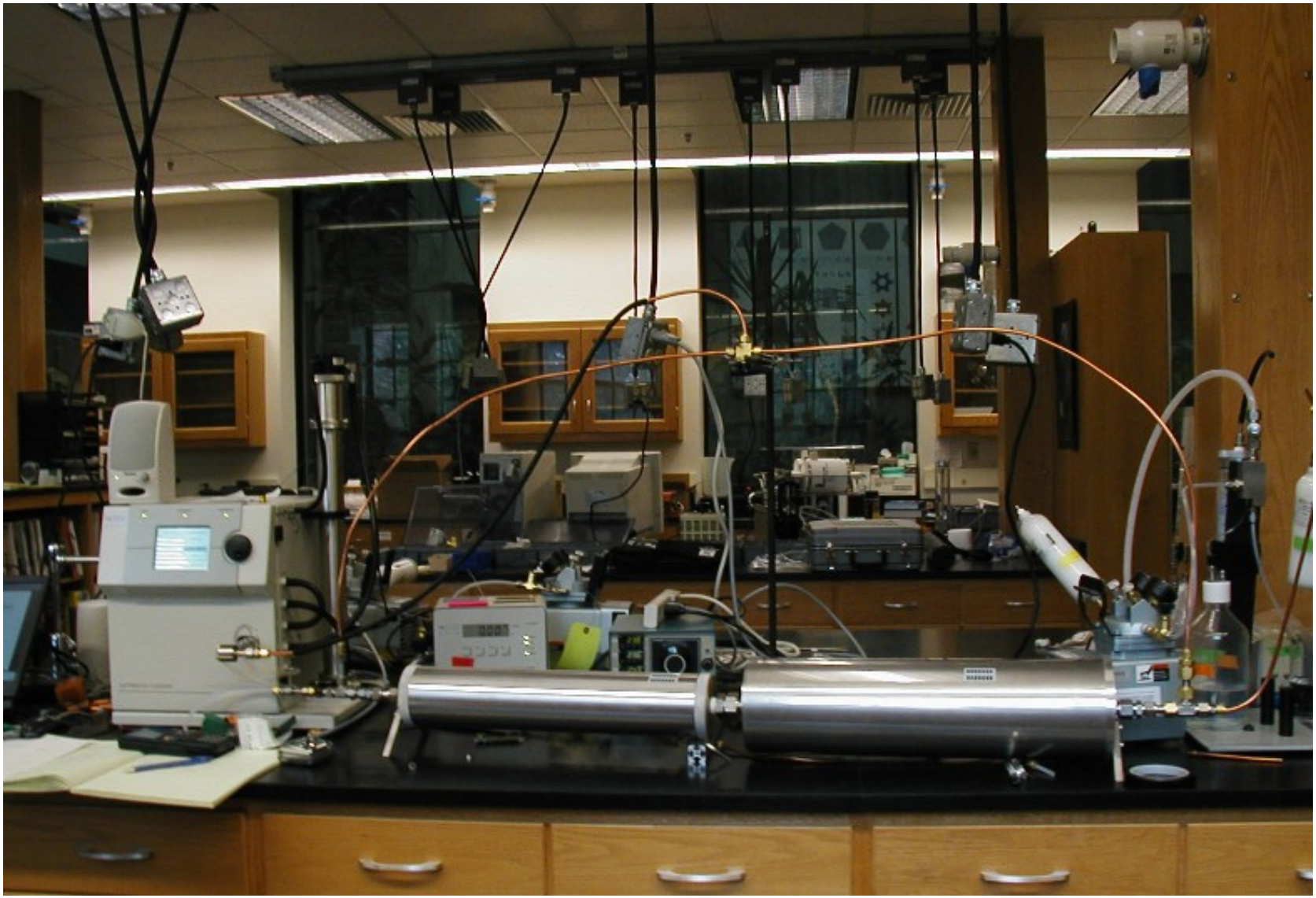
Univ. of Colorado-Boulder, Univ. of Manchester, Aerodyne Research, UC-Riverside, Georgia Tech, NOAA CMDL

Chebogue Pt. Data Analysis Mtg – NOAA 3/10/2005

Part I: Thermodenuder-AMS

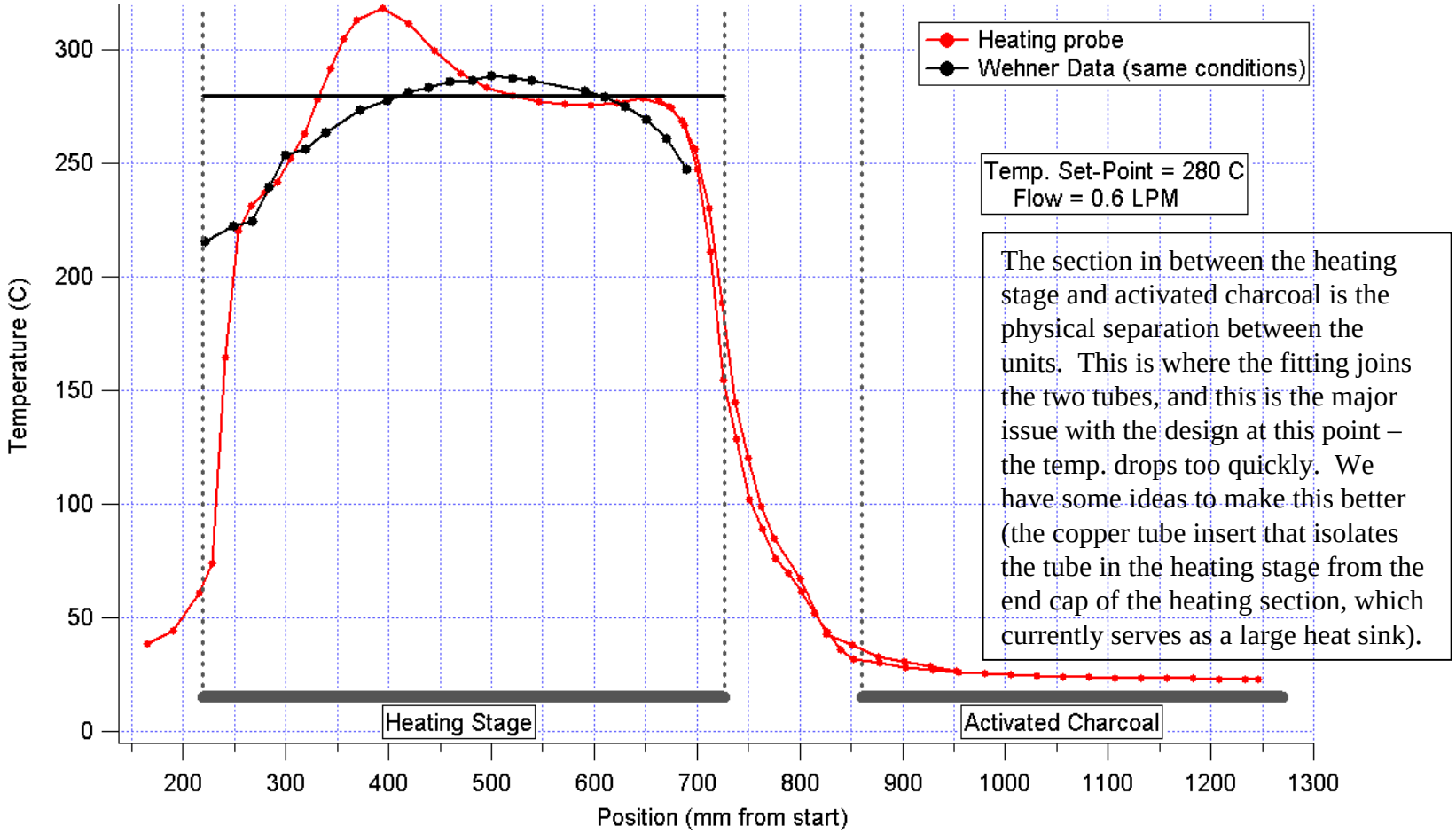
- Idea: measure change in aerosol composition as a function of volatilization temperature
- Focus on organics, “polymers”?

