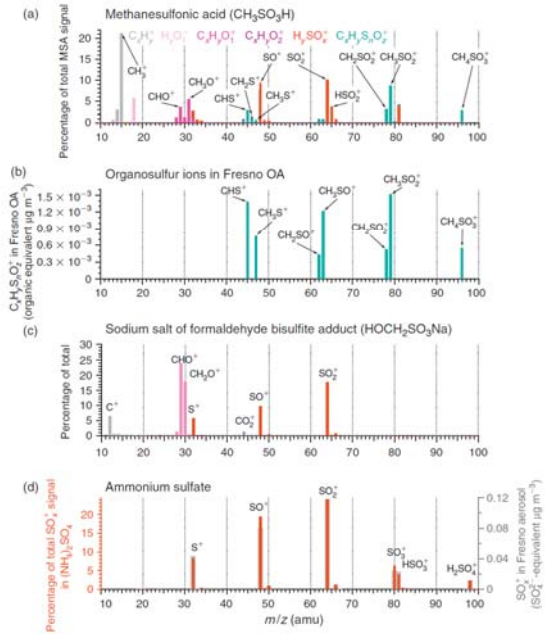

Fig. 9. High-resolution aerosol mass spectrometer (HR-AMS) spectra of (a) methanesulfonic acid (MSA, CH_3SO_3H), (b) average signals of the organosulfur ions detected in Fresno OA, (c) sodium hydroxymethanesulfonate ($HOCH_2SO_3Na$) and (d) ammonium sulfate and the average sulfate signals detected in ambient Fresno aerosol. Note water and ammonium ions are excluded in (d).

Ge, X., Q. Zhang, Y. Sun, C. R. Ruehl, and A. Setyan (2012), Effect of Aqueous-Phase Processing on Aerosol Chemistry and Size Distribution in Fresno, California, during Wintertime, *Environmental Chemistry*, *9*(3), 221-235, doi:10.1071/EN11168.

UC DAVIS
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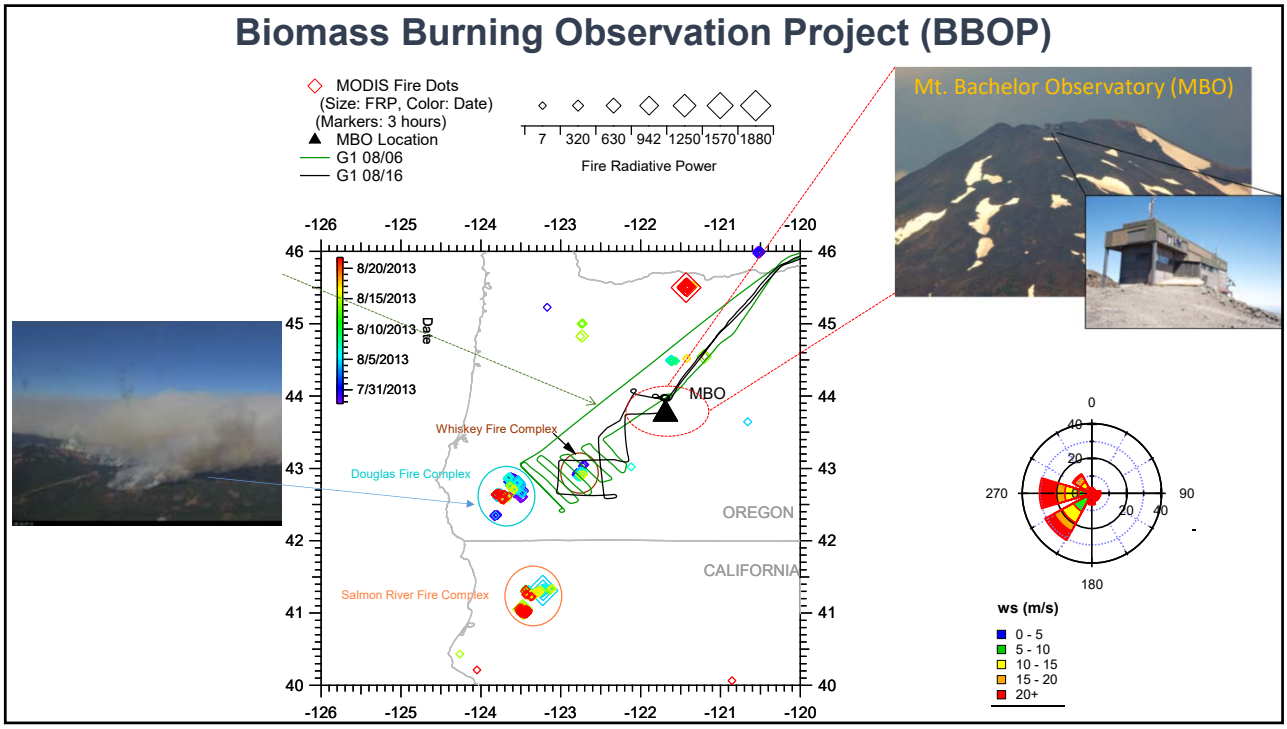
PMF Analysis of AMS Data: *New Strategies*

