Preliminary Modeling of SOA during CARES

Jerome Fast

SOA Formation Breakout Session

Thanks to CARES scientists for data used in this study including:
John Shilling, Art Sedlacek, Chen Song, Qi Zhang, and Stephen Springston

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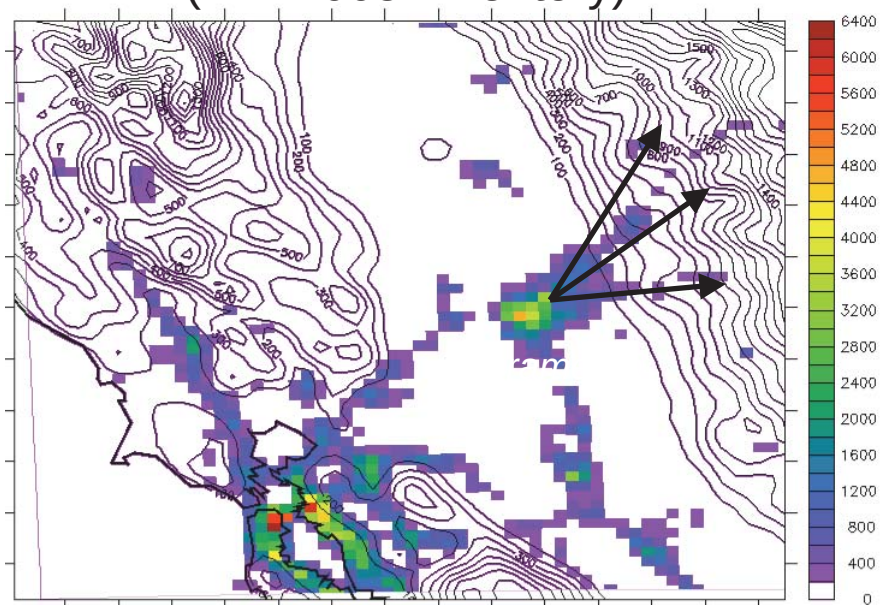
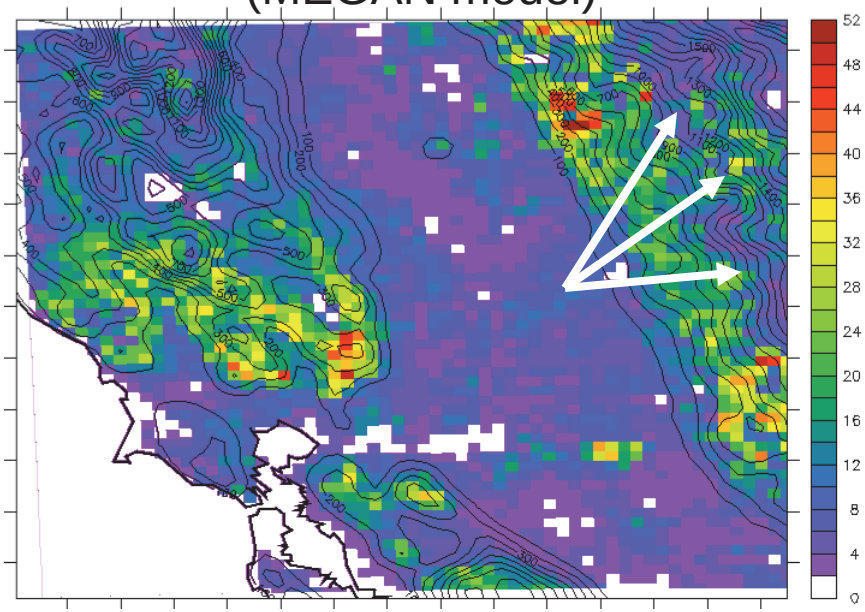
Goals

- How do anthropogenic and biogenic precursors interact to form SOA?