Themodenuder

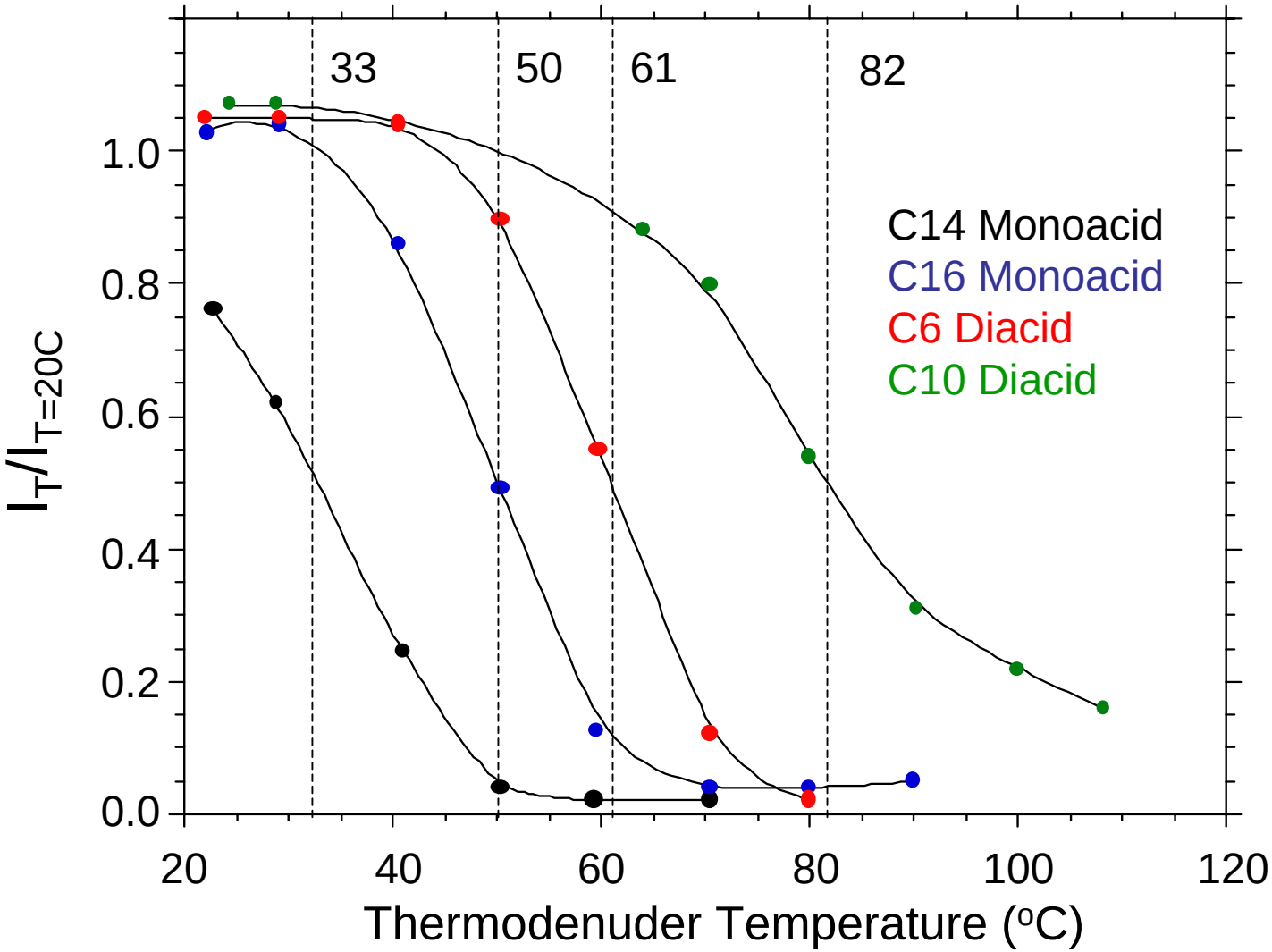


Design after Wehner et al. *J. Aerosol Sci*. 33: 1087-1093.(2002)

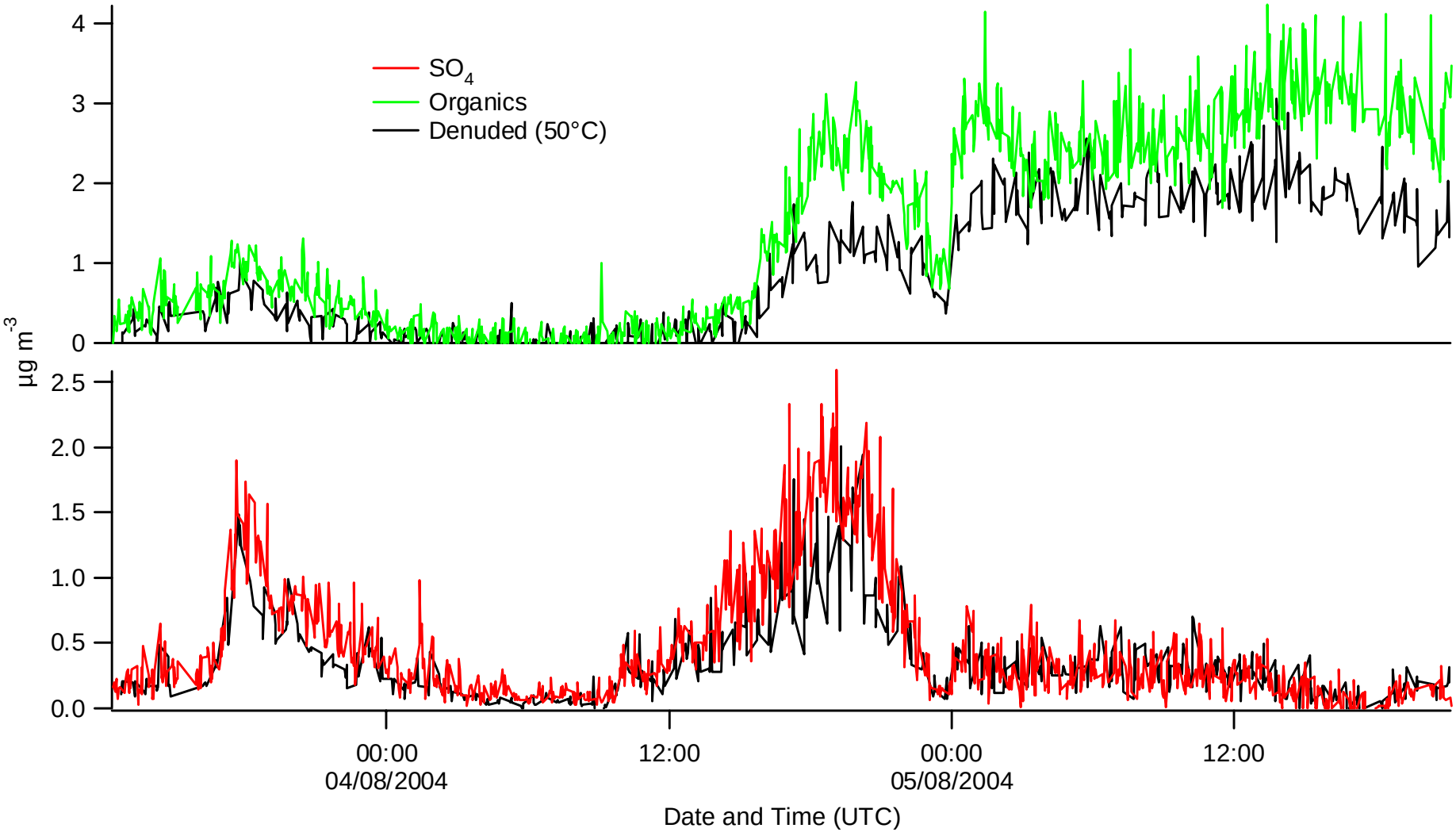
Thermodenuder Temperature Profile



Thermodenuder/TDPBMS
Monocarboxylic and Dicarboxylic Acids



TD-AMS Time Series



- Appears consistent with VTDMA and TAG/Org fraction

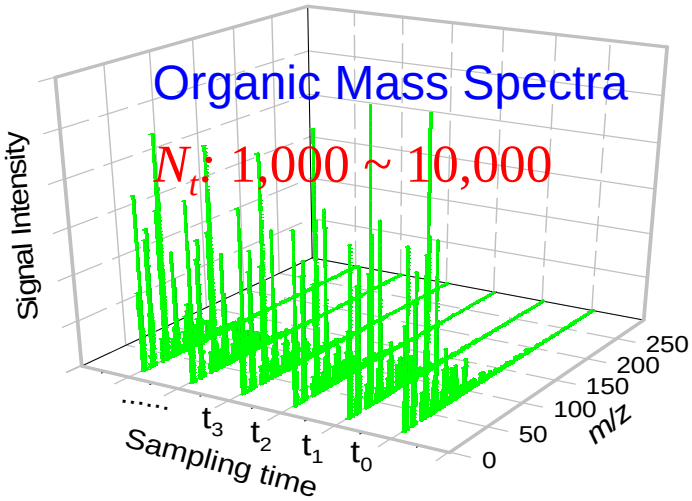
Part II: Organic Component Analysis

- Some chemical resolution *on the whole organic aerosol*
- Apply method developed for urban areas
- "Custom" Principal Component Analysis
- Qi Zhang applying this to 25+ worldwide datasets

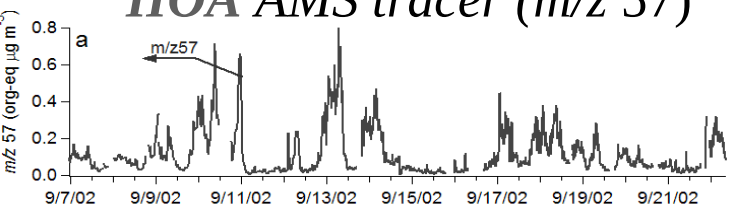
OOA HOA Quantification Algorithm (*see Poster* ***12PA-11***)

OOA: Oxygenated OA

HOA: Hydrocarbon-like OA



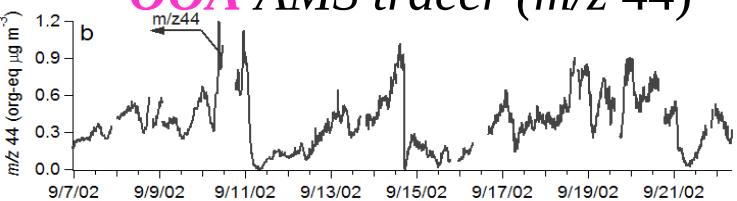
HOA AMS tracer (m/z 57)

