

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

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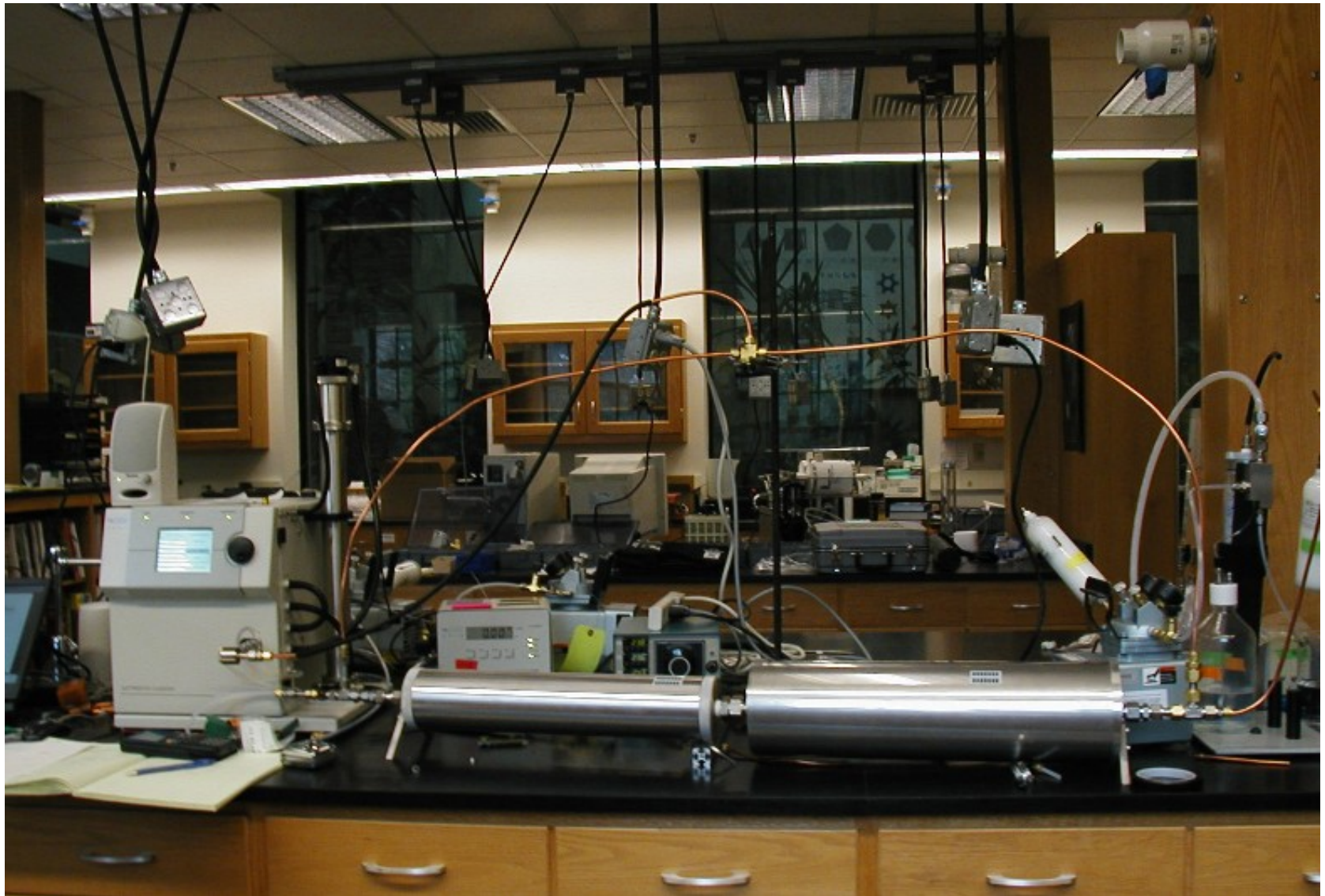
Univ. of Colorado-Boulder, Univ. of Manchester, Aerodyne Research, UC-Riverside, Georgia Tech, NOAA CMDL

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

Part I: Thermodesorber-AMS

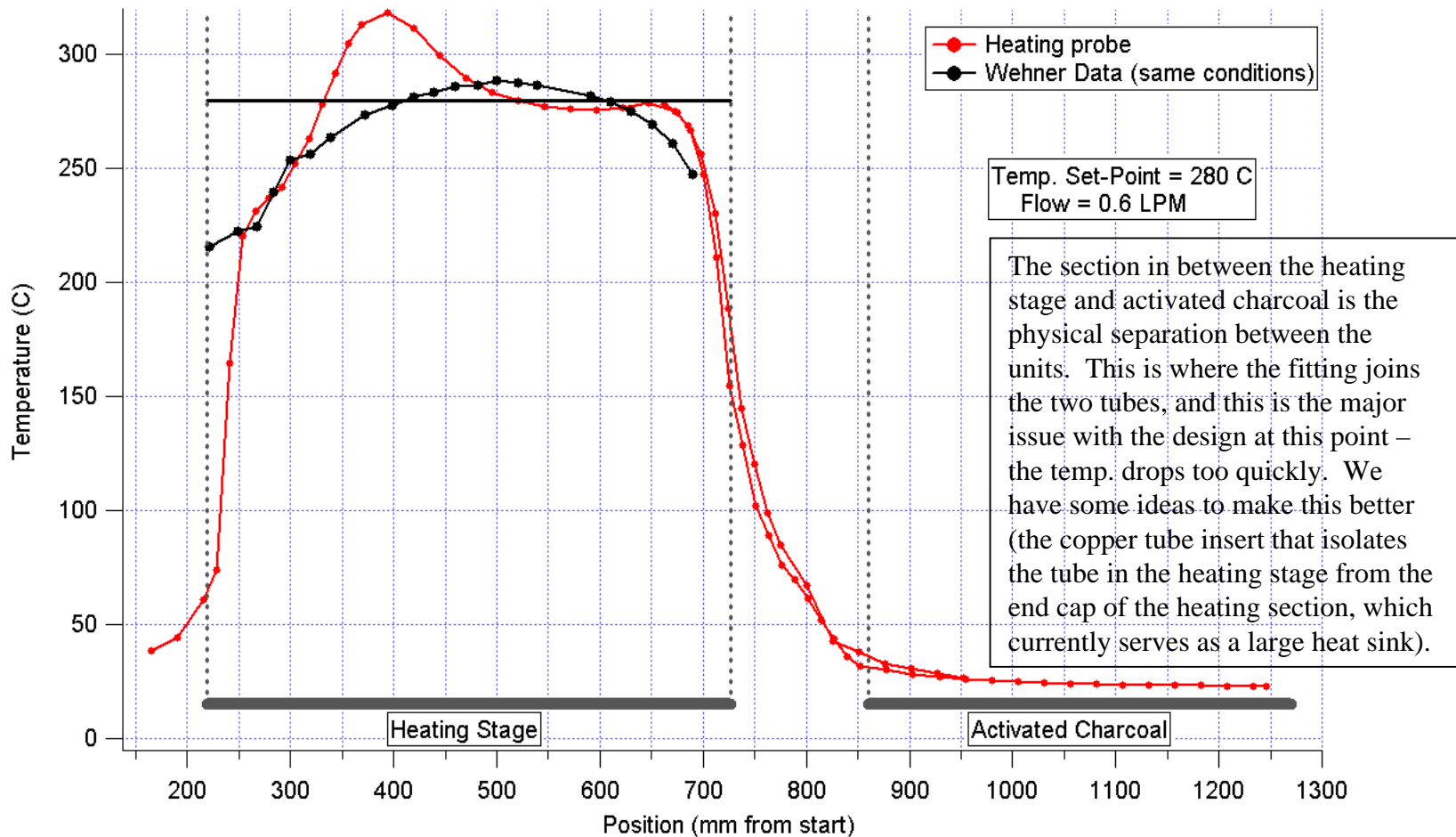
- Idea: measure change in aerosol composition as a function of volatilization temperature
- Focus on organics, “polymers”?