CO Emission Rates
(NEI 2005 Inventory)



Isoprene Emission Rates
(MEGAN model)



- Utilize data collected during the 2010 CARES campaign to evaluate model predictions, test parameterizations, and perform sensitivity simulations of SOA evolution

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CARES

- CARES supersites
- G-1 flight paths
- radar wind profilers
- surface meteorological monitoring
- surface PM2.5 monitoring

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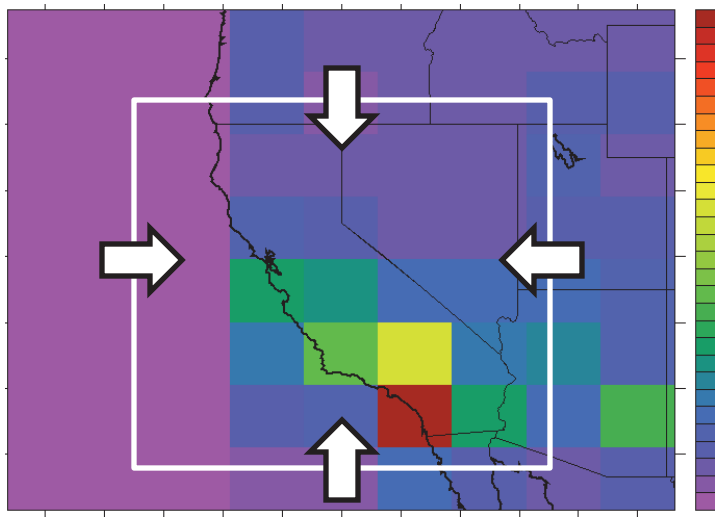
Modeling Approach

WRF-Chem:

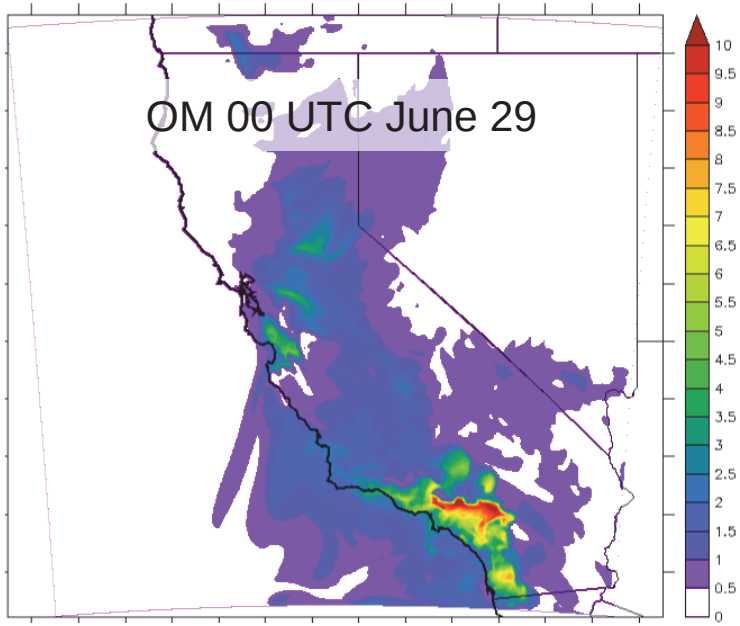
- Same configuration as operational CARES forecasts CARES, except chemistry
- Δx = 4 km, domain encompassing California
- See *Fast et al*., ACPD [2011], to be submitted soon
- Initial and boundary conditions from MOZART to account for long-range transport
- Anthropogenic emissions from NEI 2005 and biogenic emissions from MEGAN, no biomass burning emissions presently (likely to be small locally)

MOZART Organic Matter

from Louisa Emmons (NCAR)