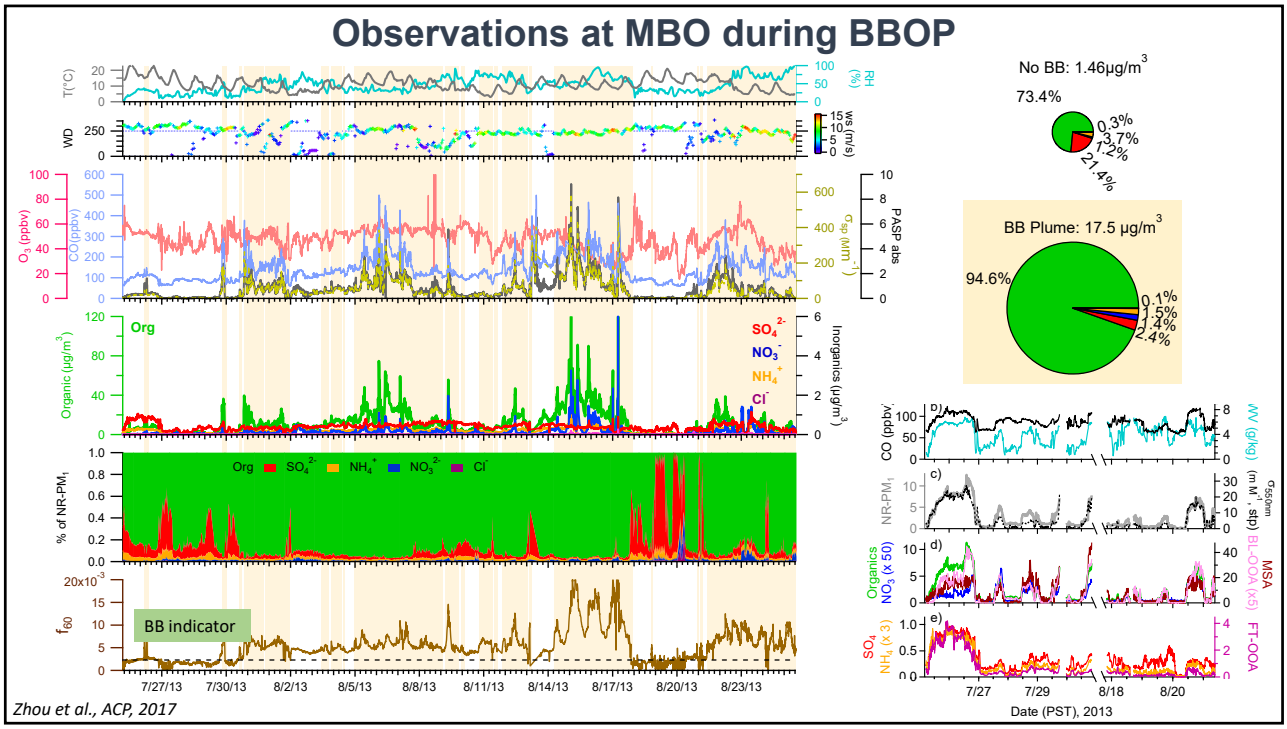
Qi Zhang
University of California, Davis