Themodenuder

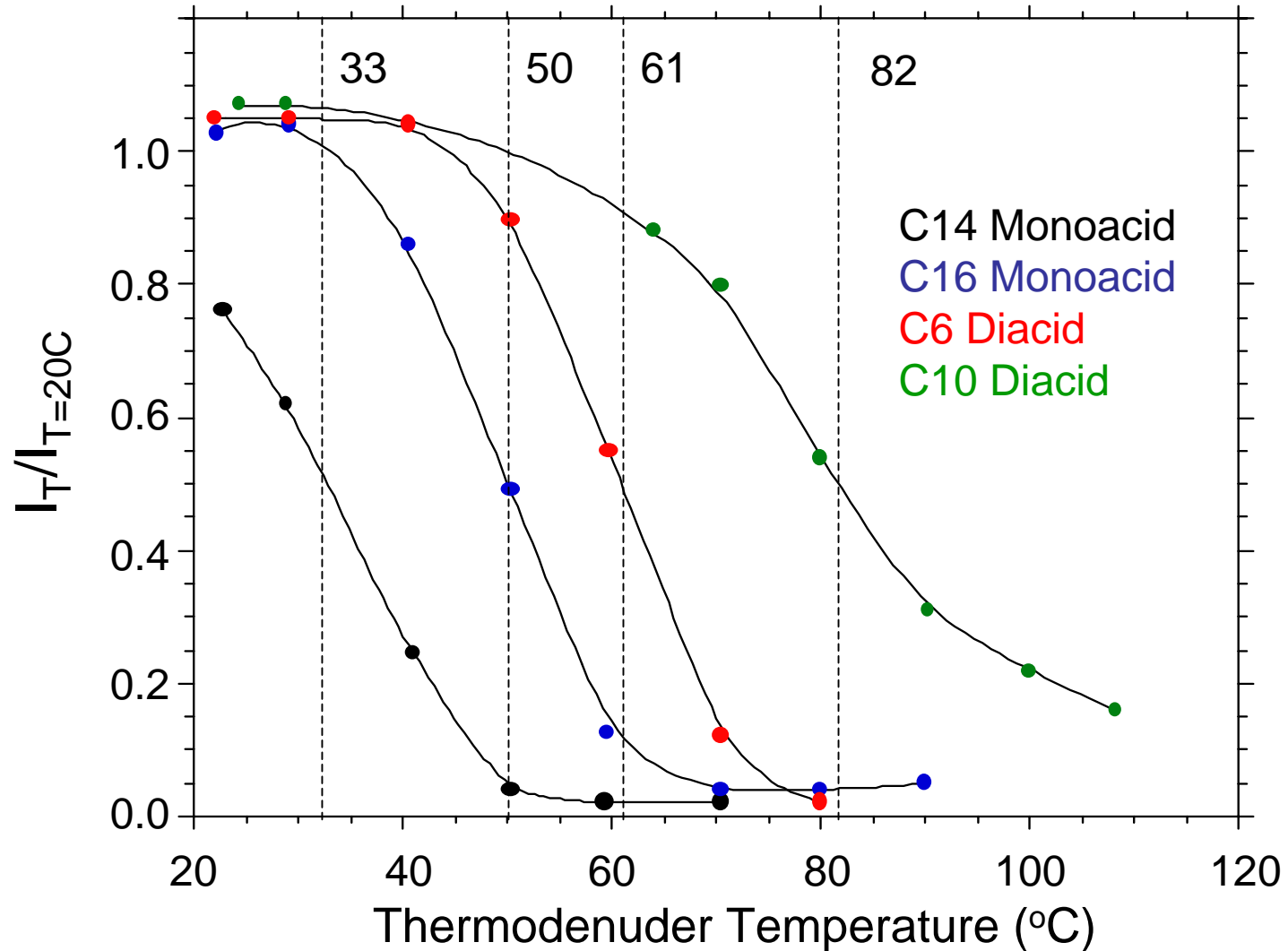


Design after Wehner et al. *J. Aerosol Sci.* 33: 1087-1093.(2002)

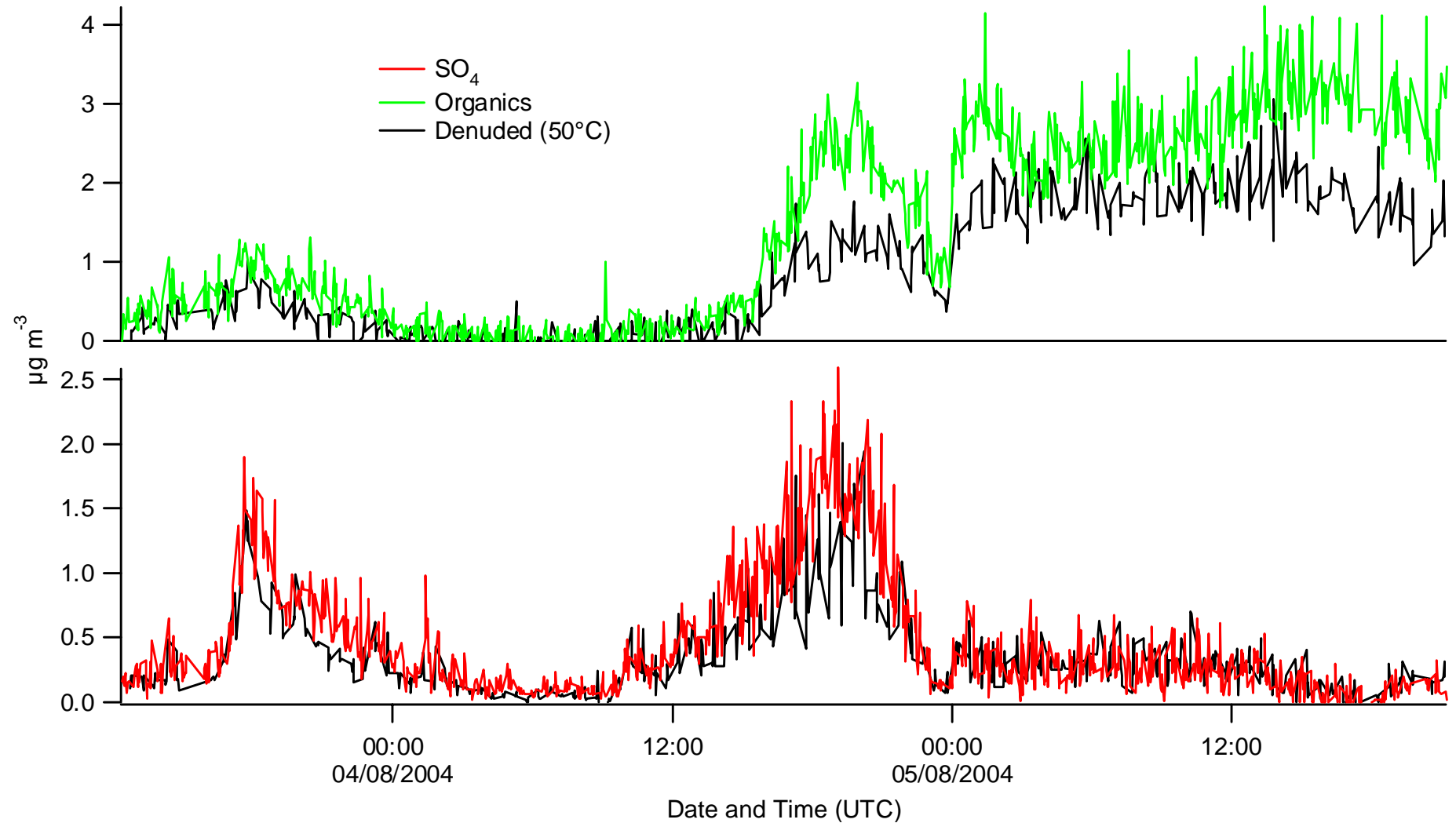
Thermodenuder Temperature Profile



Thermodenuder/TDPBMS Monocarboxylic and Dicarboxylic Acids



TD-AMS Time Series

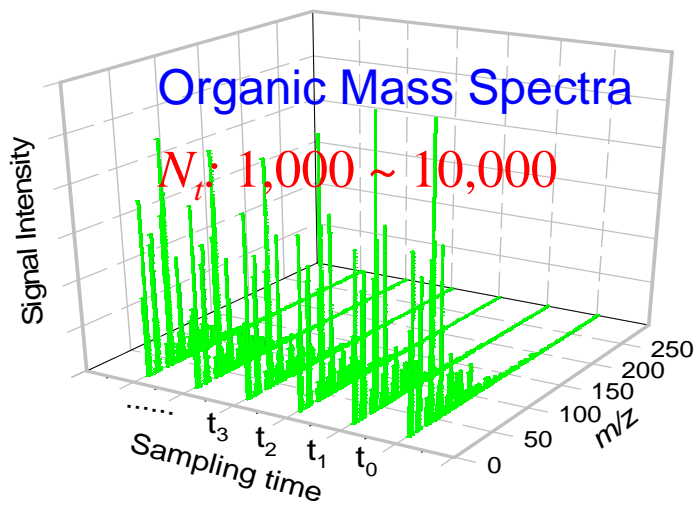


- Appears consistent with VTDMA and TAG/Org fraction

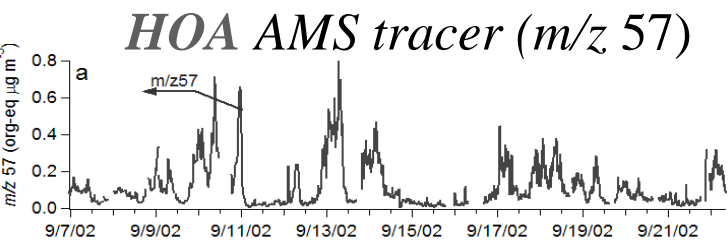
Part II: Organic Component Analysis

- 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)