WRF-Chem Domain



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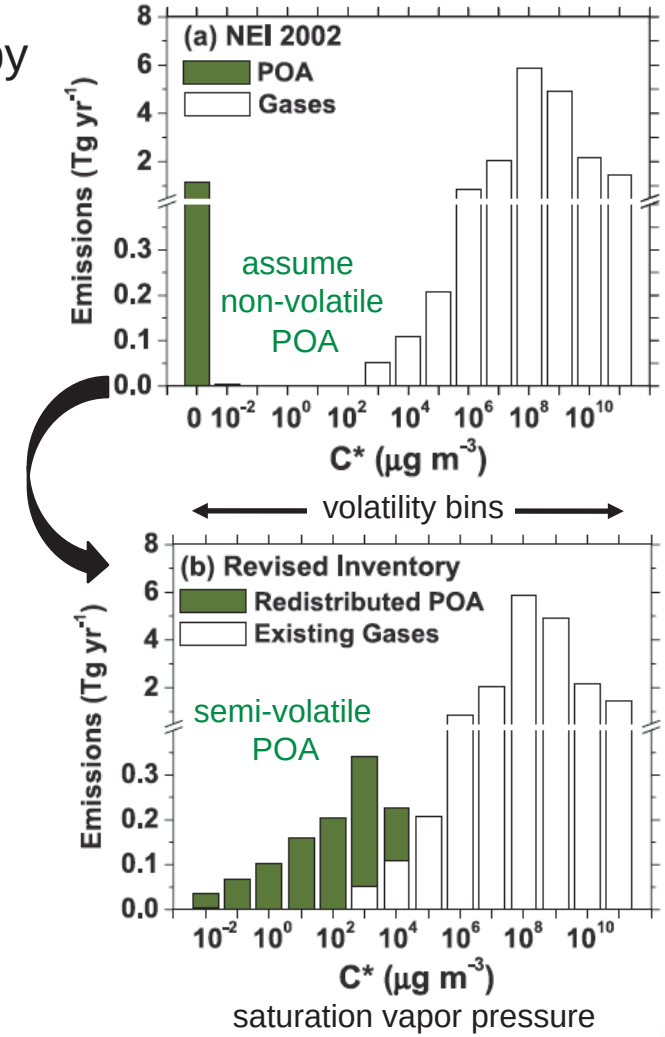
Organic Aerosol Approach

Organic Aerosol Treatment in WRF-Chem:

- Modified *Robinson et al*. [2007] volatility basis set by adding 2 oxygen atoms per generation of oxidation
- # of volatility bins: 9 for **fresh** and 8 for **aged**
- Separate volatility species for **fossil** and **biomass burning** sources
- Predict both **oxygen** and **carbon** mass for each volatility species to obtain O:C ratios
- Traditional anthropogenic and biogenic SOA (4-product VBS set) using yields from *Tsimpidi et al*. [2010] with no further aging
- prognostic SOA species: currently **380 for 4 size bins**, (684 for 8 size bins)
- Coupled with SAPRC-99 gas-phase mechanism and MOSAIC aerosol model
- Dry deposition for all species treated the same