May 11, 2017, AMS Users' Meeting -- Beijing

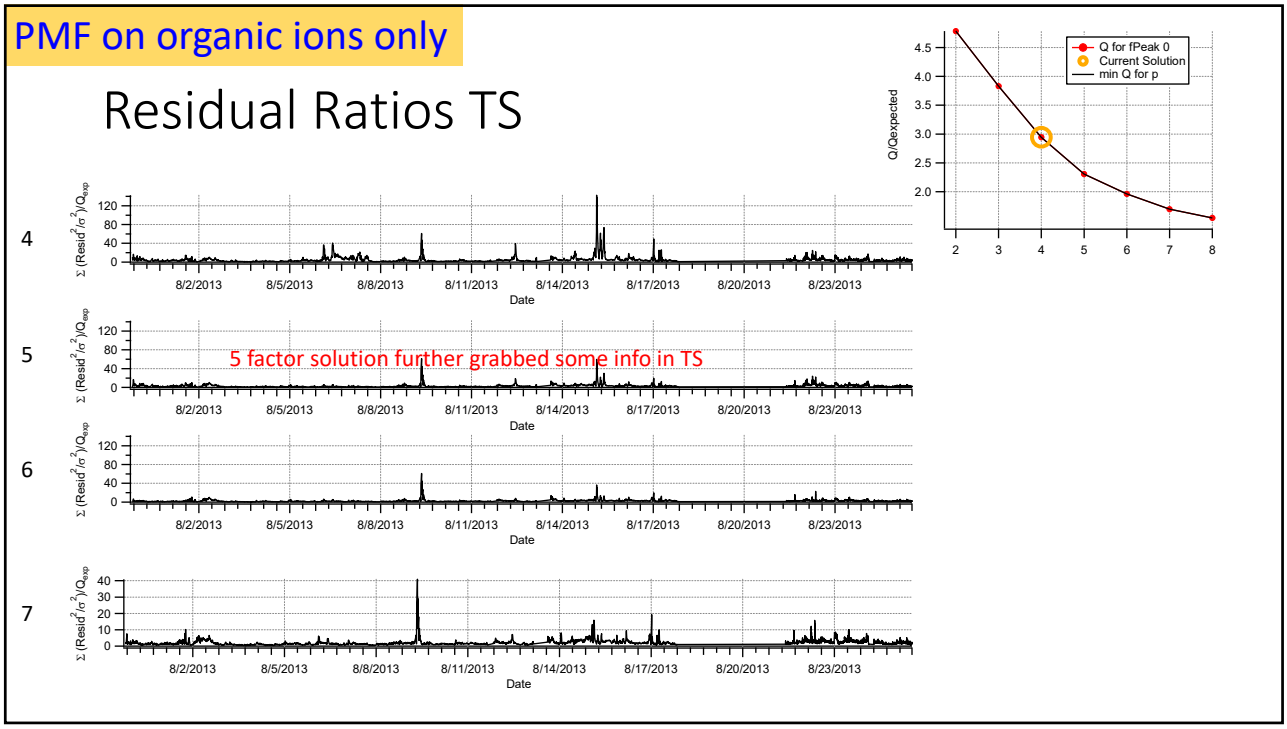
Two methods

- Analysis of combined organic and inorganic ions
  - Include good S/N inorganic ions (NO^+, NO_2^+, NH_2^+, NH_3^+, SO^+, SO_2^+ …)
  - to better extract physically meaningful factors and reduce mixing of factors.
  - Additional inorganic signal to assist interpretation of factors.
- Rolling window analysis of long term data