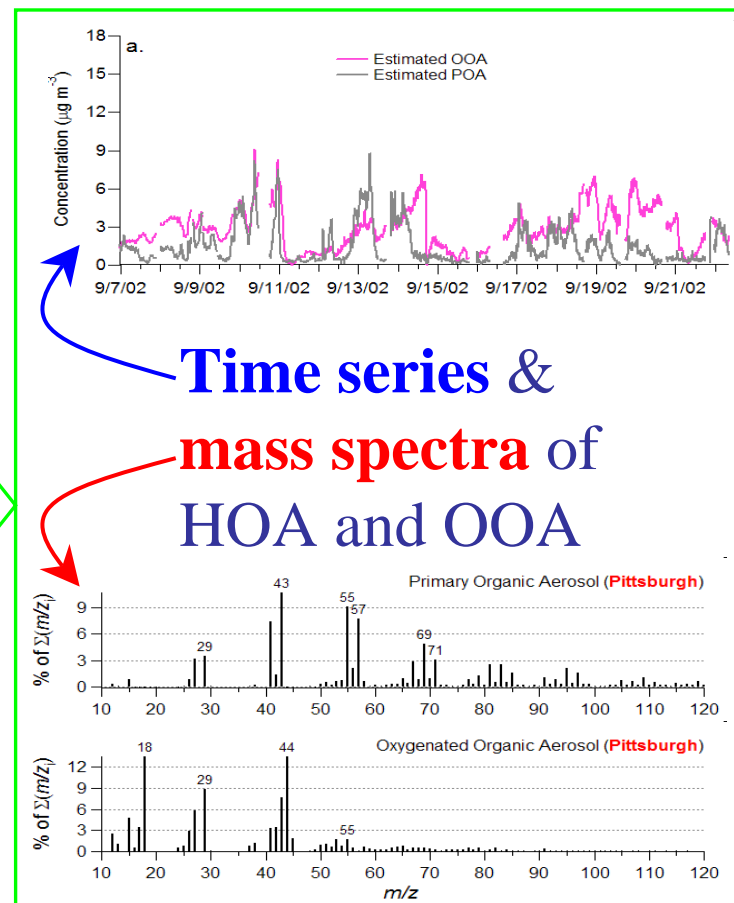
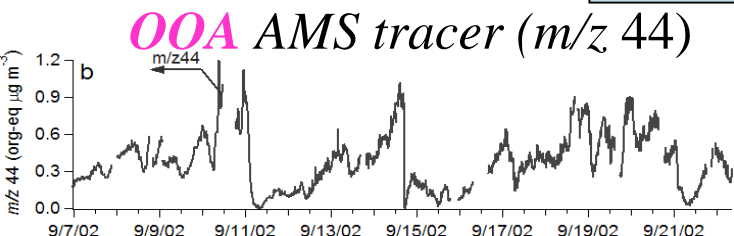


OOA: Oxygenated OA
HOA: Hydrocarbon-like OA

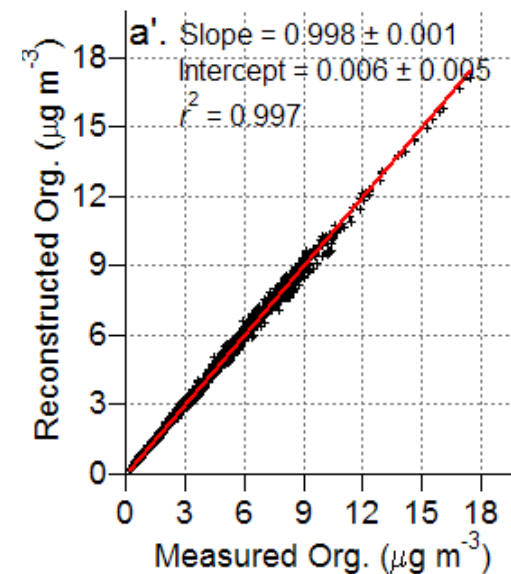
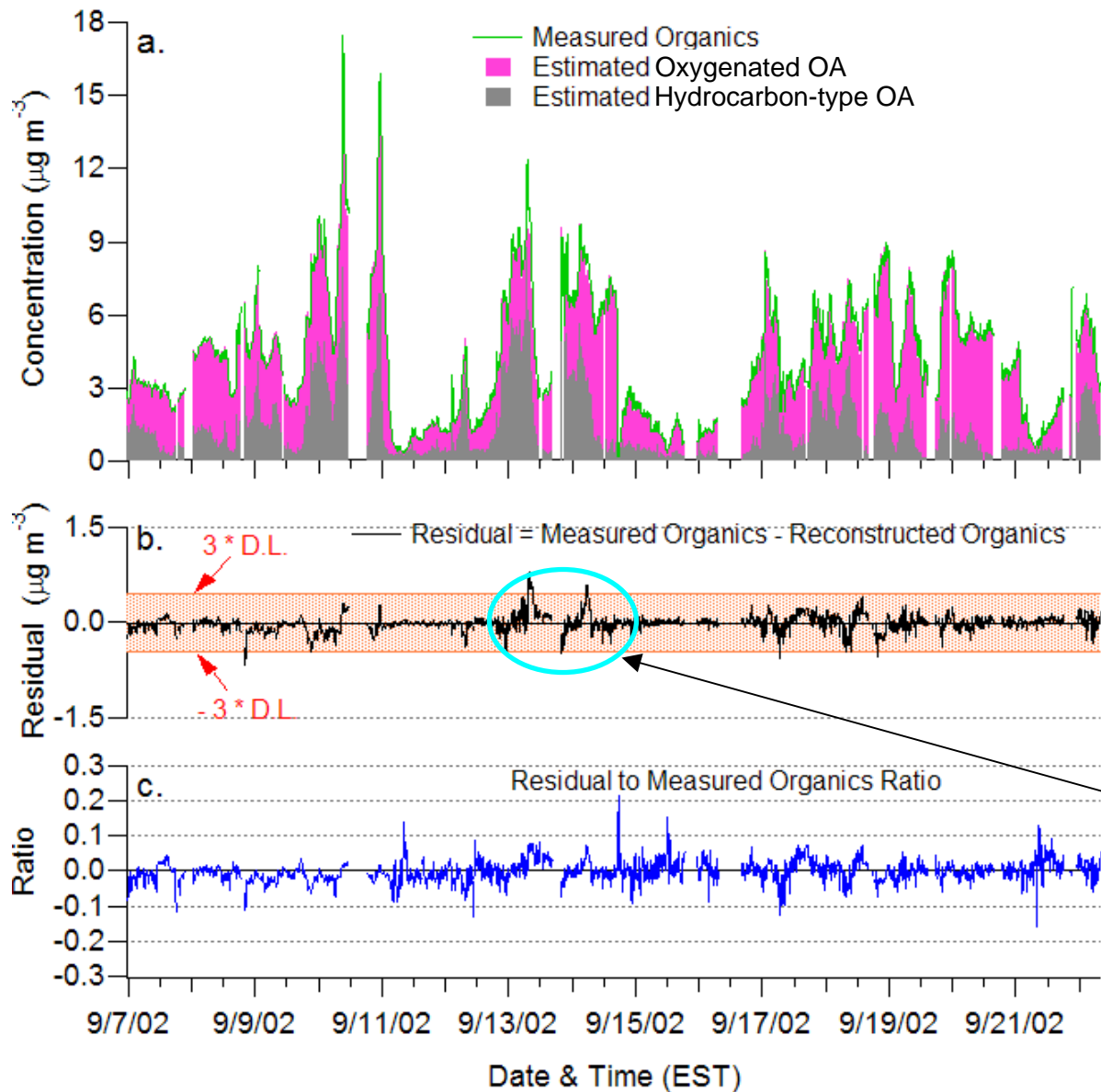