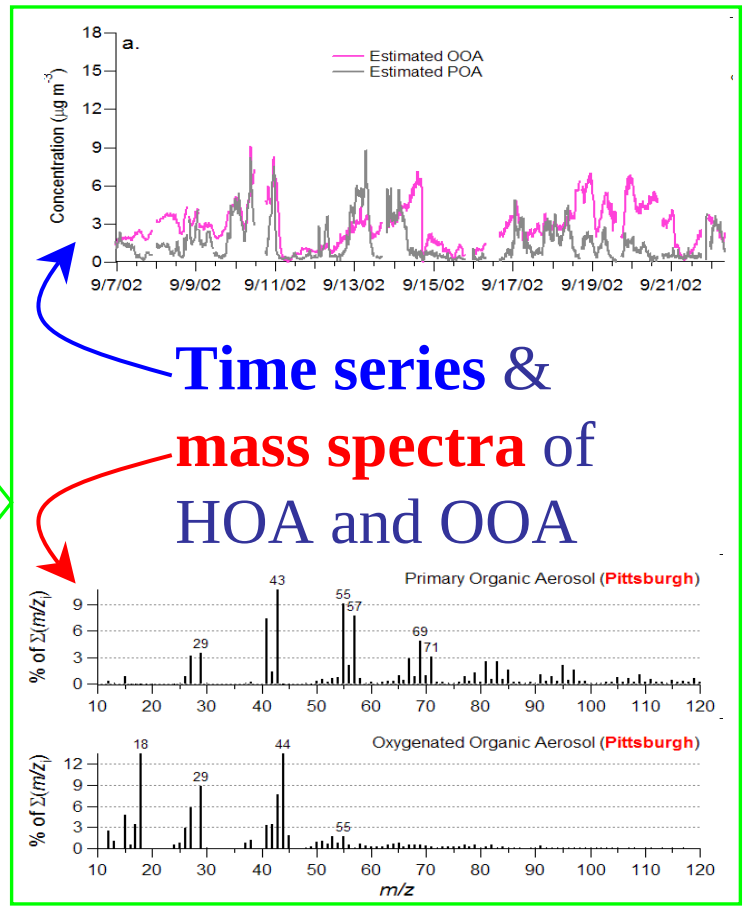


Initial guess of HOA & OOA temporal variability

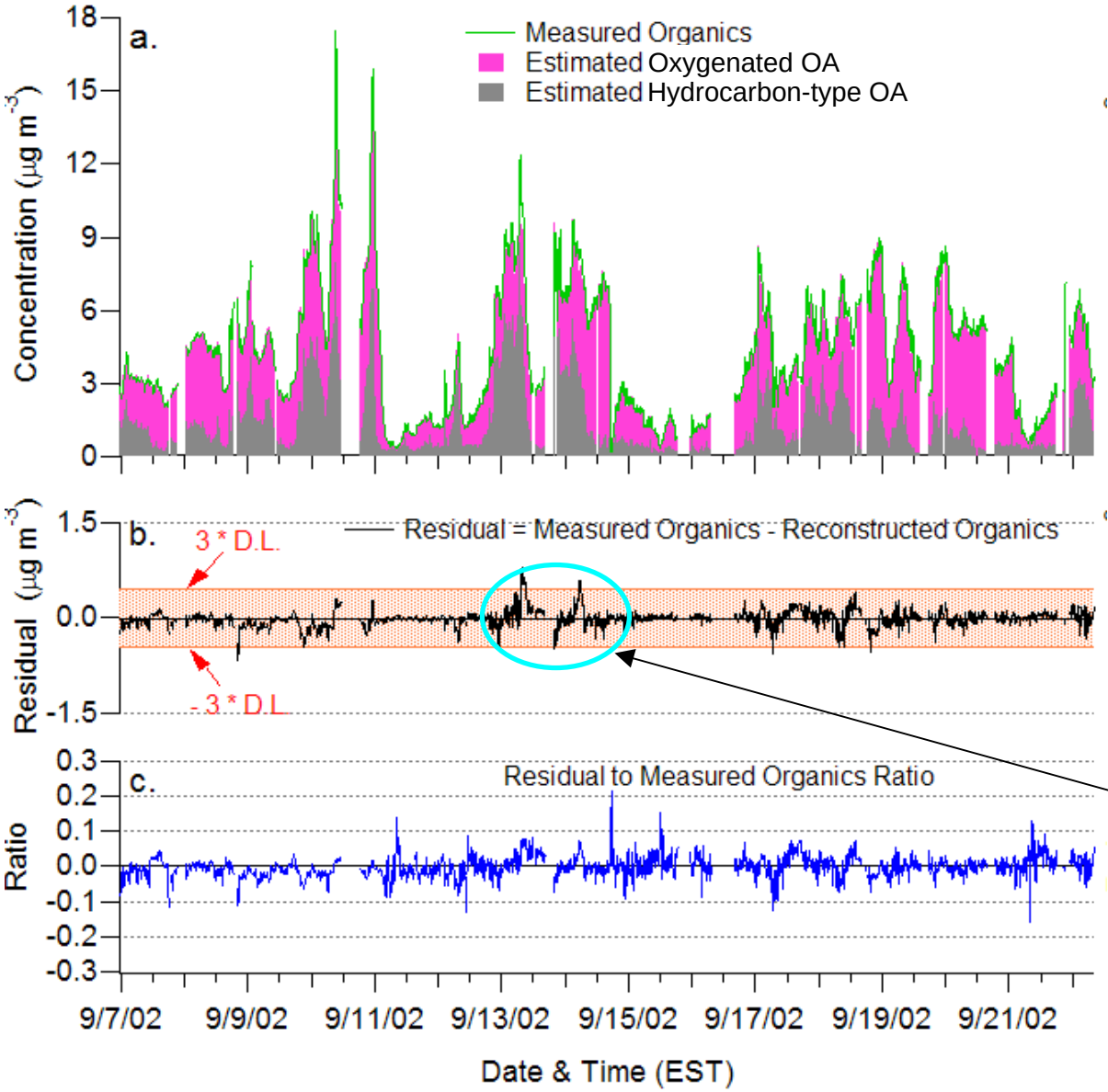
Custom *Iterative* Principal Component Analysis

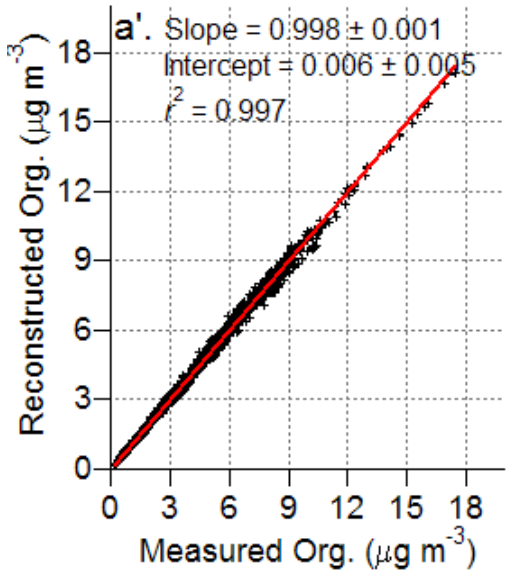
OOA AMS tracer (m/z 44)