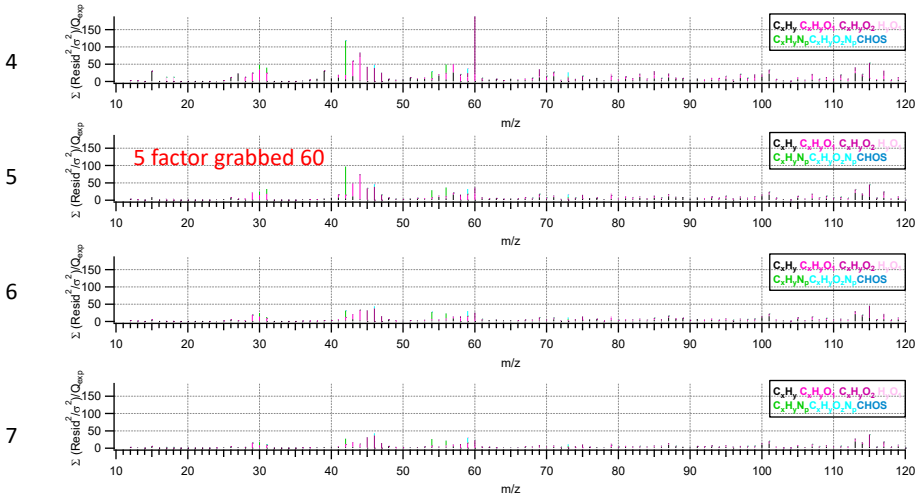


PMF on organic ions only

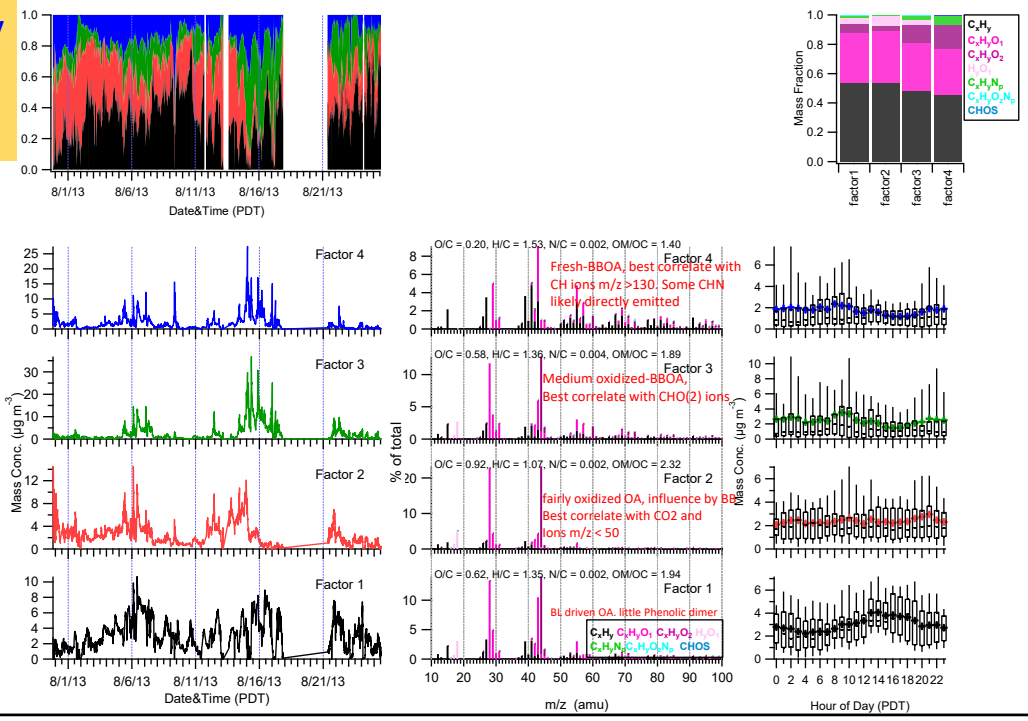


PMF on organic ions only

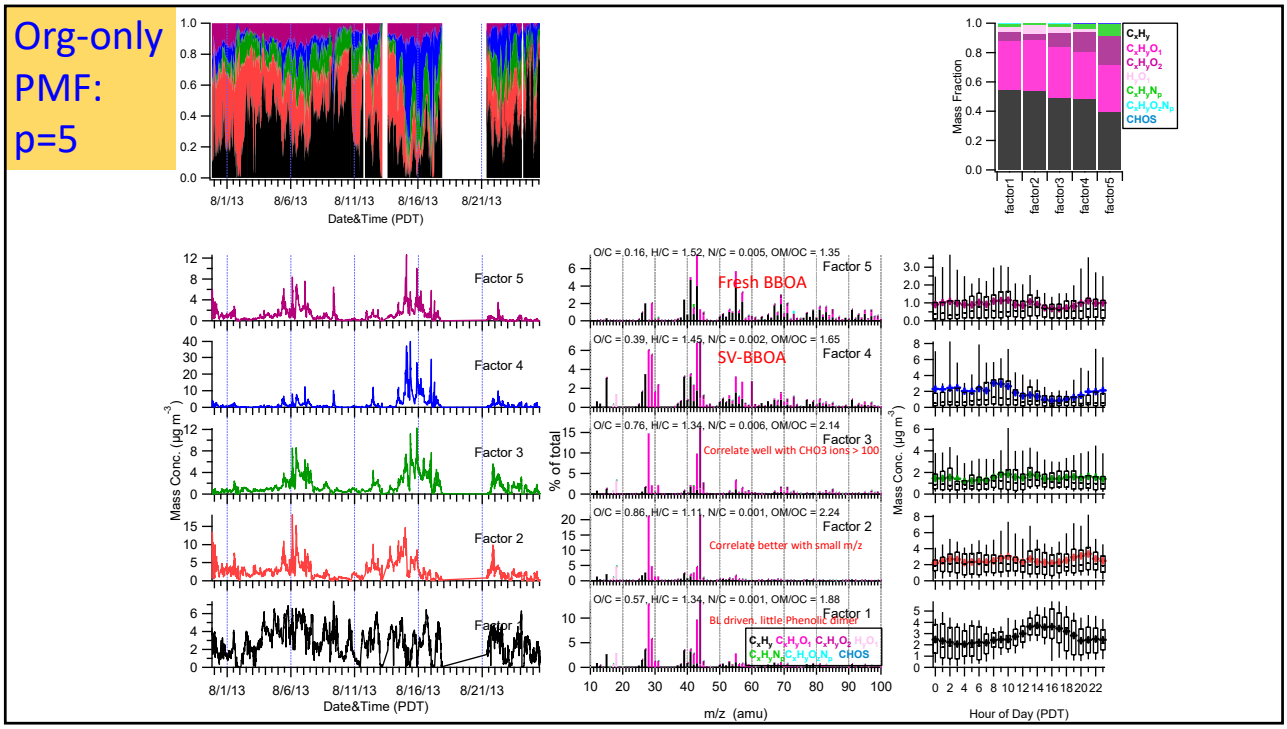
Residual Ratio m/z



