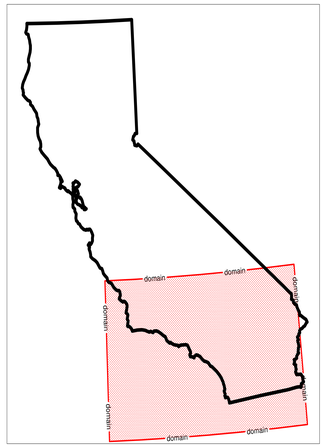
Modeling Organic Aerosol: Using Regional-scale Models to Characterize GEOS-Chem

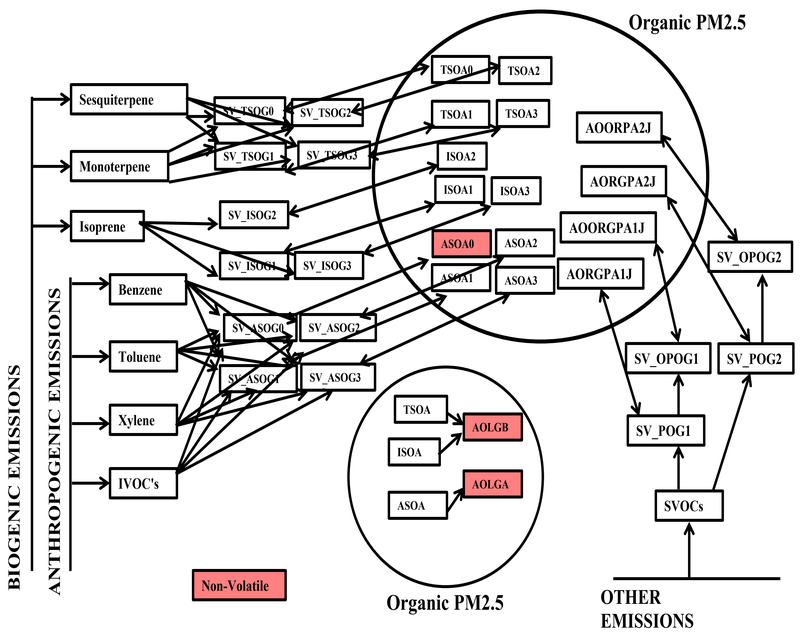
Joseph J. Ensberg (jensberg@caltech.edu), Jill S. Craven,
Havala O. T. Pye, and John H. Seinfeld
Division of Chemistry and Chemical Engineering and Division of Engineering and Applied Science

Motivation

- The Los Angeles mega-city has consistently exhibited some of the highest particulate matter levels in the United States.
- During May 2010, an intensive field experiment, known as the California Nexus (CalNex) campaign, was carried out to study the chemistry and physics of gas and aerosol-phase pollution.
- The organic aerosol treatment in GEOS-Chem is one of the most sophisticated frameworks in both regional and global scale models.
- To apply the organic aerosol treatment of GEOS-Chem on an urban scale, its aerosol module has been implemented into the Community Multi-scale Air Quality Model (CMAQv4.7.1) (Binkowski and Roselle 2003).
- Additional updates made to CMAQ will be reimplemented into GEOS-Chem.