See Shrivastava et al., ACP [2010] for more details

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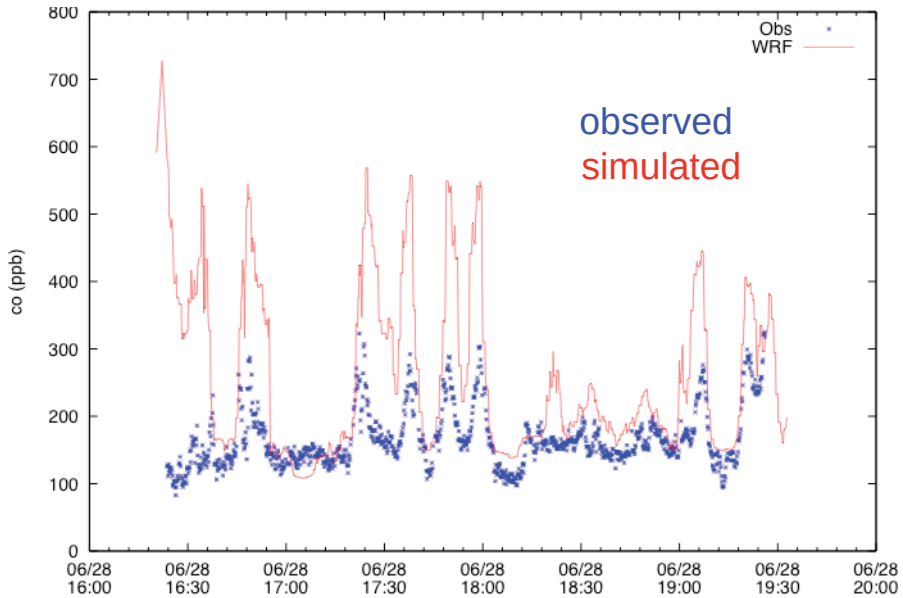
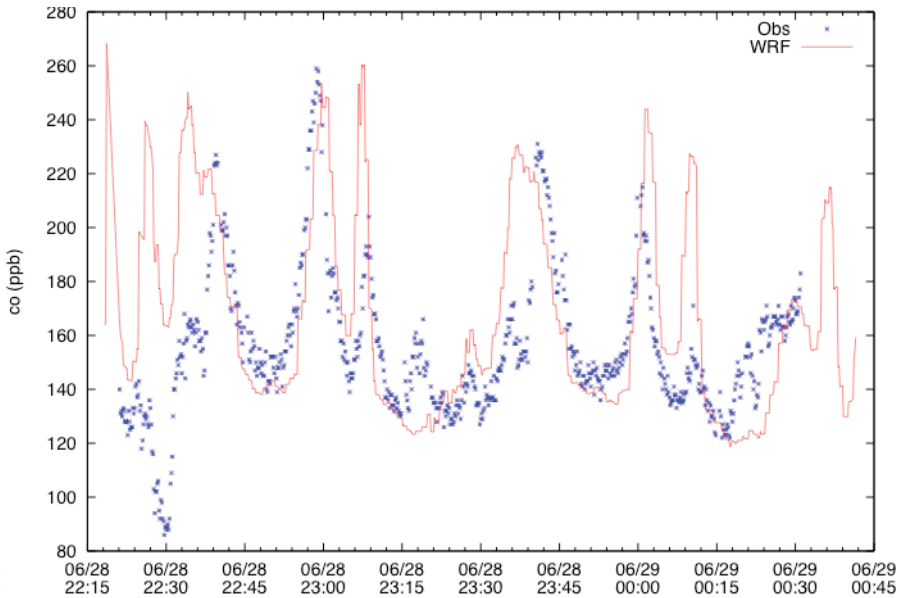
June 28

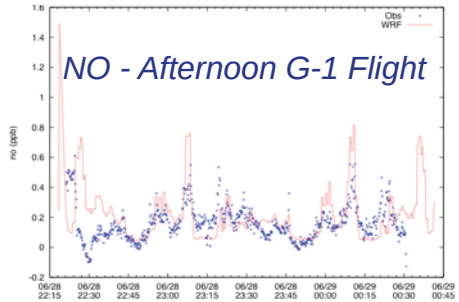
Southwesterly Winds – Transport Predicted Well on This Day