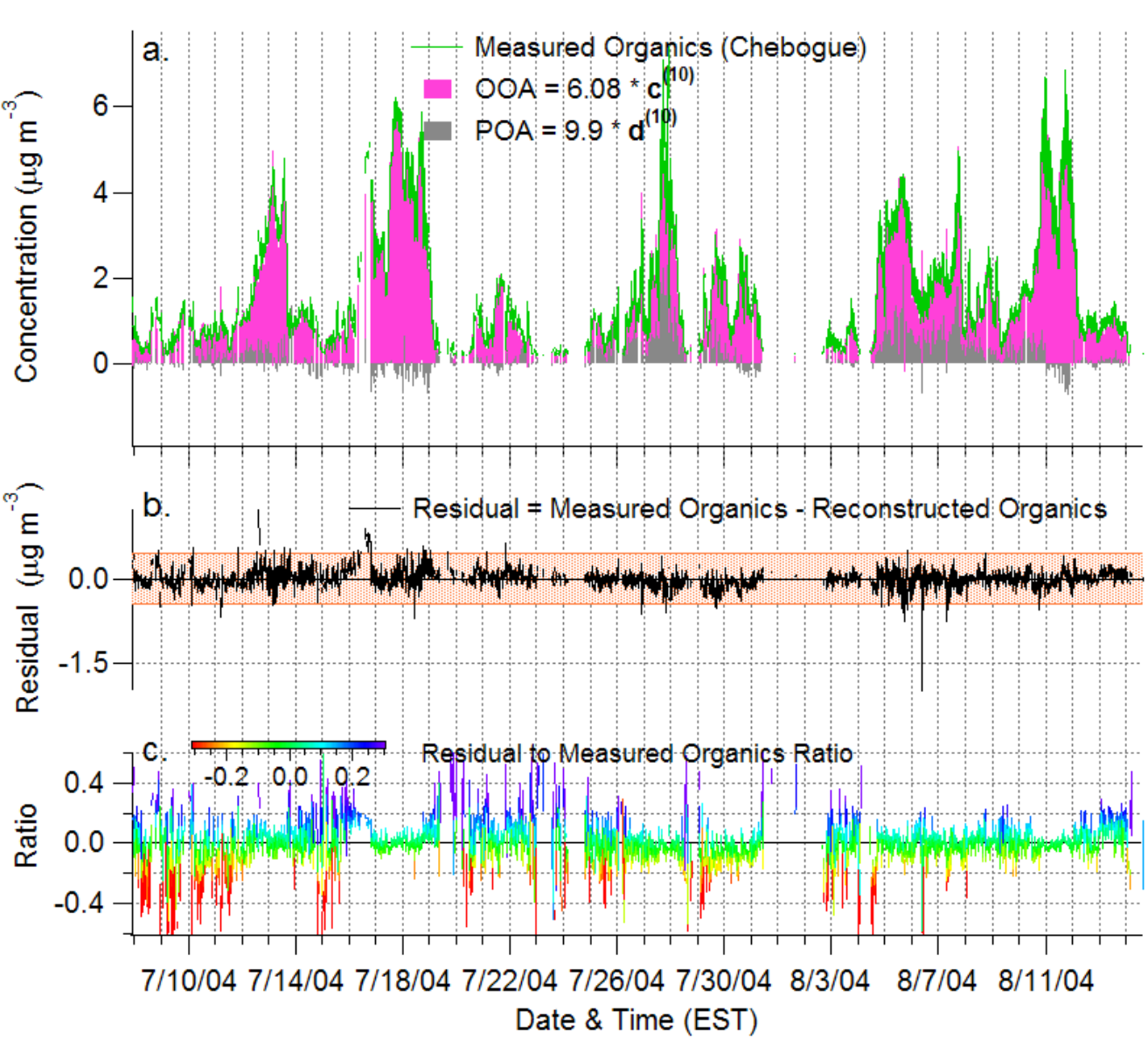
HOA and OOA Time Series in Pittsburgh

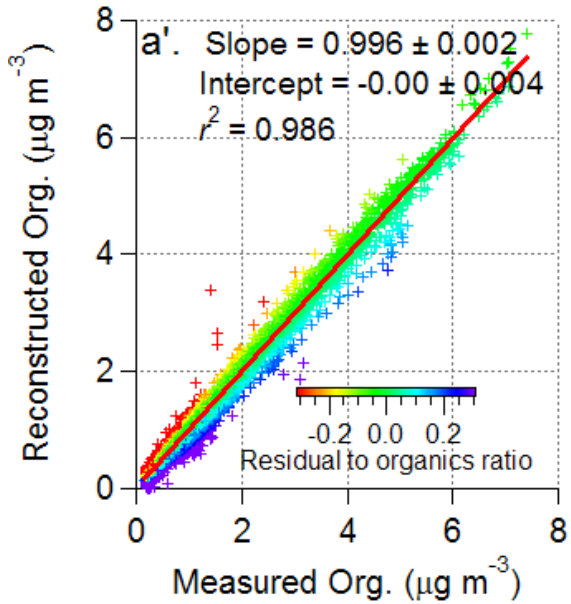


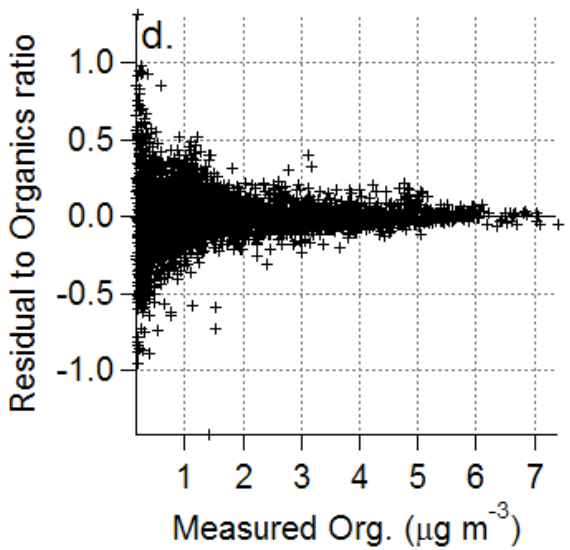


Indications of other (small) components.