Initial guess of
HOA & OOA
temporal variability

Custom *Iterative*
Principal
Component
Analysis

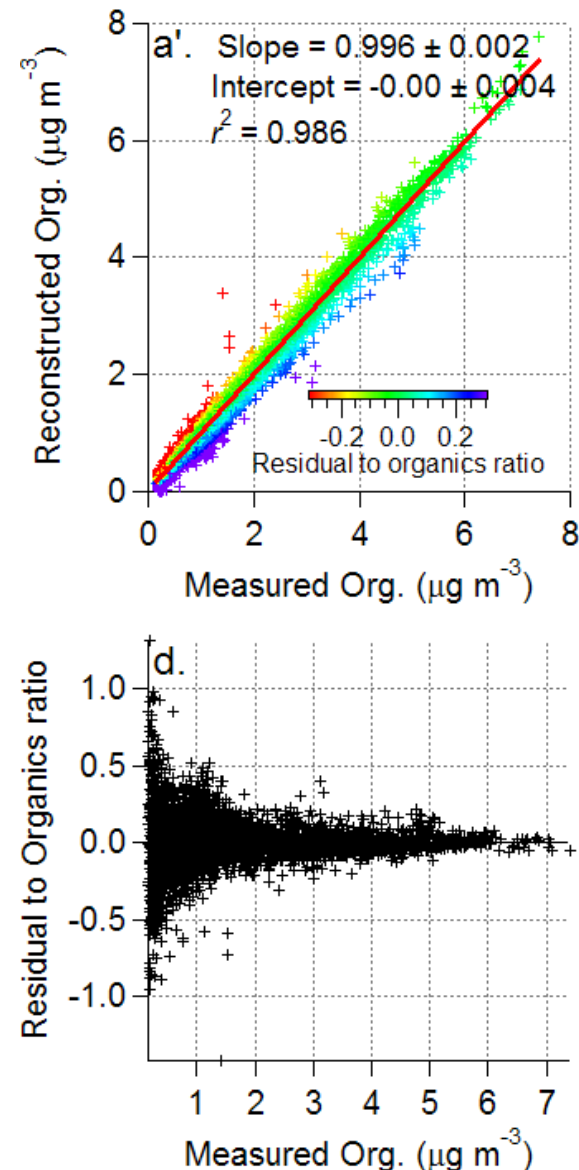
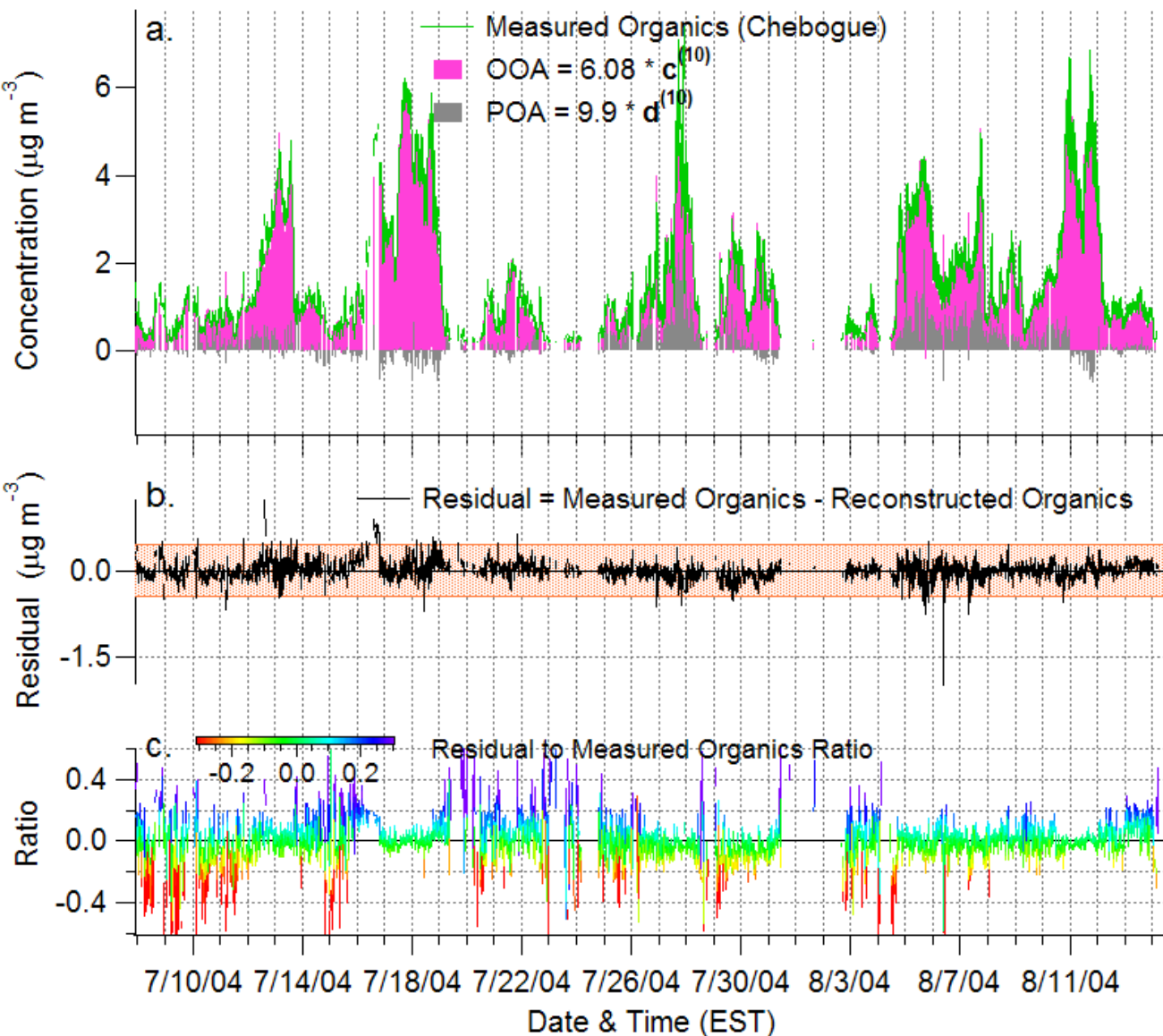


HOA and OOA Time Series in Pittsburgh

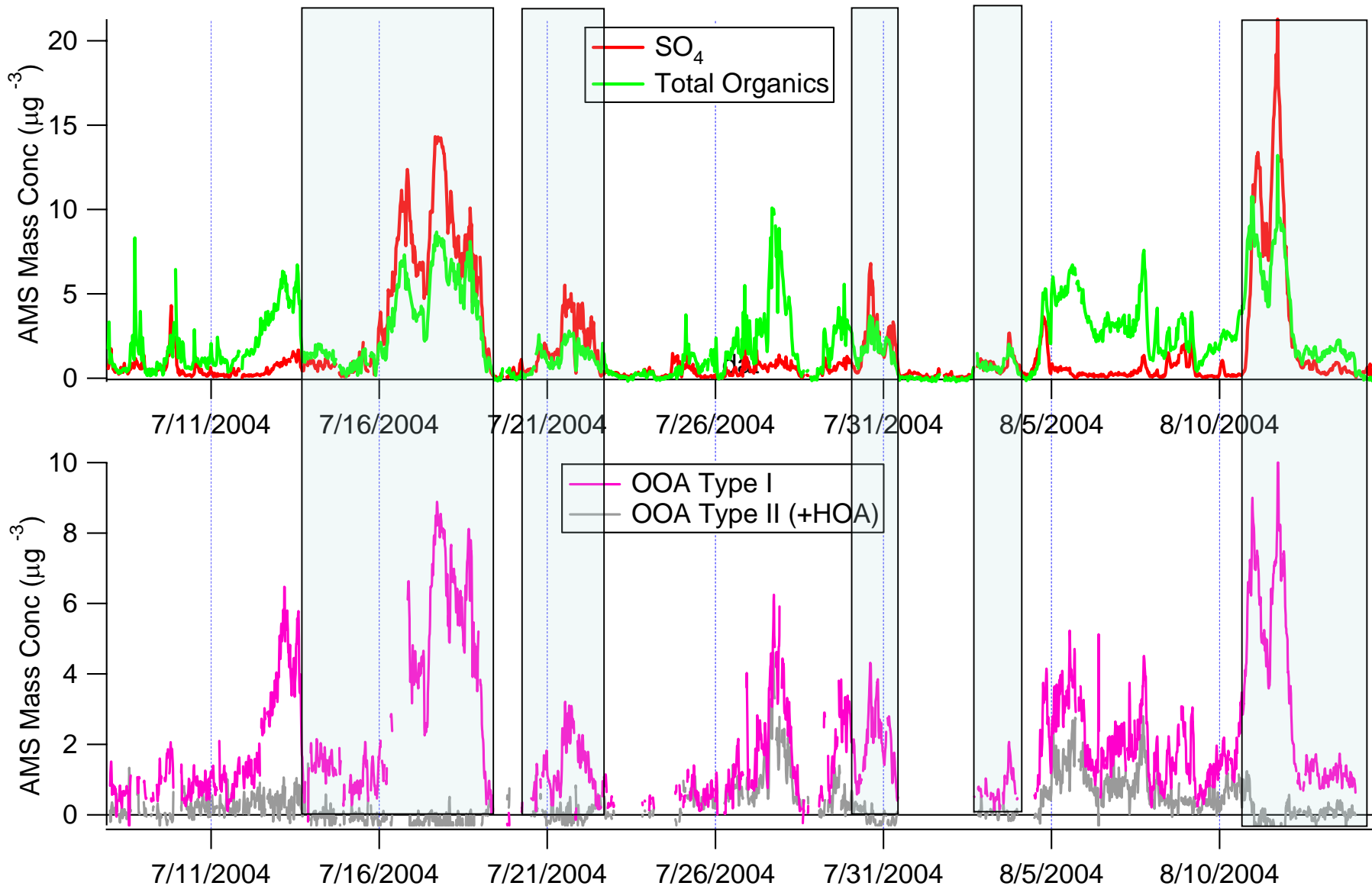


Indications of other (small) components.