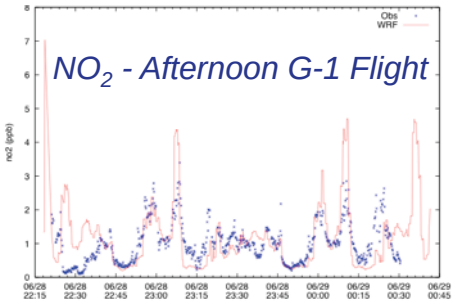
CO - Morning G-1 Flight

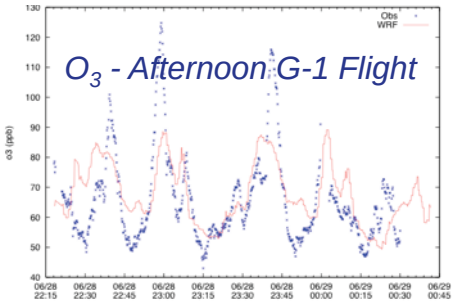


CO - Afternoon G-1 Flight









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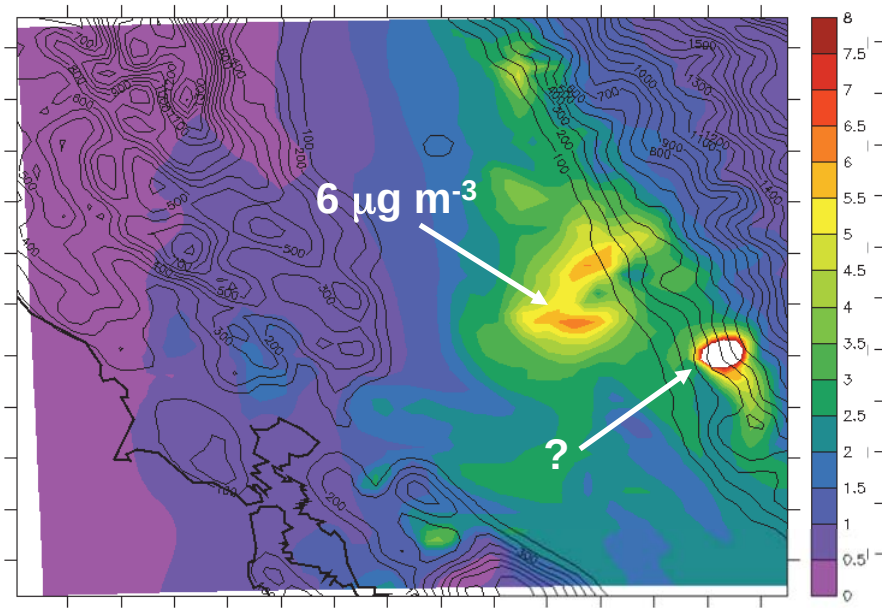
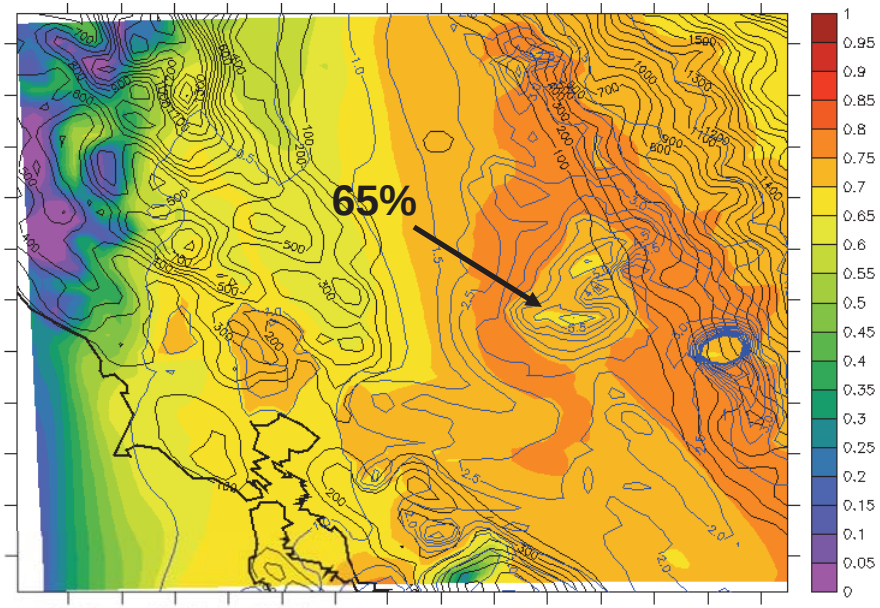
18 UTC June 28

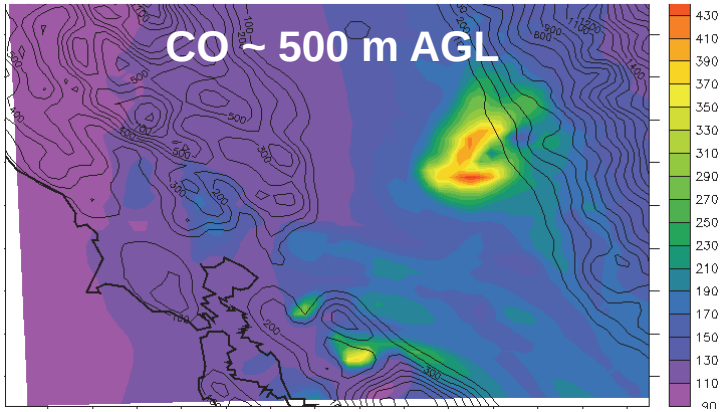
Regional Variation in Organic Matter (OM)