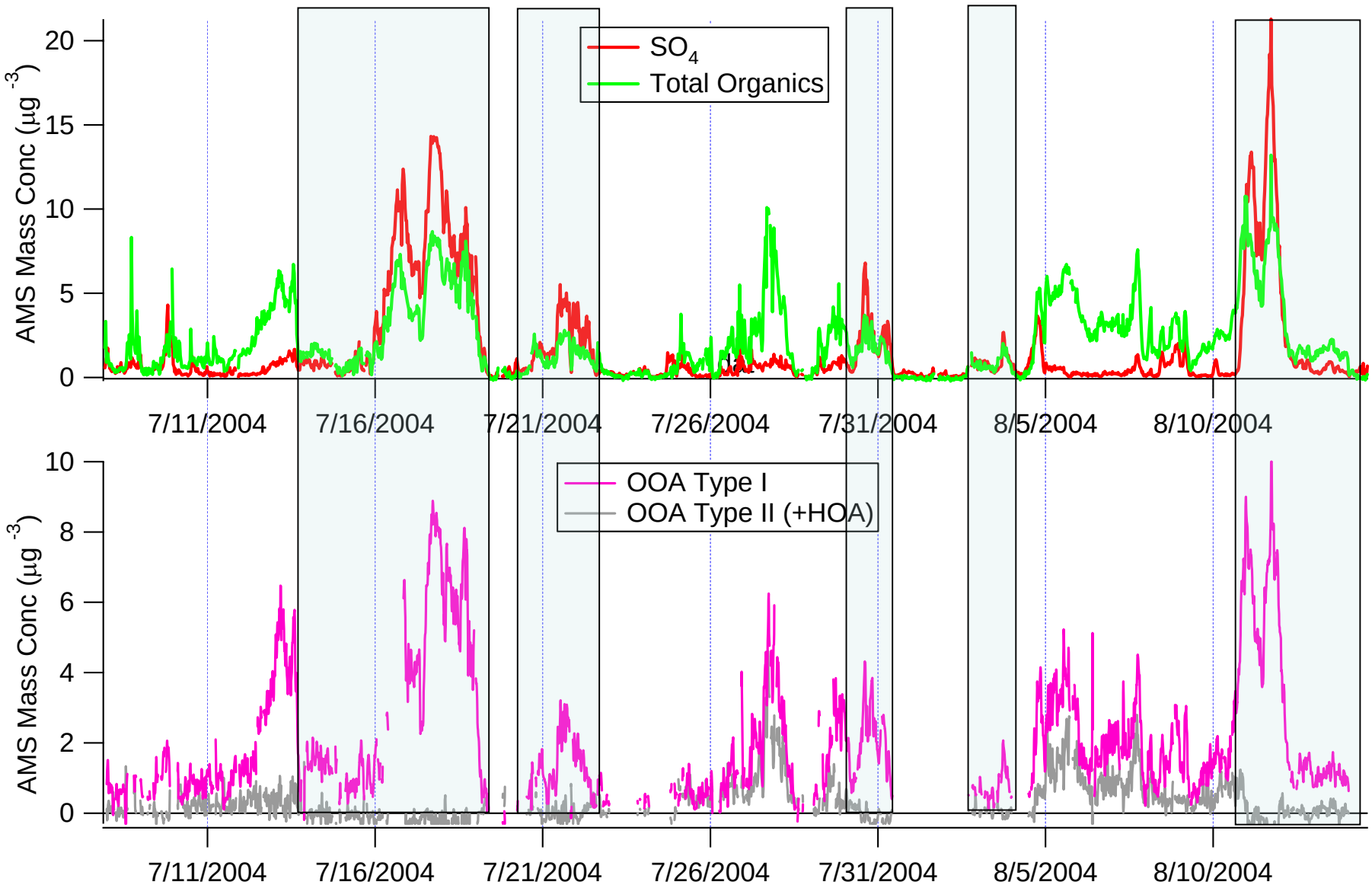
Chebogue: Results of First Pass







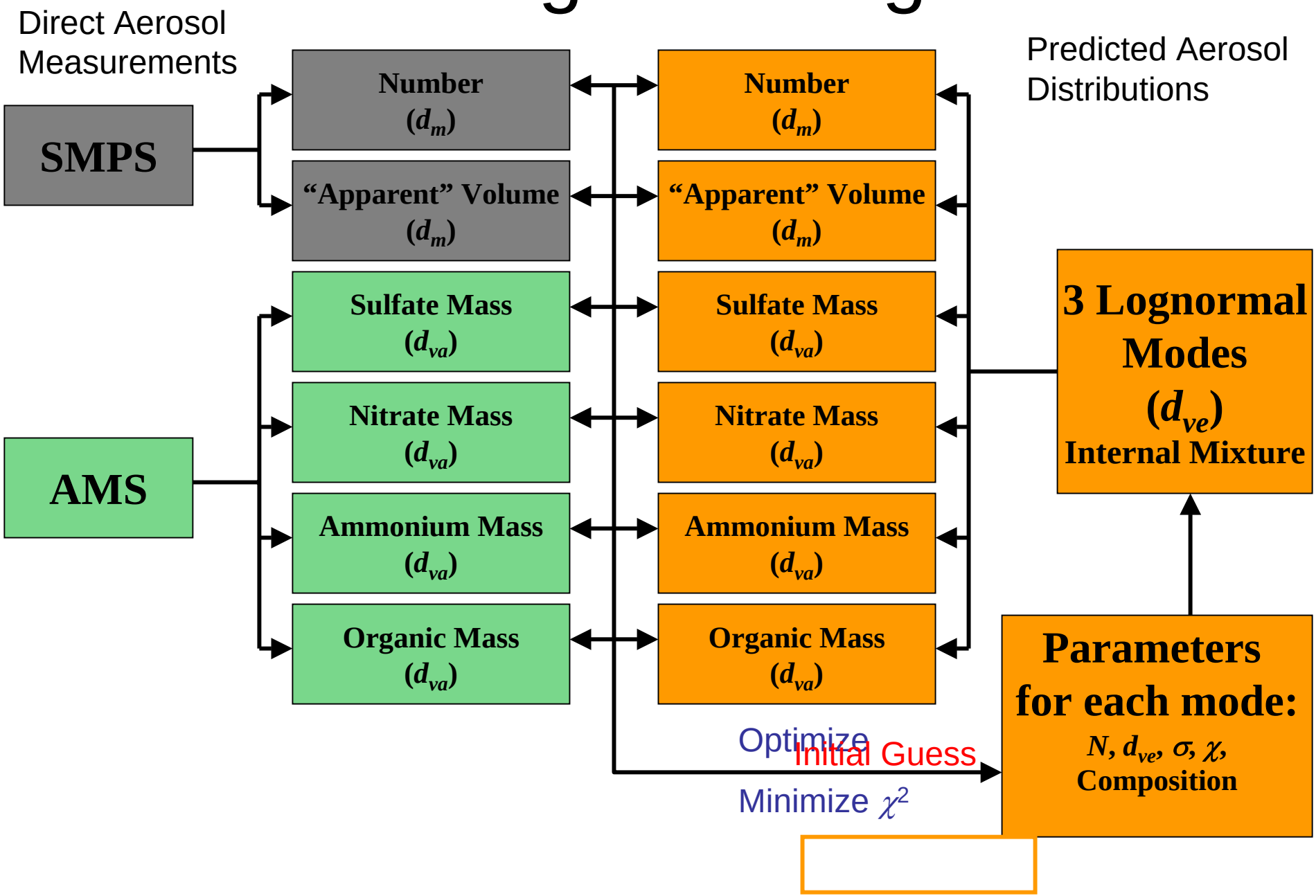
SO_4/Org vs Org Components

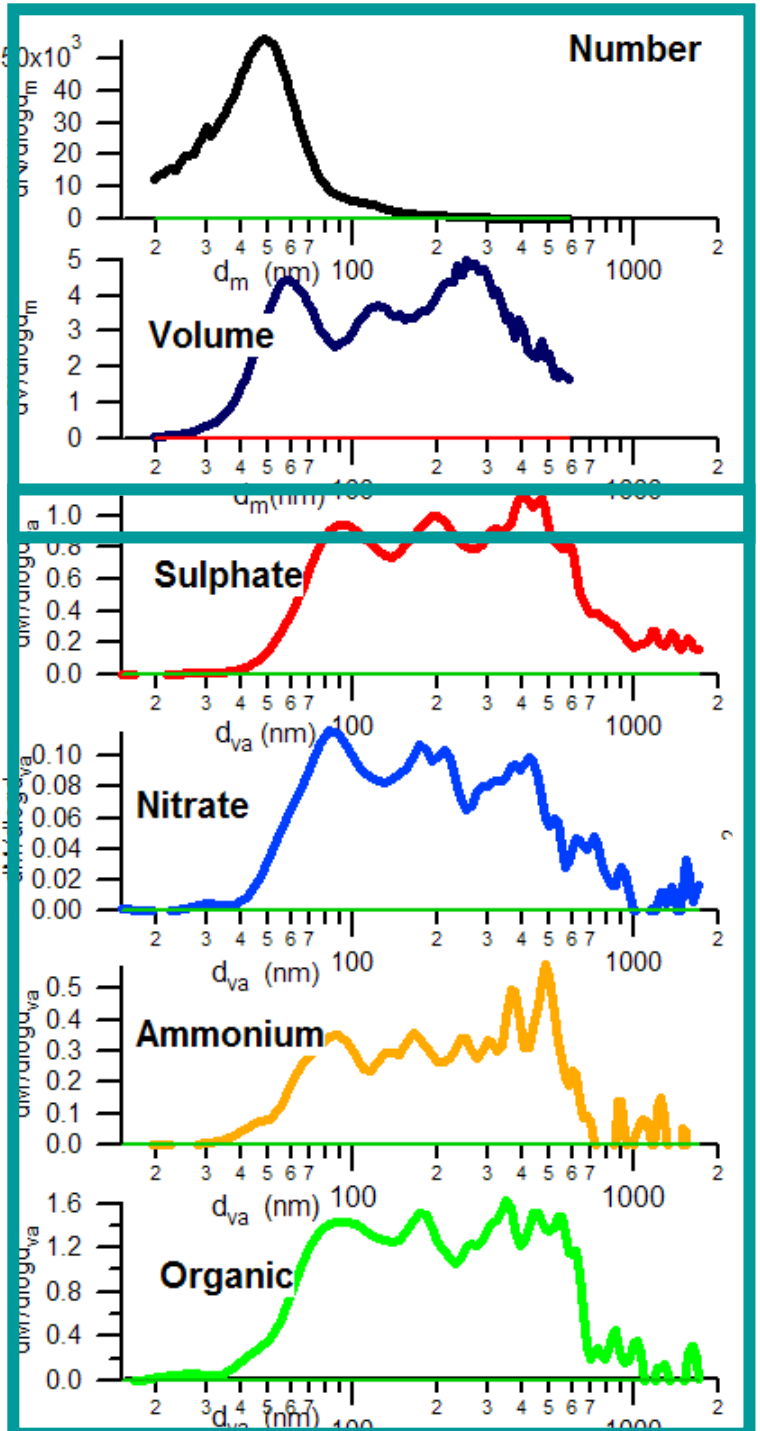


Part III: Aerosol-CCN Closure

- Apply method developed for urban areas
- “Custom” Principal Component Analysis
- Qi Zhang applying this to 25+ worldwide datasets