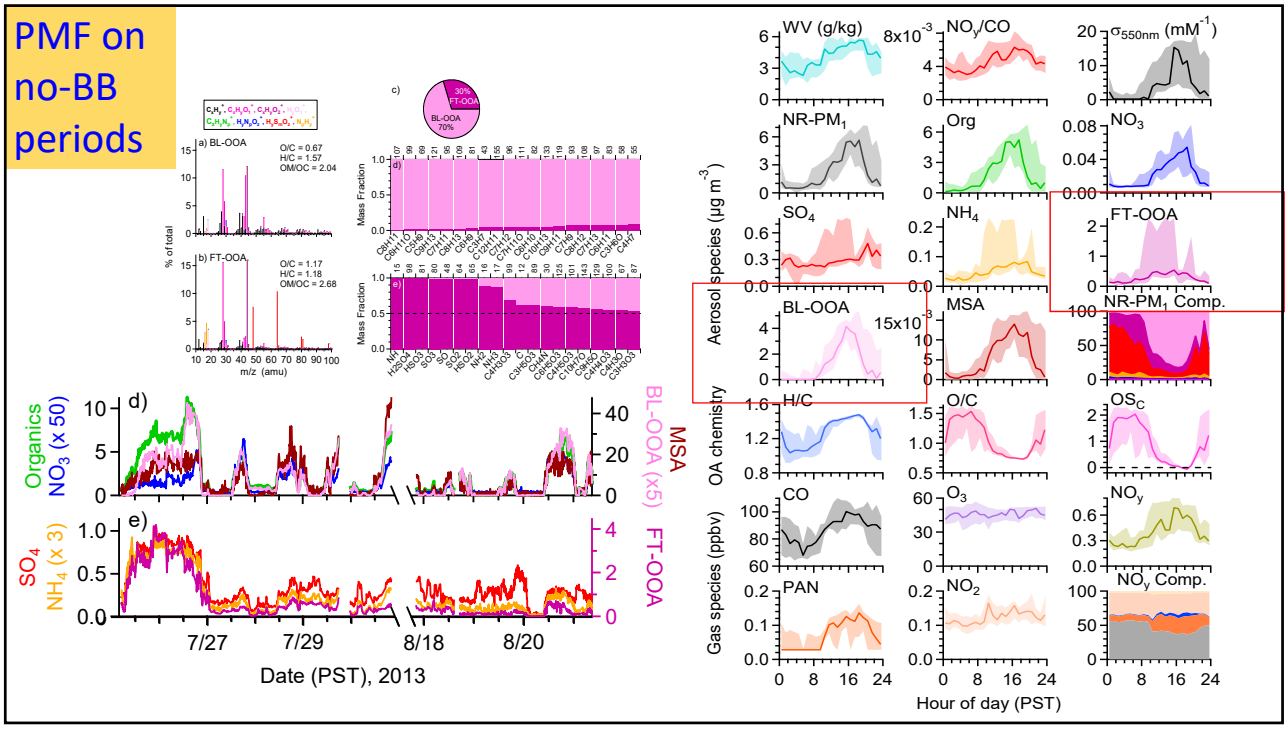
Org-only PMF: p=4



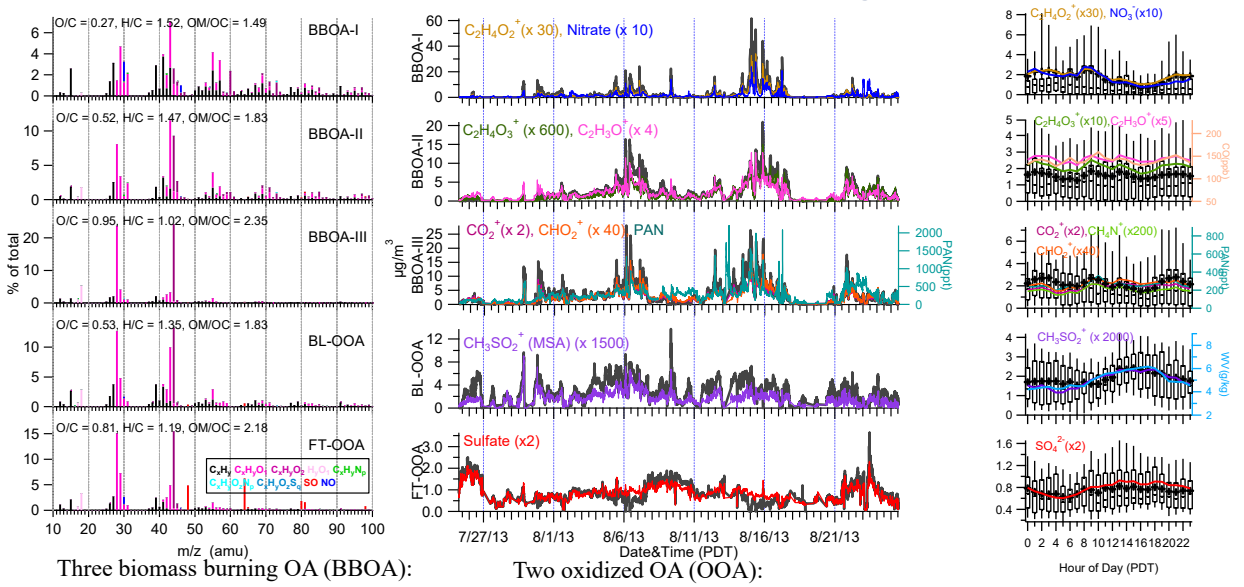
Org-only PMF: p=5



PMF on no-BB periods



OA Factors Observed at MBO during BBOP



Three biomass burning OA (BBOA):