OM ~ 500 m AGL



SOA Fraction ~ 500 m AGL





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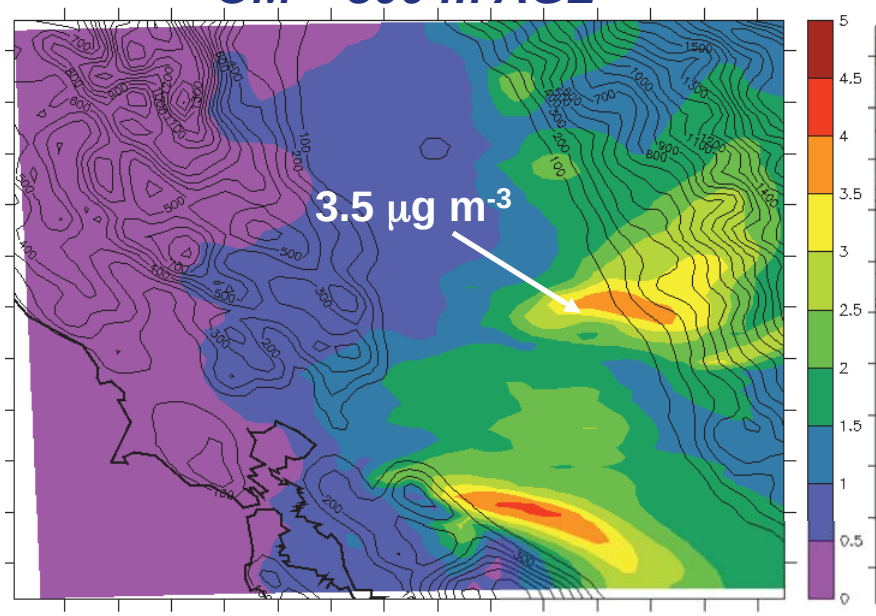
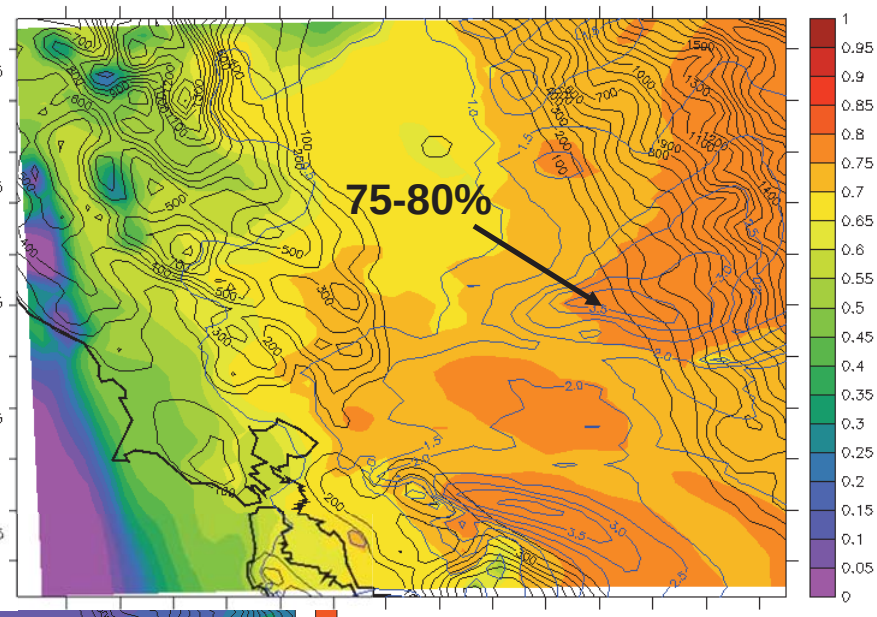
00 UTC June 29