Chebogue: Results of First Pass



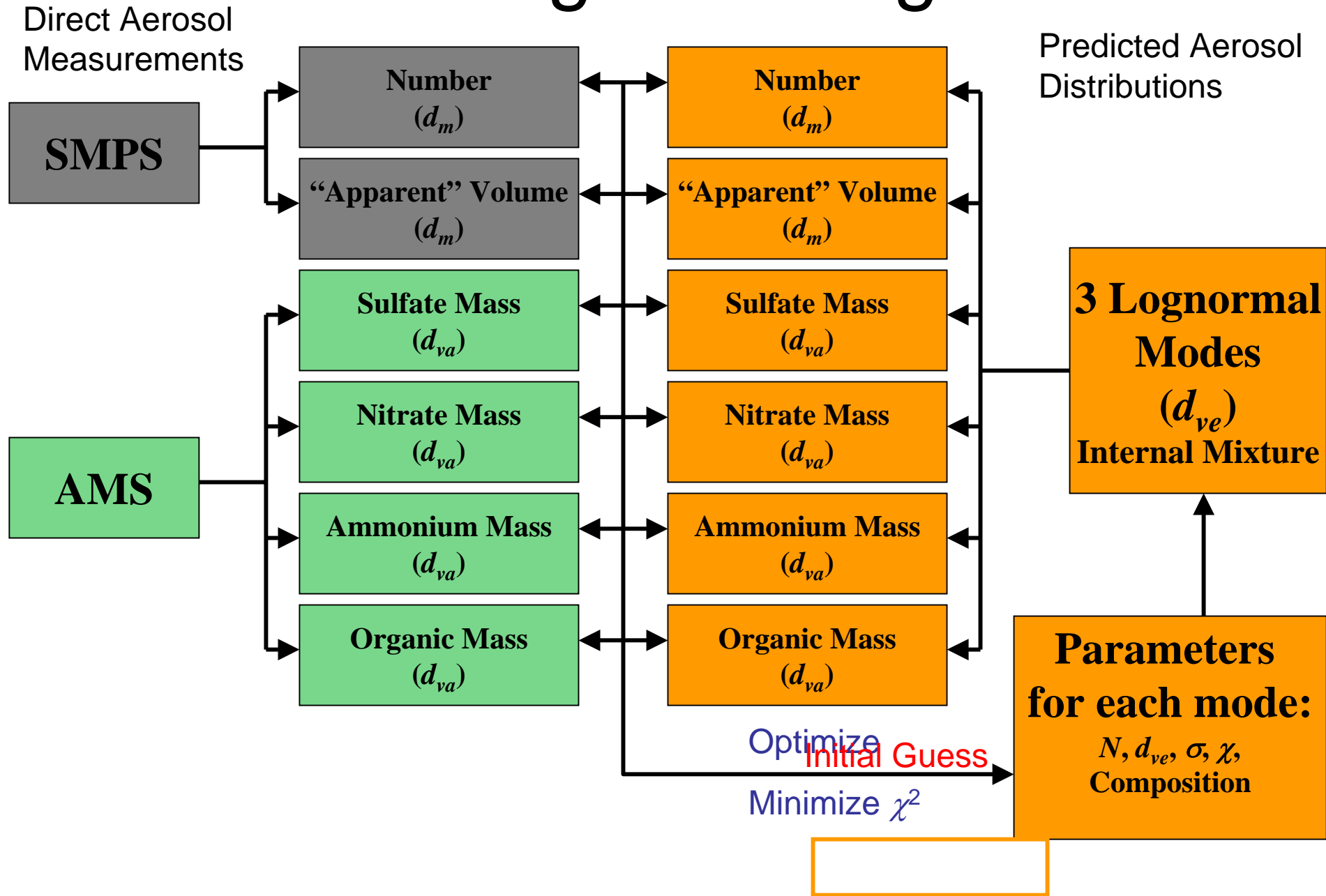
SO₄/Org vs Org Components

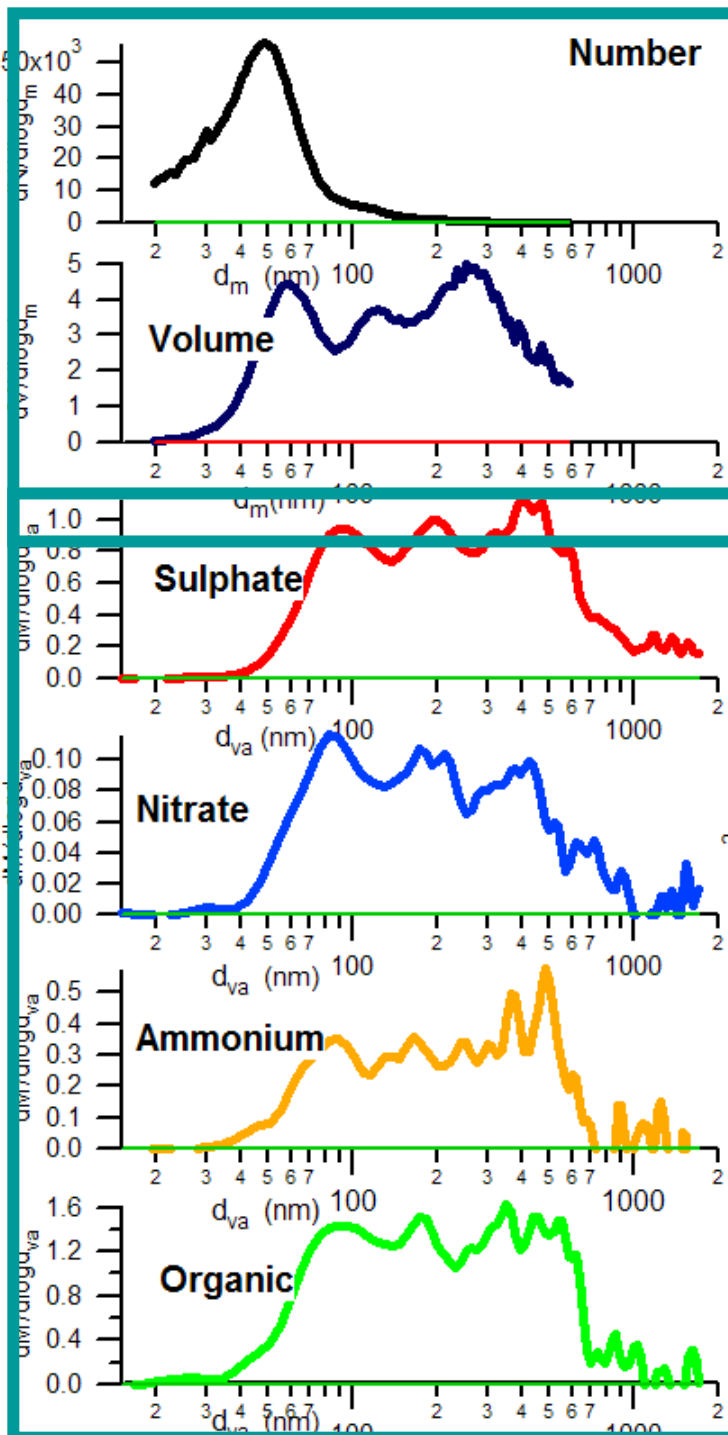


Part III: Aerosol-CCN Closure

- 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

Direct Aerosol Measurements

SMPS

AMS

APS

OPC

Other Data

Derive Optimum Complete Aerosol Representation

Data Integration Model

N & M Chemical Size Distrib.

Predict Properties of Interest

“Closure” Analyses

Mie Theory

CCN Model

Hygros. Model

LIDAR Pred.

L. Abs. Pred.

L. Scat. Pred.

CCN Pred.

Hygros. Pred.