Data Integration Algorithm





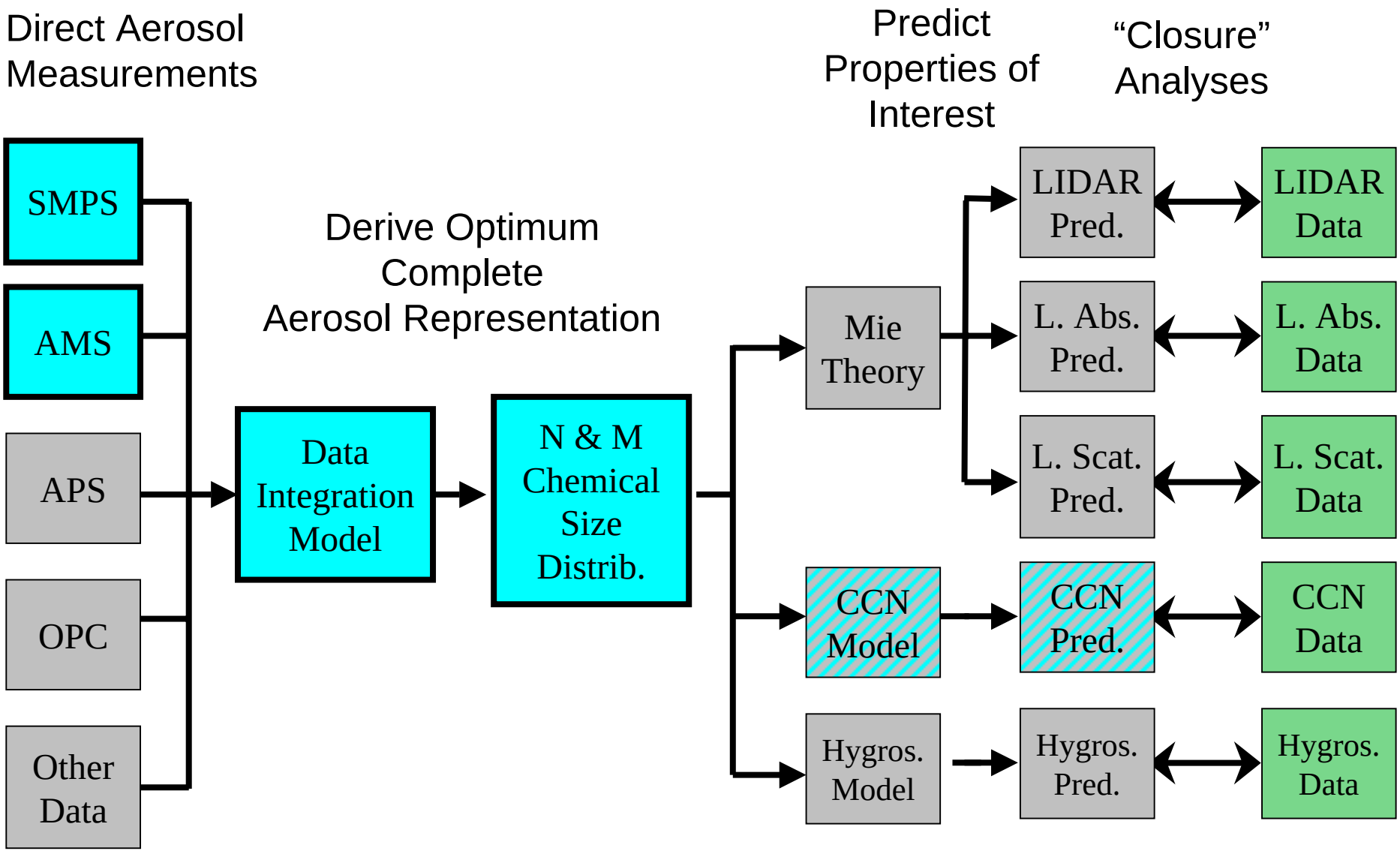
Lognormal Parameters

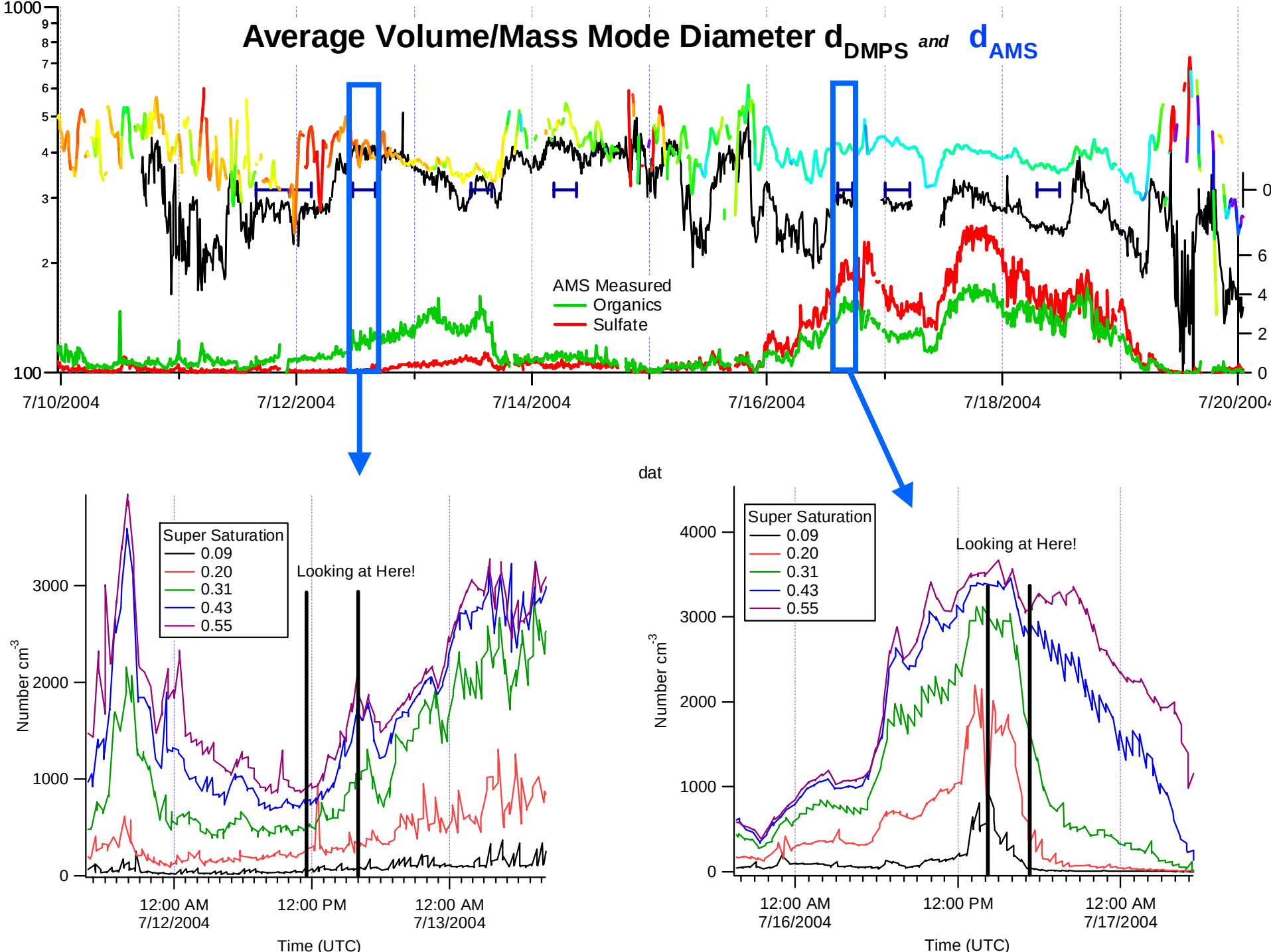
Mode Composition

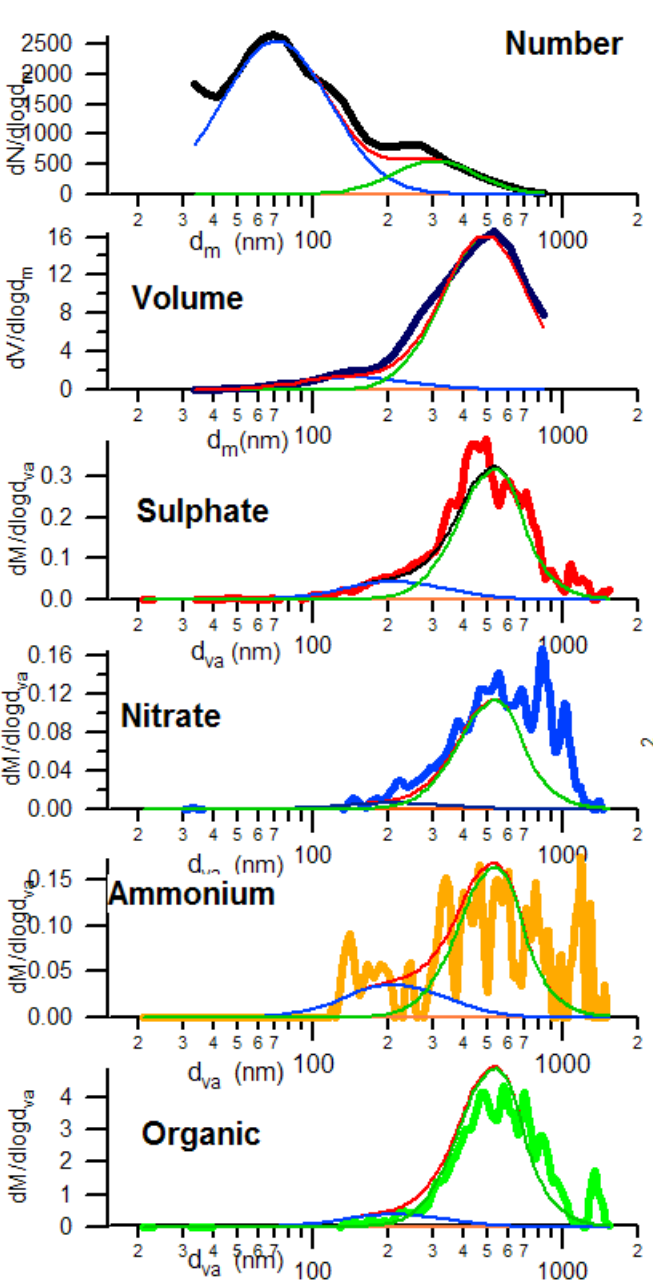
Where the error is

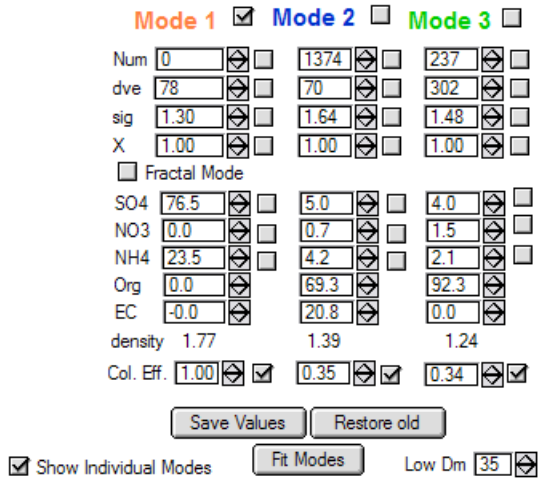
Overall Fit to AMS Data

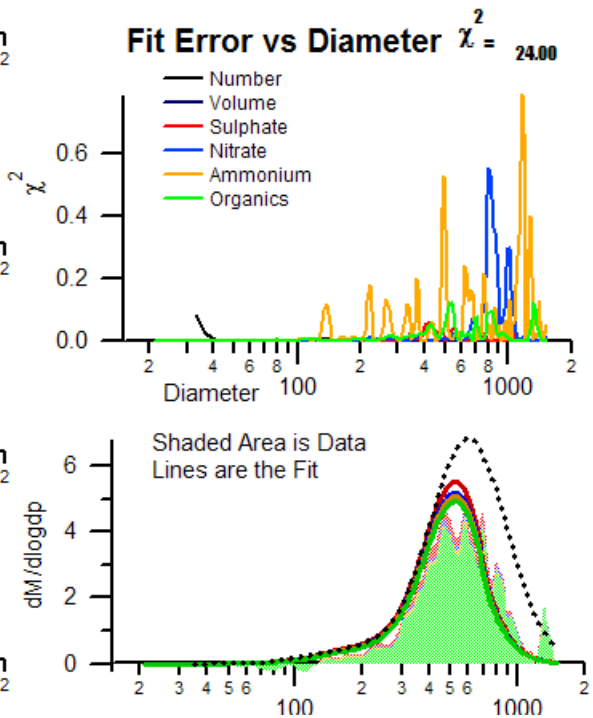
Closure Strategy




Average Volume/Mass Mode Diameter d DMPS and d AMS
1000
9
8
7
6
5
4
3
2
100
AMS Measured
Organics
Sulfate
7/10/2004
7/12/2004
7/14/2004
7/16/2004
7/18/2004
7/20/2004
Super Saturation
0.09
0.20
0.31
0.43
0.55
Looking at Here!
Number cm-3
3000
2000
1000
0
12:00 AM
7/12/2004
12:00 PM
12:00 AM
7/13/2004
Time (UTC)
dat
Super Saturation
0.09
0.20
0.31
0.43
0.55
Looking at Here!
4000
3000
2000
1000
0
Number cm-3
12:00 AM
7/16/2004
12:00 PM
12:00 AM
7/17/2004
Time (UTC)