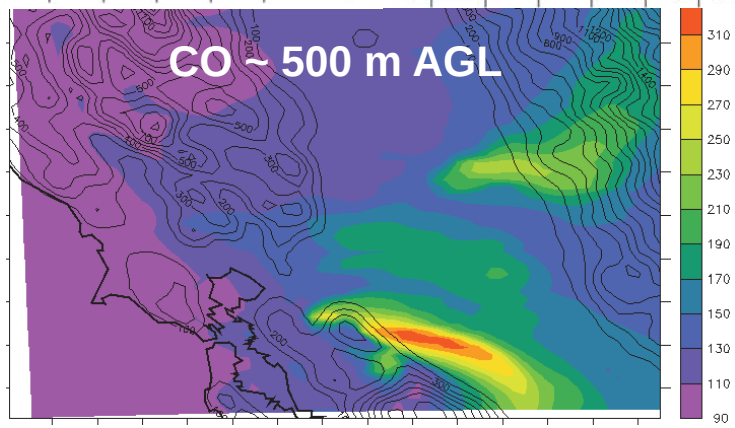
Regional Variation in Organic Matter (OM)

OM ~ 500 m AGL



SOA Fraction ~ 500 m AGL





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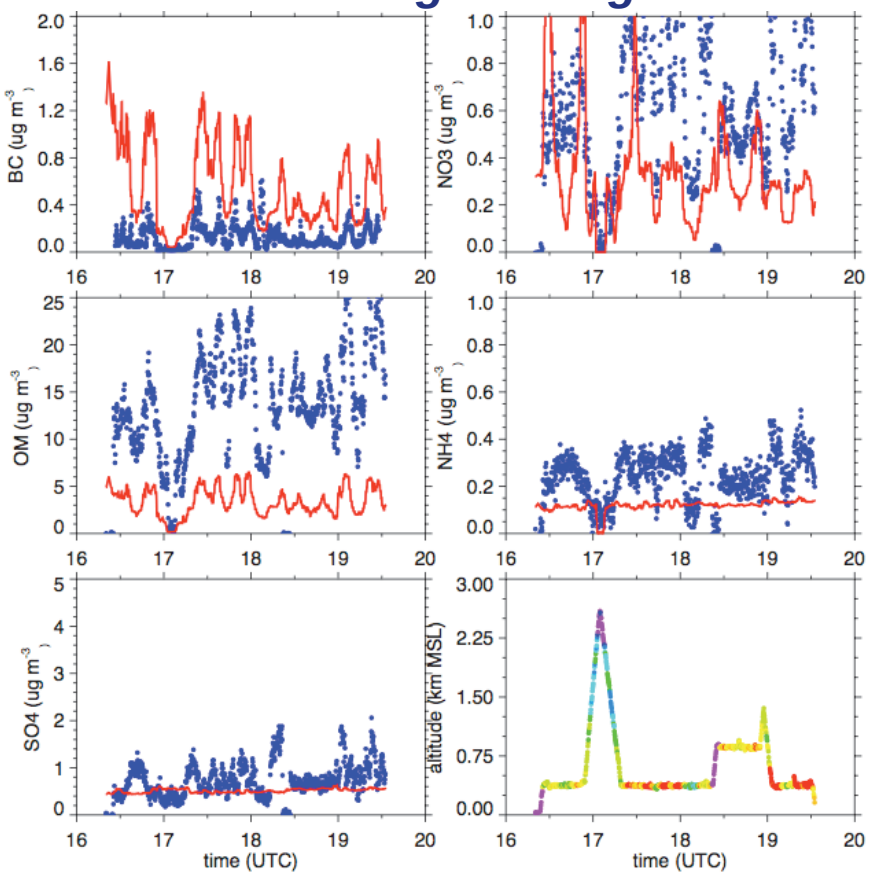
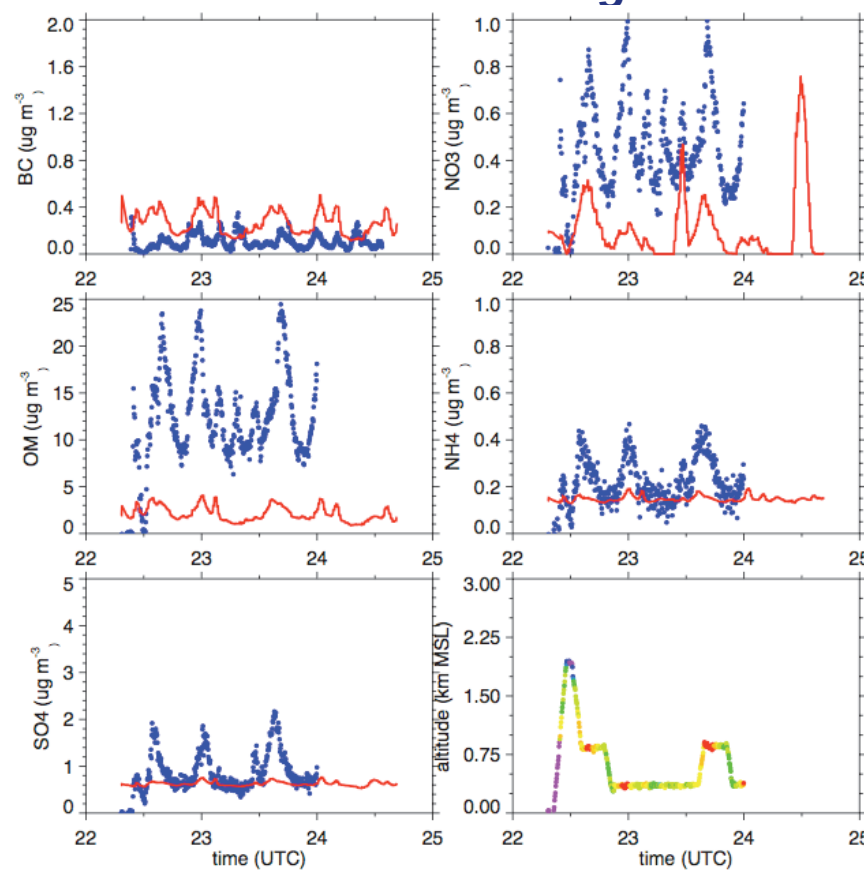
Comparison with G-1