- **BBOA-I**: Fresh BBOA
- **BBOA-II**: More oxidized BBOA
- **BBOA-III**: Highly oxidized, aged BBOA

Two oxidized OA (OOA):

- **BL-OOA**: Boundary layer oxygenated OA
- **FT-OOA**: Free tropospheric oxygenated OA

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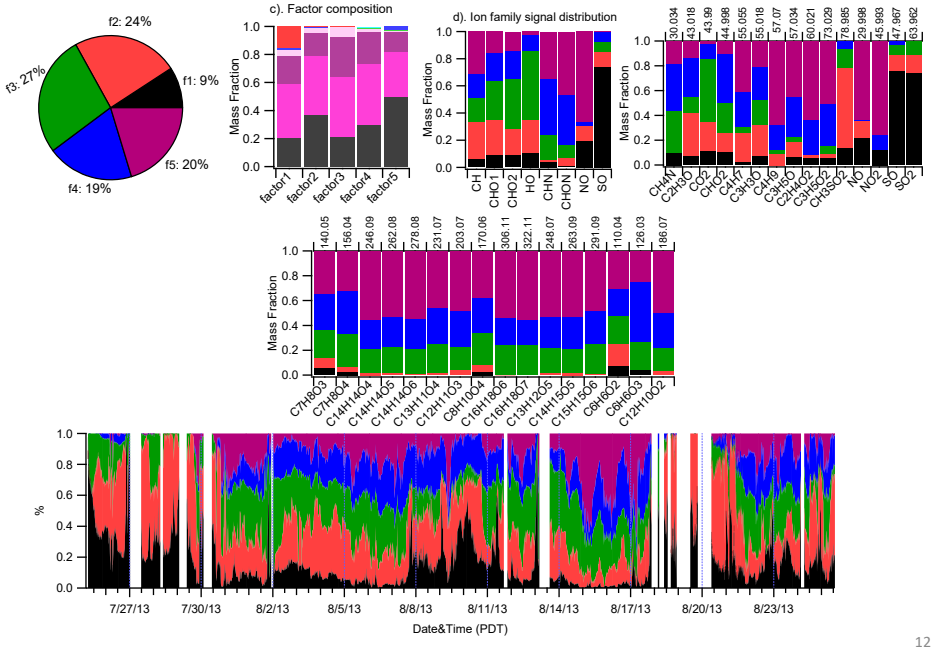
Zhou et al., 2016

PMF factors composition and signal distribution



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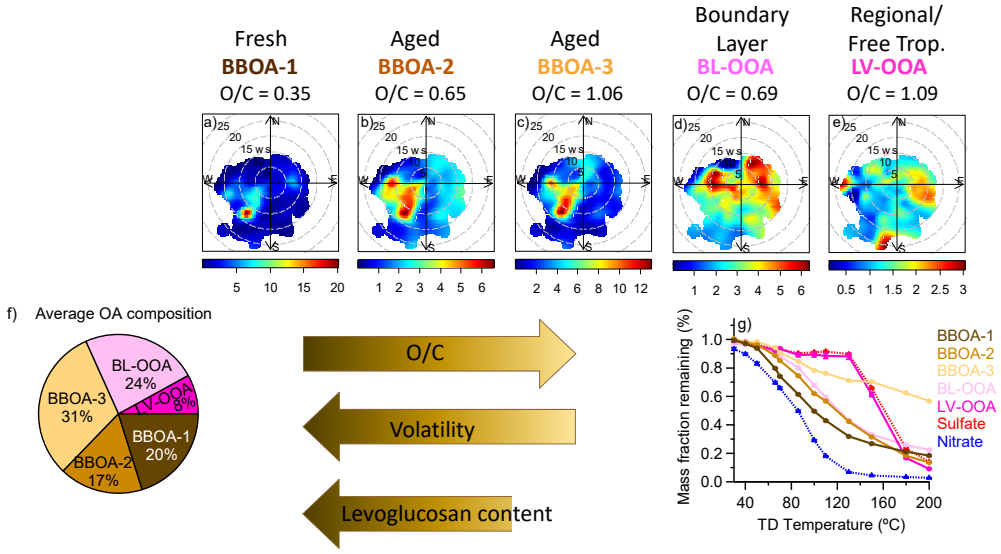
BB POA and SOA in Regional Air Masses