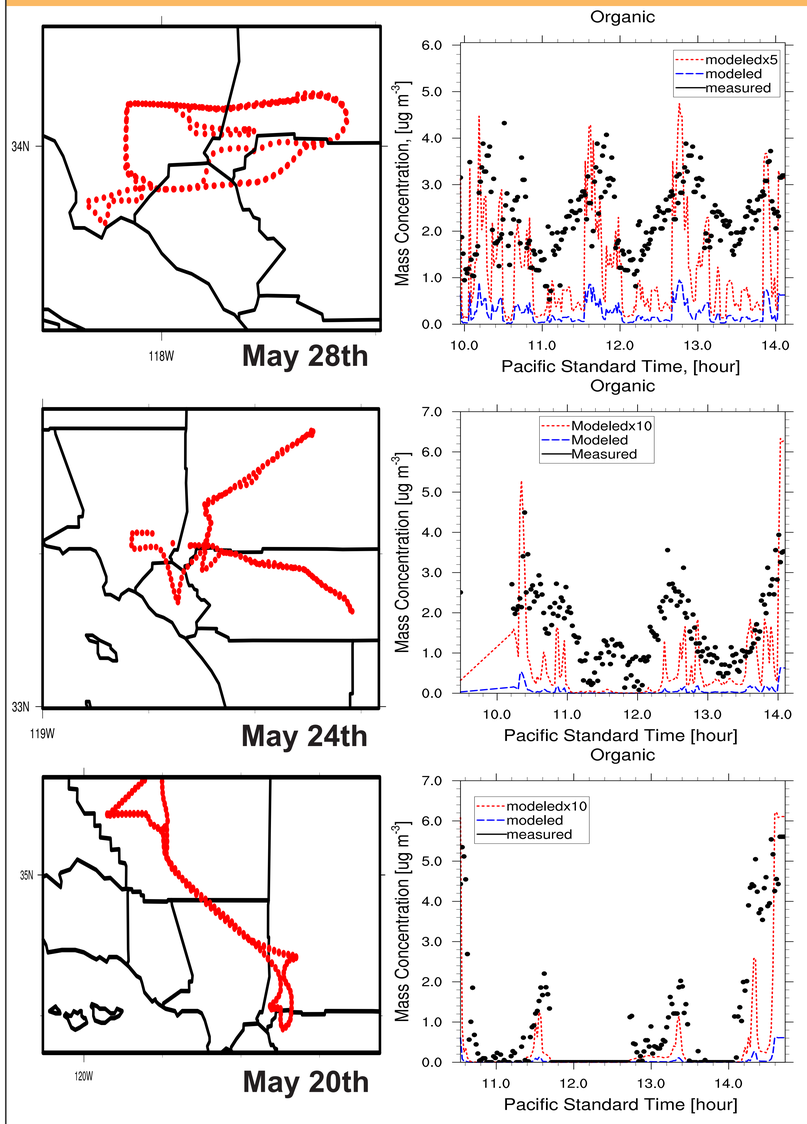


SOA from SVOCs, IVOCs, and Traditional Precursors



(Pye and Seinfeld 2010b)

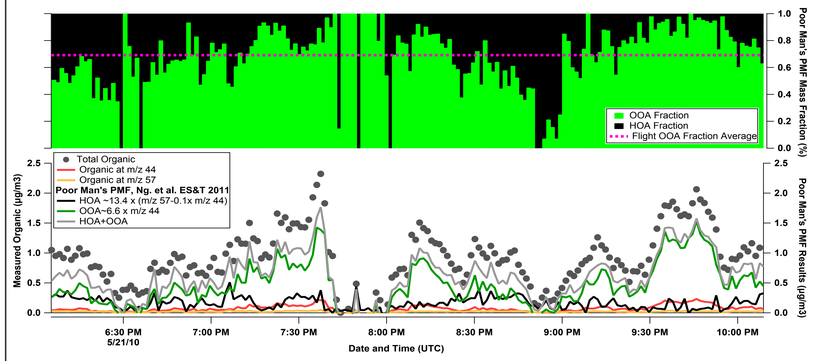
Bulk Organic Aerosol Concentrations in L. A. Basin



Future GEOS-Chem Updates

- Aging of all semi-volatile species through gas-phase photo-oxidation will be implemented into GEOS-Chem (Hodzic et al. 2010)
- Instantaneous equilibrium between SOA and semi-volatile gas-phase species will be relaxed and a dynamic mass transfer treatment will be implemented into GEOS-Chem.

POA vs. SOA using PM Positive Matrix Factorization



- Positive Matrix Factorization is a mathematical technique used to deconstruct organic aerosol mass spectra into chemically relevant factors.
- The results from this technique can produce a hydrocarbon-like OA (HOA) and an oxygenated OA (OOA) constituent.
- Poor Man's PMF is a parameterization based on several PMF data-sets that approximate PMF results to within 30% (Ng et al. 2010).
- Poor Man's PMF places an additional constraint on model performance by specifying what fraction of OA should come from POA and what fraction should come from SOA

Conclusions

- The aerosol treatment of GEOS-Chem captures the spatial distribution of OA well, but underpredicts bulk concentrations by up to an order of magnitude.
- Underpredictions may be attributable to large uncertainties in IVOC emission inventory parameterization as well as partitioning coefficients
- Volatility reduction of gas-phase species due to photo-oxidation may help increase total OA mass
- Standard models (without semi-volatile POA and IVOCS) overpredict the fraction of OA that comes from POA
- By volatilizing POA, oxidizing, and then repartitioning, the aerosol treatment of GEOS-Chem captures the correct oxidation behavior better than older models.

References and Acknowledgements

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- Ng et al. *Env. Sci. Tech.*, 45, 910-916, 2011
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