LIDAR Data

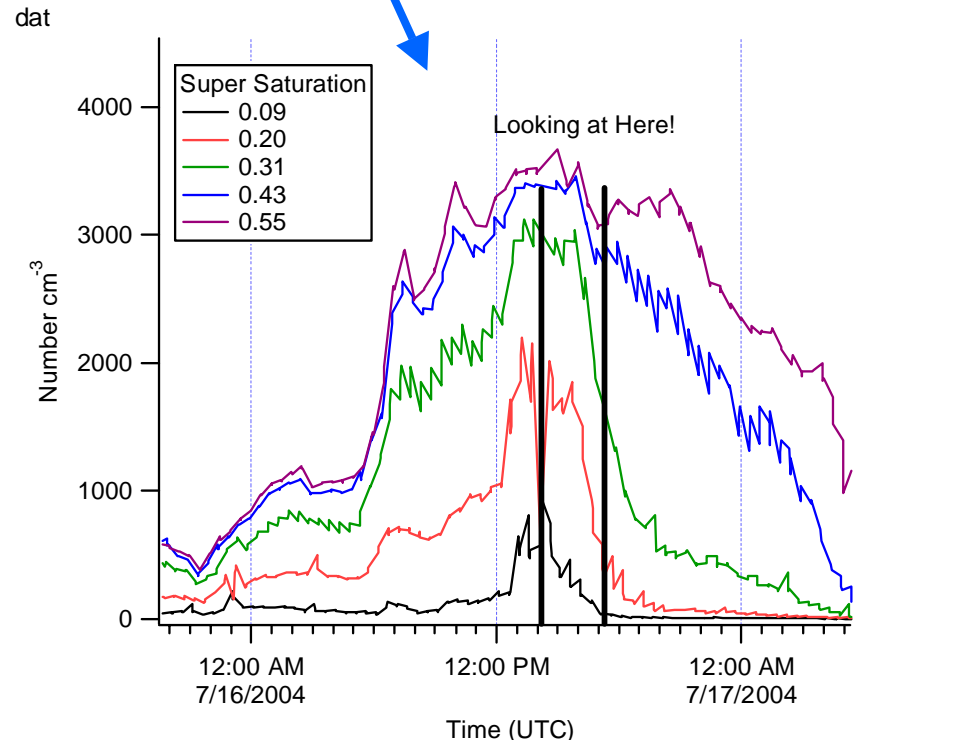
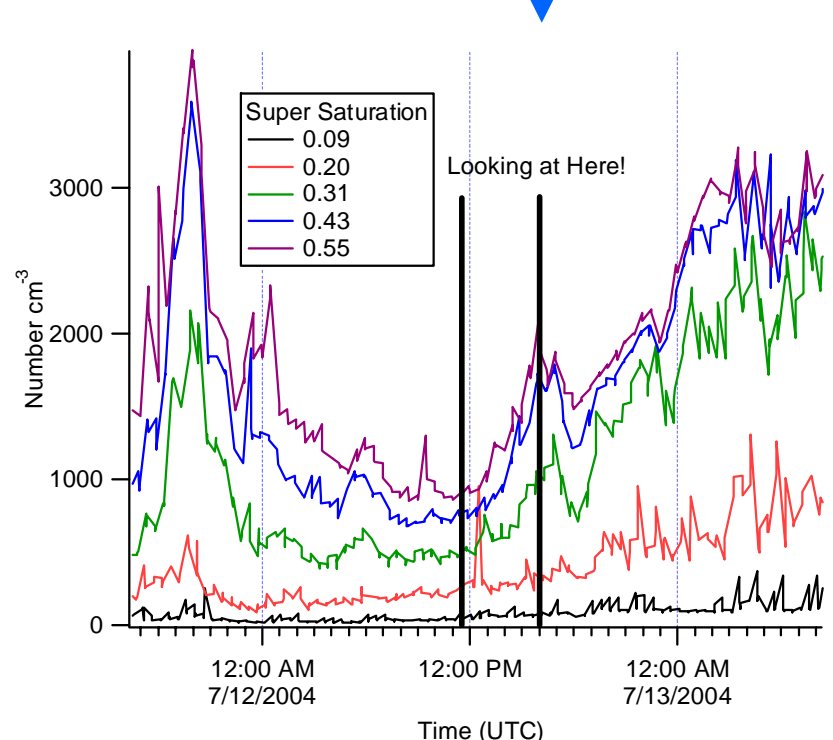
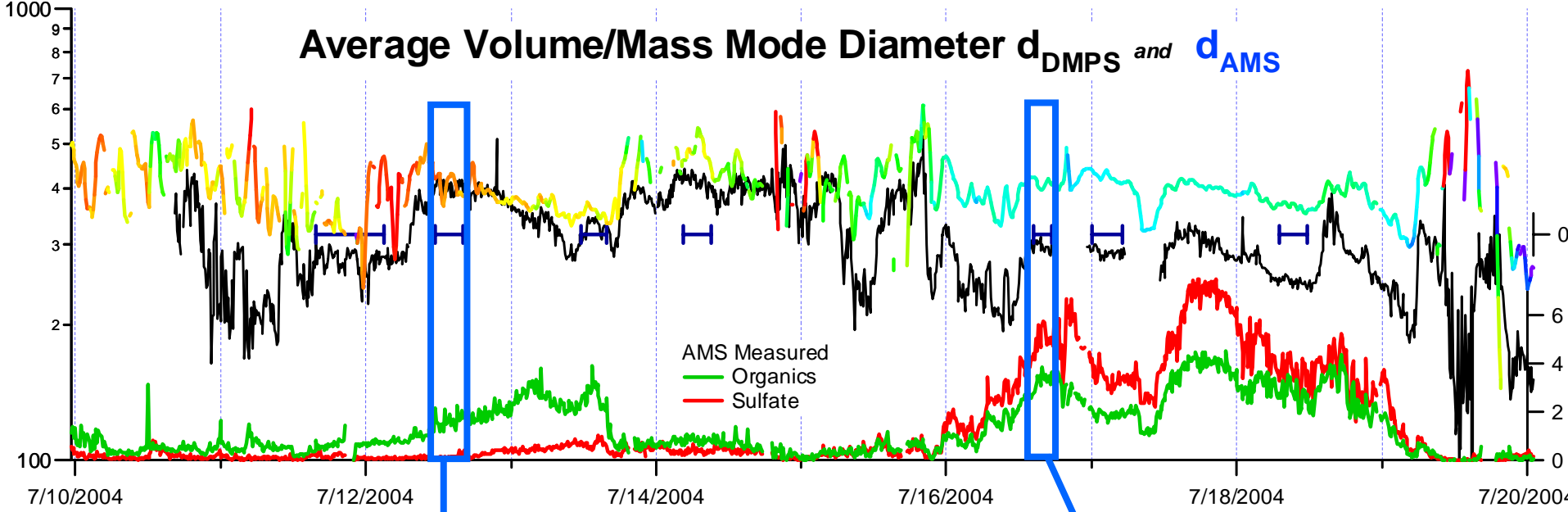
L. Abs. Data