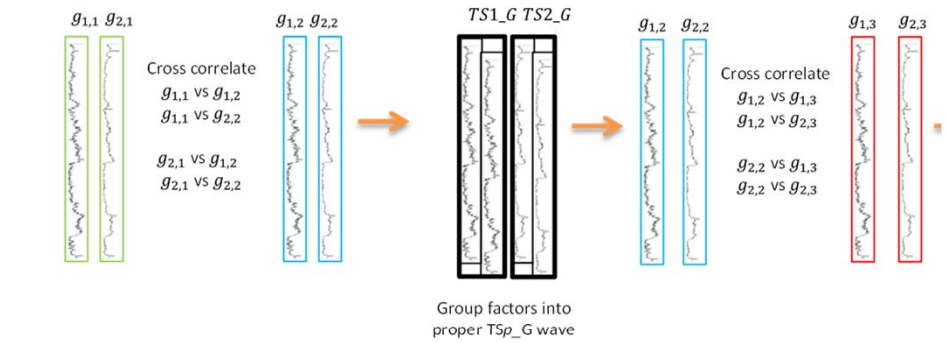
- Three types of BBOA, different chemistry and volatility
- ΣBBOA ≈70% of OA mass, ~ 60% of BBOA is secondary.

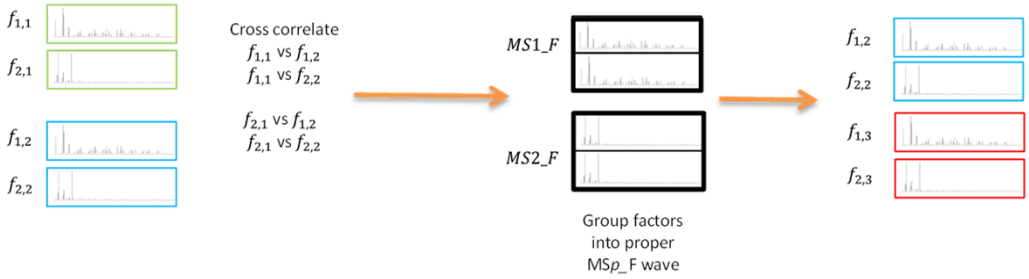
Two methods

- Analysis of combined organic and inorganic ions
  - Include good S/N inorganic ions (NO^+, NO_2^+, NH_2^+, NH_3^+, SO^+, SO_2^+ …)
  - to better extract physically meaningful factors and reduce mixing of factors.
  - Additional inorganic signal to assist interpretation of factors.

- Rolling window analysis of long term data
  - Small chunk of MS matrix, continue roll over on time axis
  - Better capture time-dependent variations of factor profiles.

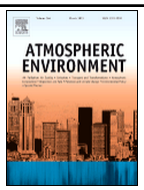
Rolling Window Analysis





15

Long-term measurements of submicrometer aerosol chemistry at the Southern Great Plains (SGP) using an Aerosol Chemical Speciation Monitor (ACSM)

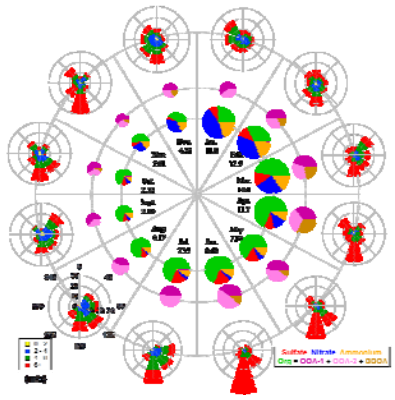


Parworth, C., Fast, J., Mei, F., Shippert, T., Sivaraman, C., Tilp, A., Watson, T., and Zhang, Q.: *Atmospheric Environment* doi:10.1016/j.atmosenv.2015.01.060, 2015.
http://www.sciencedirect.com/science/article/pii/S1352231015000837

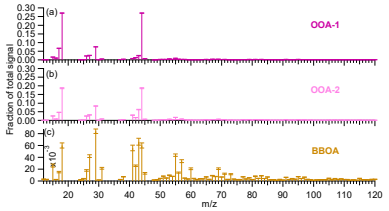
- Location: The Southern Great Plains (SGP) site of DOE's Atmospheric Radiation Measurement (ARM) program, a rural site in central Oklohoma.
- 19 months of continuous ACSM data (30 min resolution)
- Average NR-PM_1: 6.7 ± 8.9 µg m^{-3}. Org % of total: 65 ± 21%