Period 2

Lots of organics.

mode 2
Number = 1374.1
Diameter = 70
Sigma = 1.64
MF Solubles: 0.13413 MF Slightly Soluble: 0.82963

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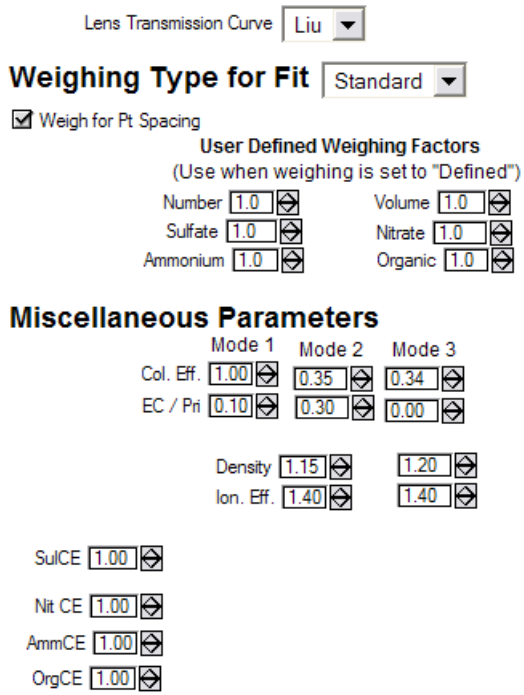
mode 3
Number = 237.17
Diameter = 297.97
Sigma = 1.5342
MF Solubles: 0.10462 MF Slightly Soluble: 0.85877



Period 2 (Organic Dominated)

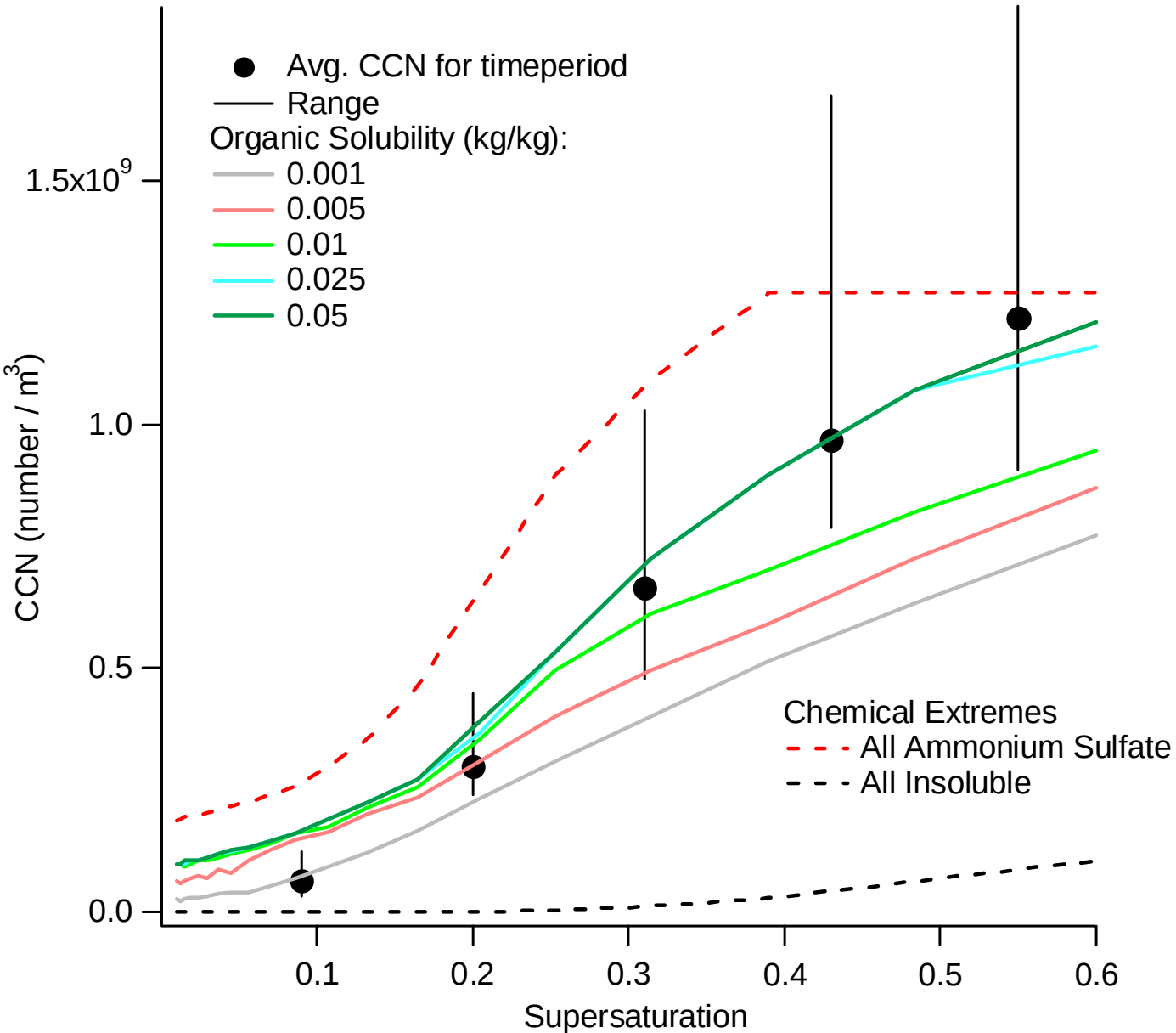
High Organics	Mode 1	Mode 2
Number (cm^{-3})	1374	237
Diameter (nm)	70	297
Sigma	1.64	1.53
MF Soluble	0.13	0.10
MF Slightly Soluble	0.83	0.86