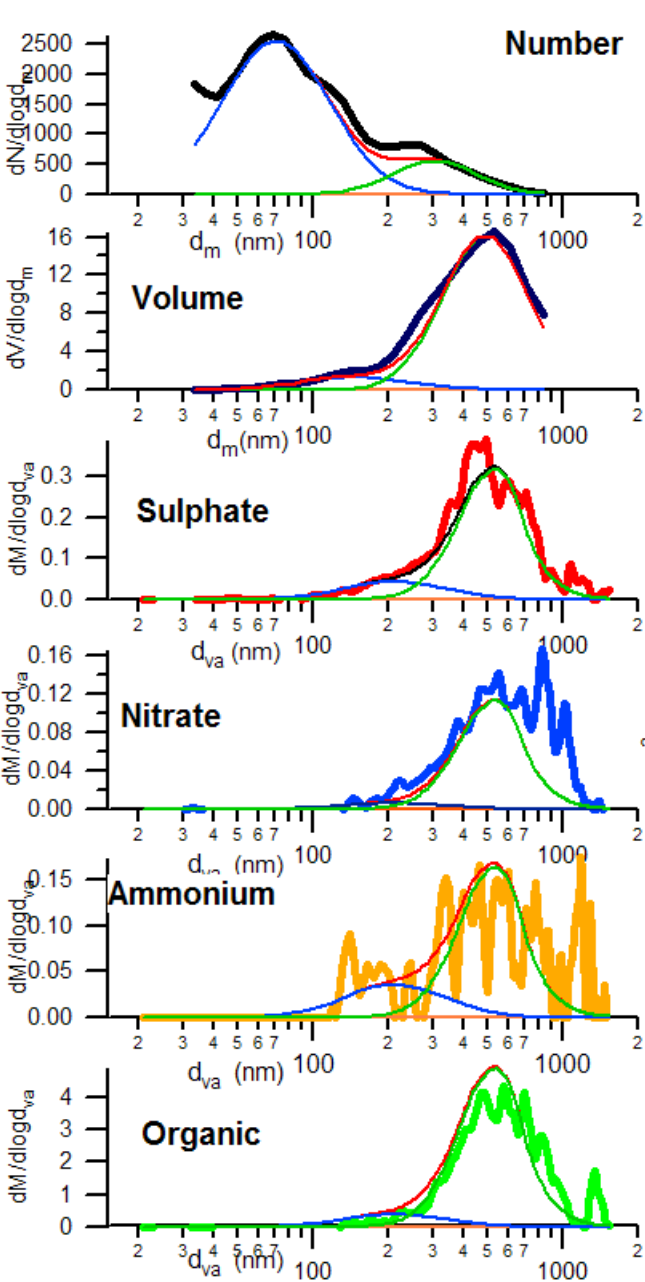
L. Scat. Data

CCN Data

Hygros. Data

Average Volume/Mass Mode Diameter d_{DMPs} and d_{AMS}





Mode 1 Mode 2 Mode 3

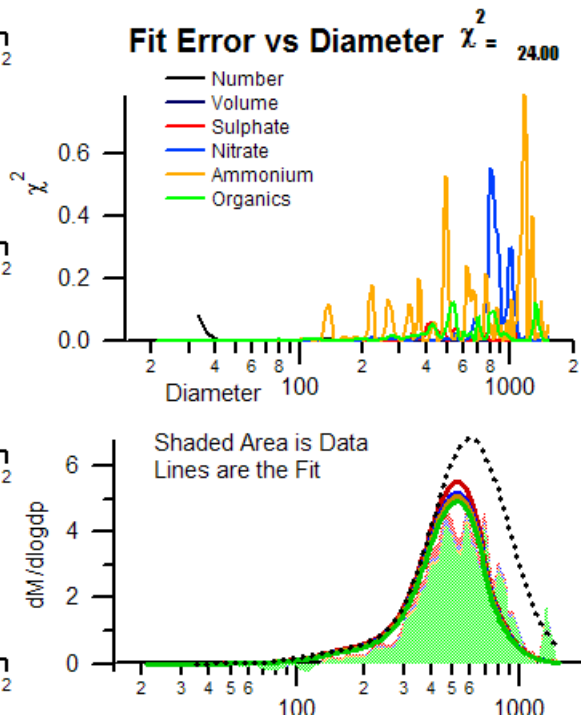
Num	0	1374	237
dve	78	70	302
sig	1.30	1.64	1.48
X	1.00	1.00	1.00

Fractal Mode

SO4	76.5	5.0	4.0
NO3	0.0	0.7	1.5
NH4	23.5	4.2	2.1
Org	0.0	69.3	92.3
EC	-0.0	20.8	0.0

density 1.77 1.39 1.24
 Col. Eff. 1.00 0.35 0.34

Show Individual Modes Low Dm 35



Period 2

Lots of organics.

mode 2

Number = 1374.1

Diameter = 70

Sigma = 1.64

MF Solubles: 0.13413 MF Slightly Soluble: 0.82963

mode 3

Number = 237.17

Diameter = 297.97

Sigma = 1.5342

MF Solubles: 0.10462 MF Slightly Soluble: 0.85877

Lens Transmission Curve Liu

Weighing Type for Fit Standard

Weigh for Pt Spacing

User Defined Weighing Factors

(Use when weighing is set to "Defined")

Number	1.0	Volume	1.0
Sulfate	1.0	Nitrate	1.0
Ammonium	1.0	Organic	1.0

Miscellaneous Parameters

	Mode 1	Mode 2	Mode 3
Col. Eff.	1.00	0.35	0.34
EC / Pri	0.10	0.30	0.00
Density	1.15	1.20	
Ion. Eff.	1.40	1.40	

SulCE 1.00

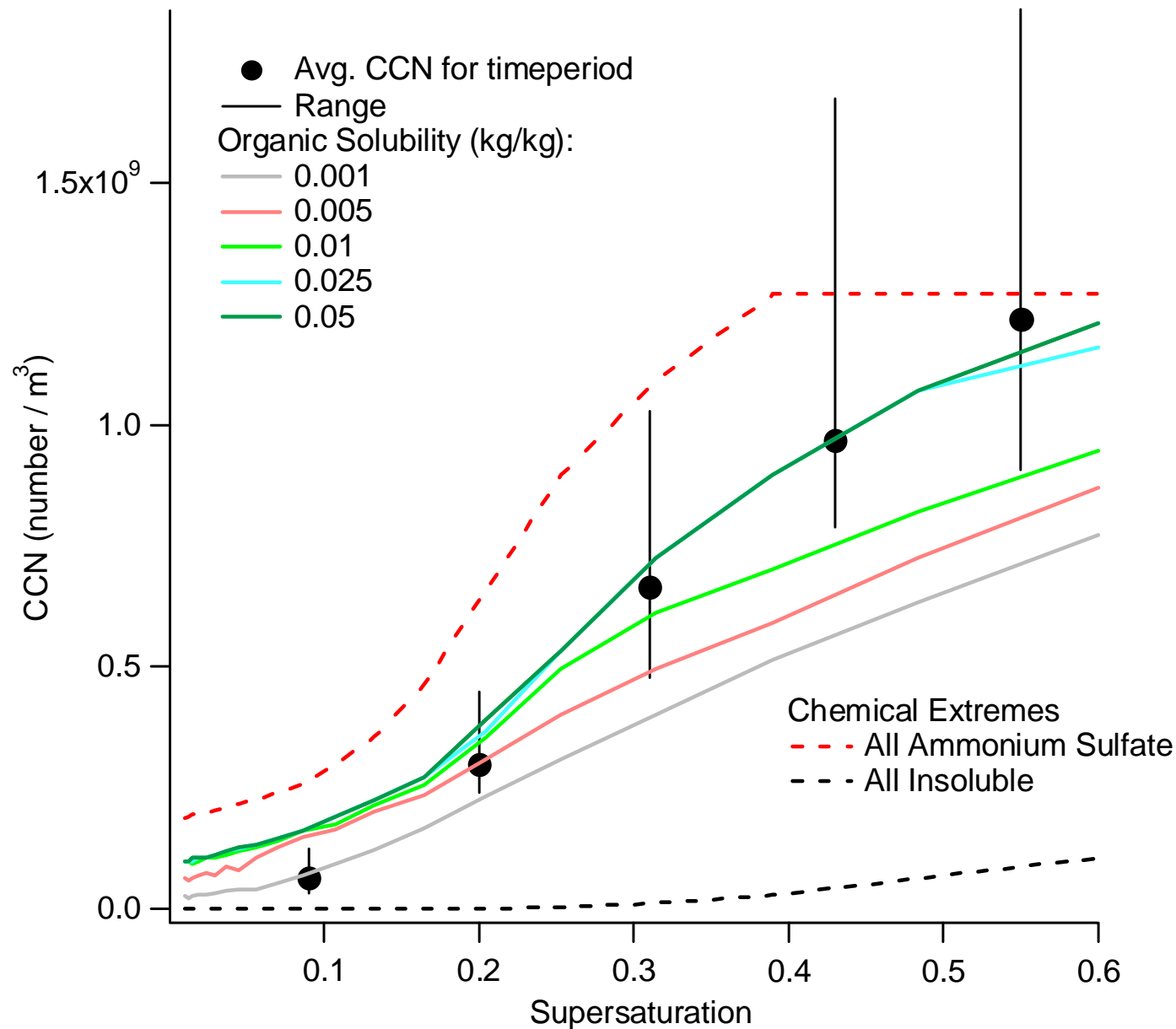
Nit CE 1.00

AmmCE 1.00

OrgCE 1.00

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

Period 2 (Organic Dominated)



Water Acc. Coeff = 0.04

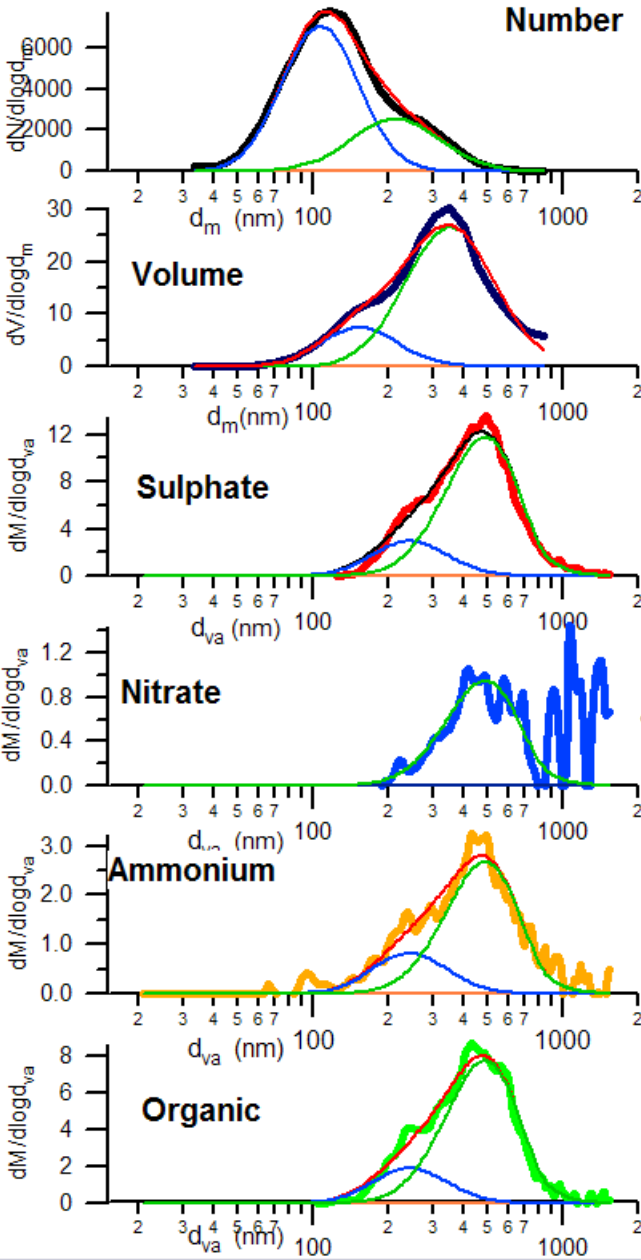
Residence Time = 10 s

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

Van Hoft Fac. = 2 (for Org)