Rolling Window PMF Methodology

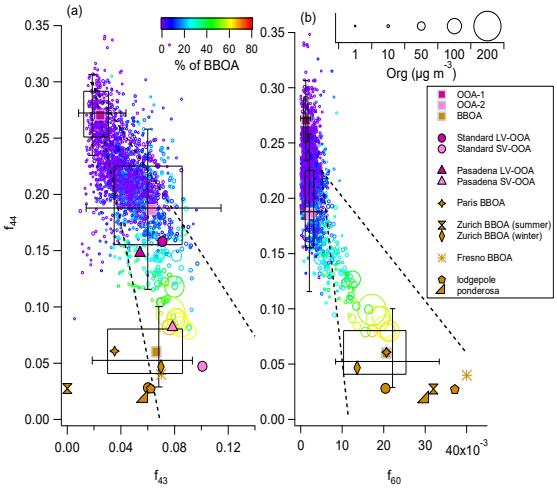
- Standard pretreatment method applied (Ulbrich et al., 2009)
- Rolling window size flexible, 2 weeks used here
- Data increment is 1 day until end of data reached
- 2 or 3 factor solutions possible for this rural site: BBOA (if f_{60} > 0.008) and two types of OOA
- Rolling window length
  - 1-week not enough data
  - 2 & 3 weeks show similar results
  - 2-weeks contains enough data to capture dynamic variations of aerosols and is representative of avg. lifecycle of aerosols in atmosphere



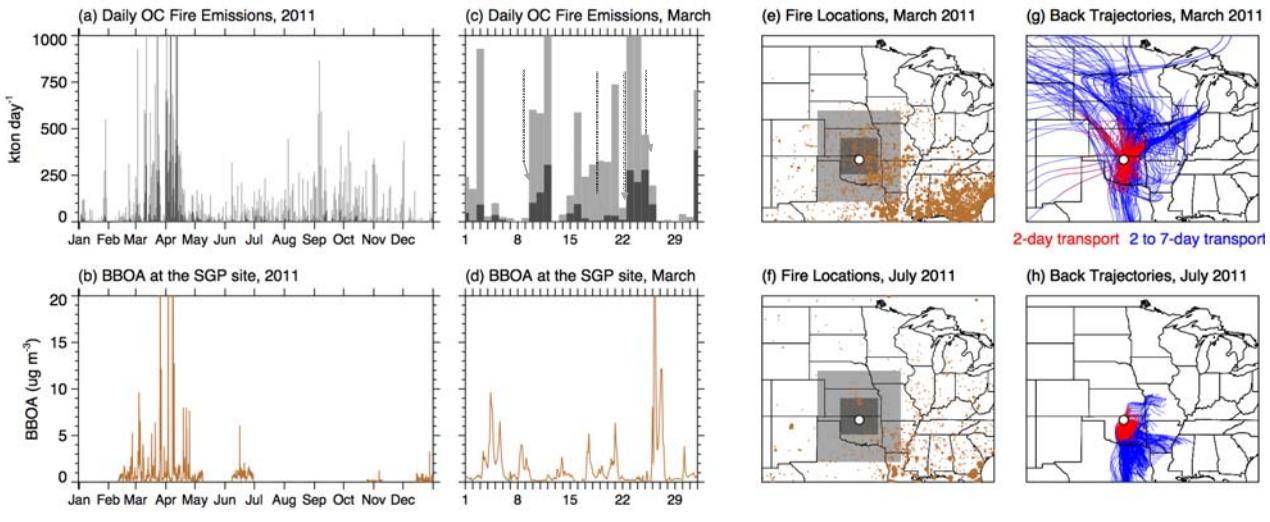
Monthly variations in average NR-PM$_1$ concentration, composition, and wind data for one year (2011)



Average OA mass spectra over entire study with standard error bars from rolling window analysis.



Box and whisker plots show range in values of each factors obtained from rolling window analysis.



Acknowledgements

Shan Zhou, Caroline Parworth, Yele Sun

Sonya Collier, Xinlei Ge, , Jianzhong Xu, Hwajin Kim, Lu Yu

References:

Sun, Y. L., Q. Zhang, J. J. Schwab, T. Yang, N. L. Ng, and K. L. Demerjian (2012), Factor analysis of combined organic and inorganic aerosol mass spectra from high resolution aerosol mass spectrometer measurements, *Atmospheric Chemistry and Physics*, *12*(18), 8537-8551, doi:10.5194/acp-12-8537-2012.

Parworth, C., J. Fast, F. Mei, T. Shippert, C. Sivaraman, A. Tilp, T. Watson, and Q. Zhang (2015), Long-term measurements of submicrometer aerosol chemistry at the Southern Great Plains (SGP) using an Aerosol Chemical Speciation Monitor (ACSM), *Atmospheric Environment*, *106*, 43-55, doi:http://dx.doi.org/10.1016/j.atmosenv.2015.01.060.

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Zhou, S., S. Collier, D. A. Jaffe, N. L. Briggs, J. Hee, A. J. Sedlacek Iii, L. Kleinman, T. B. Onasch, and Q. Zhang (2017), Regional Influence of Wildfires on Aerosol Chemistry in the Western US and Insights into Atmospheric Aging of Biomass Burning Organic Aerosol, *Atmos. Chem. Phys.*, *17*, 2477-2493, doi:10.5194/acp-17-2477-2017.