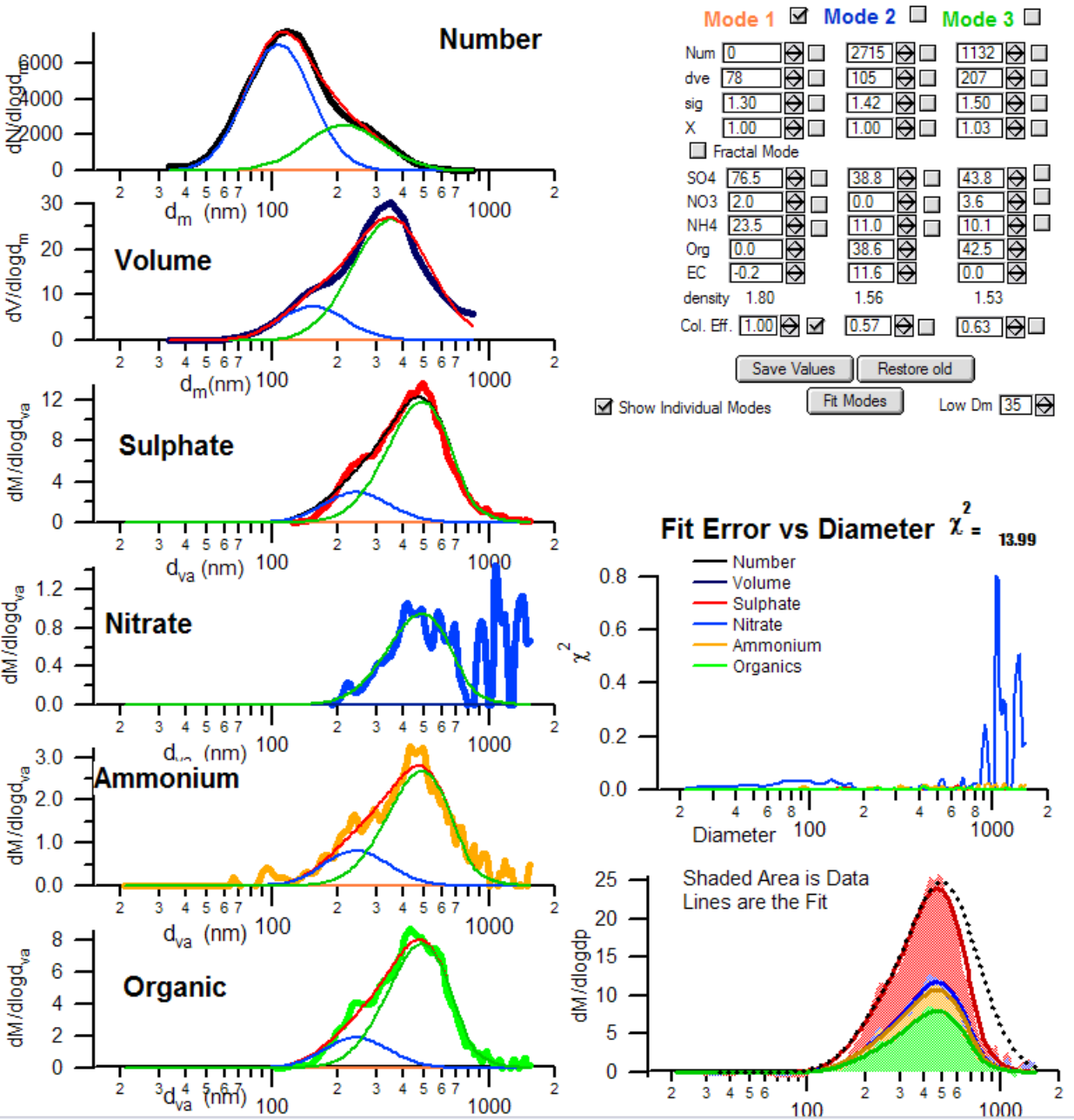
Water Acc. Coeff = 0.04

Residence Time = 10 s

(based on parabolic flow and 15% dead time to reach SS)

Van Hoft Fac. = 2 (for Org)





Period 5

Lots of Sulfate

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mode 2
Number = 2715.1 /cm3
Diameter = 105.34 nm
Sigma = 1.4174
MF Solubles: 0.58821 MF Slightly Soluble: 0.40131

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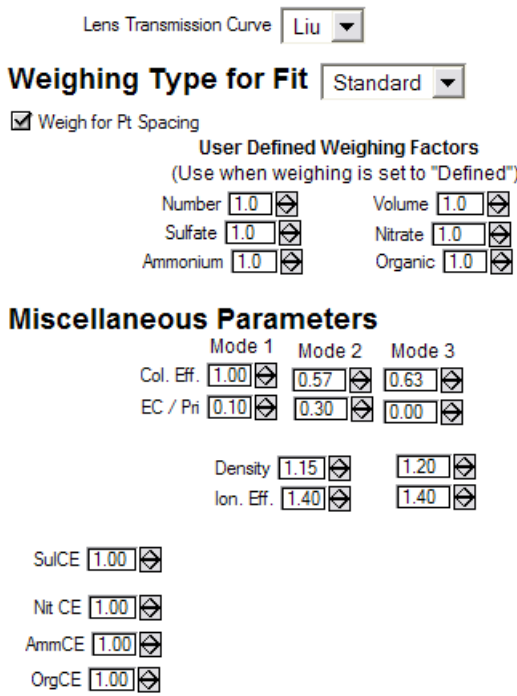
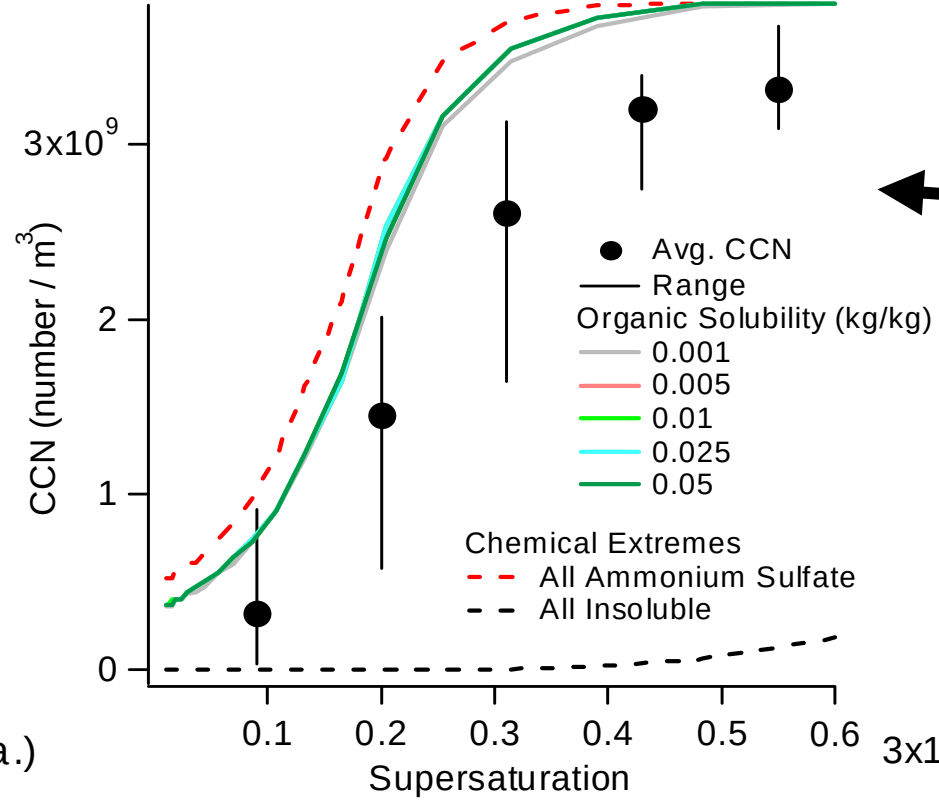
mode 3
Number = 1132.6 /cm3
Diameter = 207.13 nm
Sigma = 1.5033
MF Solubles: 0.65966 MF Slightly Soluble: 0.33014

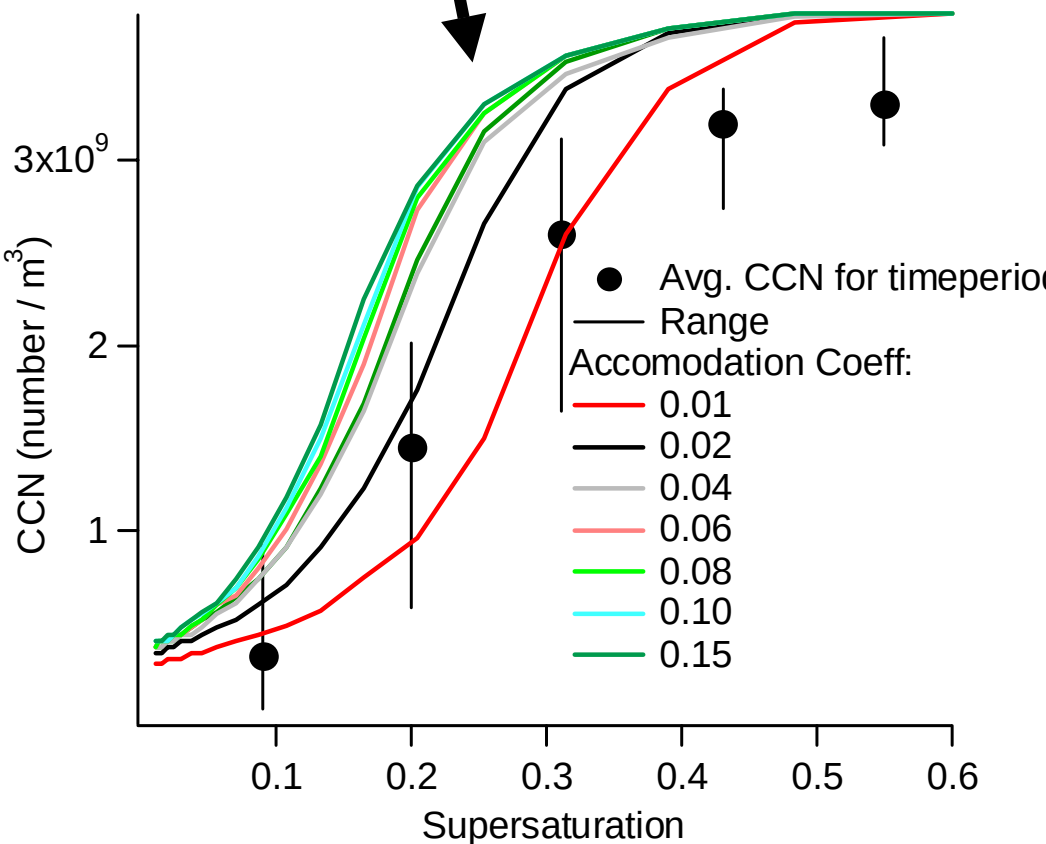


Period 5 High Amm Sulfate



Calculated CCN spectrum is independent of Organic Solubility

CCN Spectra is sensitive to Acc. Coeff. Is this reasonable? Organic Film?



High Sulfate	Mode 1	Mode 2
Number (cm^{-3})	2715	1132
Diameter (nm)	105	207
Sigma	1.42	1.50
MF Soluble	0.59	0.66
MF Slightly Soluble	0.40	0.33

Conclusions + Future Work

- TD-AMS
  - So far appears consistent with trends of study
  - Next: full analysis of magnitude & chemistry of volatiliz.
  - Compare to VTDMA and TAG/Org fraction
- Organic component analysis
  - Mostly OOA, two types, correlated with other obs.
  - Developing procedures to separate 3rd component
- CCN closure
  - Reasonable results, but lots of “knobs”
  - Next: Mike Cubison, OPC size dist
- Light scattering closure
- Hygroscopicity closure