Period 5

Lots of Sulfate



Mode 1 Mode 2 Mode 3

Num	0	2715	1132
dve	78	105	207
sig	1.30	1.42	1.50
X	1.00	1.00	1.03

Fractal Mode

SO4	76.5	38.8	43.8
NO3	2.0	0.0	3.6
NH4	23.5	11.0	10.1
Org	0.0	38.6	42.5
EC	-0.2	11.6	0.0

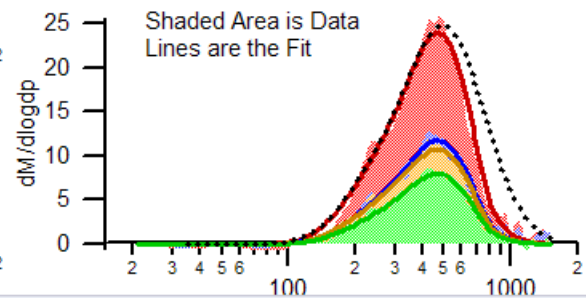
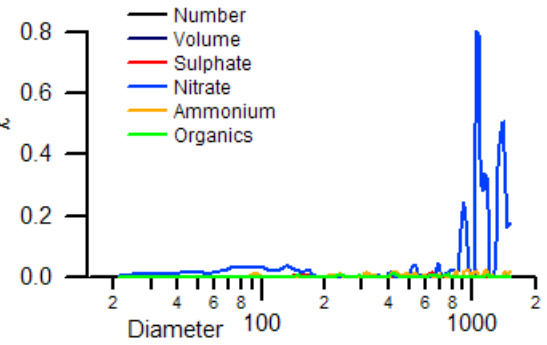
density 1.80 1.56 1.53

Col. Eff. 1.00 0.57 0.63

Save Values Restore old

Show Individual Modes Low Dm

Fit Error vs Diameter $\chi^2 = 13.99$



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

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

Lens Transmission Curve

Weighing Type for Fit

Weigh for Pt Spacing

User Defined Weighing Factors
 (Use when weighing is set to "Defined")

Number	1.0	Volume	1.0
Sulfate	1.0	Nitrate	1.0
Ammonium	1.0	Organic	1.0

Miscellaneous Parameters

	Mode 1	Mode 2	Mode 3
Col. Eff.	1.00	0.57	0.63
EC / Pri	0.10	0.30	0.00
Density	1.15	1.20	
Ion. Eff.	1.40	1.40	

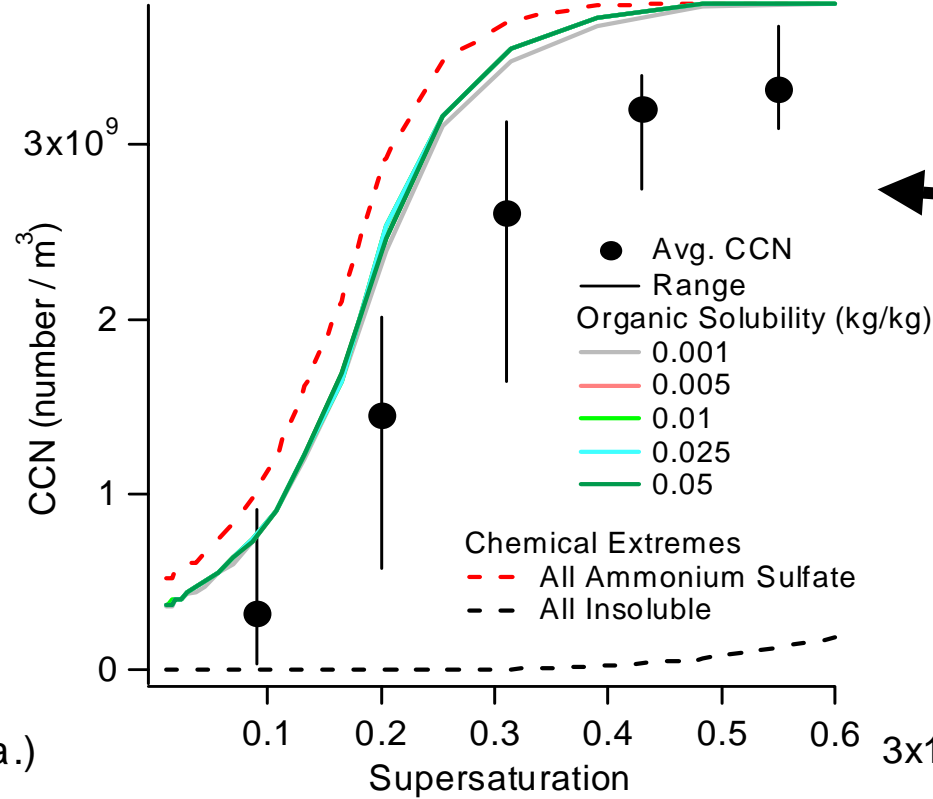
SulCE

Nit CE

AmmCE

OrgCE

Period 5 High Amm Sulfate

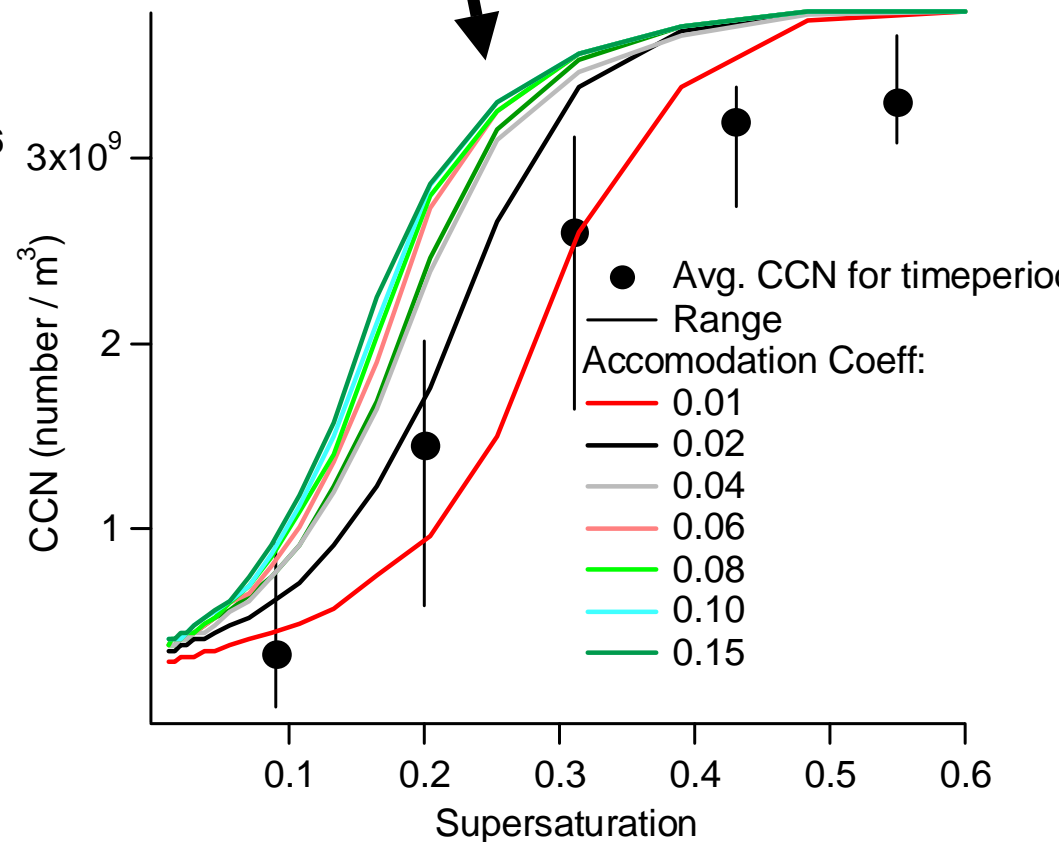


Calculated CCN spectrum is independent of Organic Solubility

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

a.)

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