Aerosols Not Predicted as Well as CO, NO, NO_2, and Ozone

Morning G-1 Flight



Afternoon G-1 Flight



- BC too high (emissions problem?)
- OM too low

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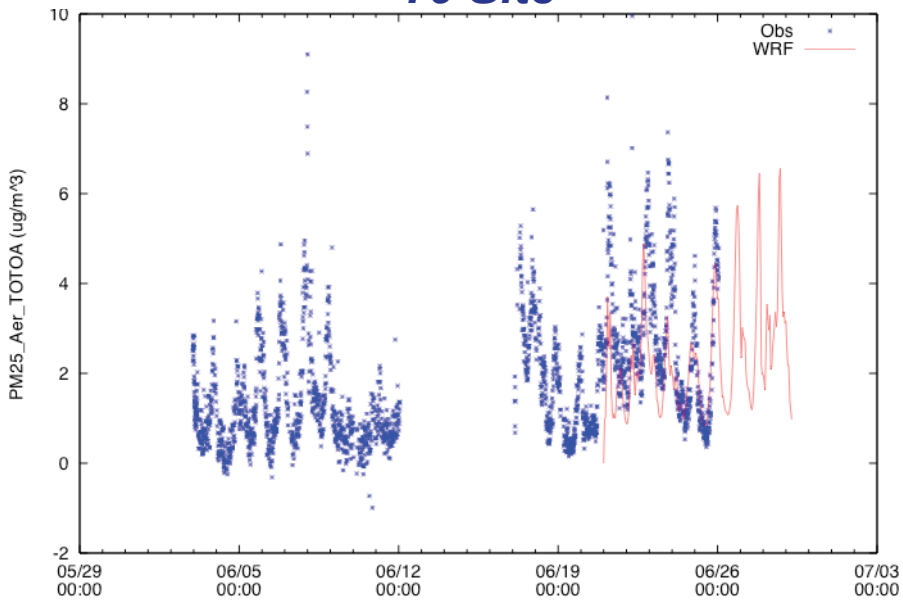
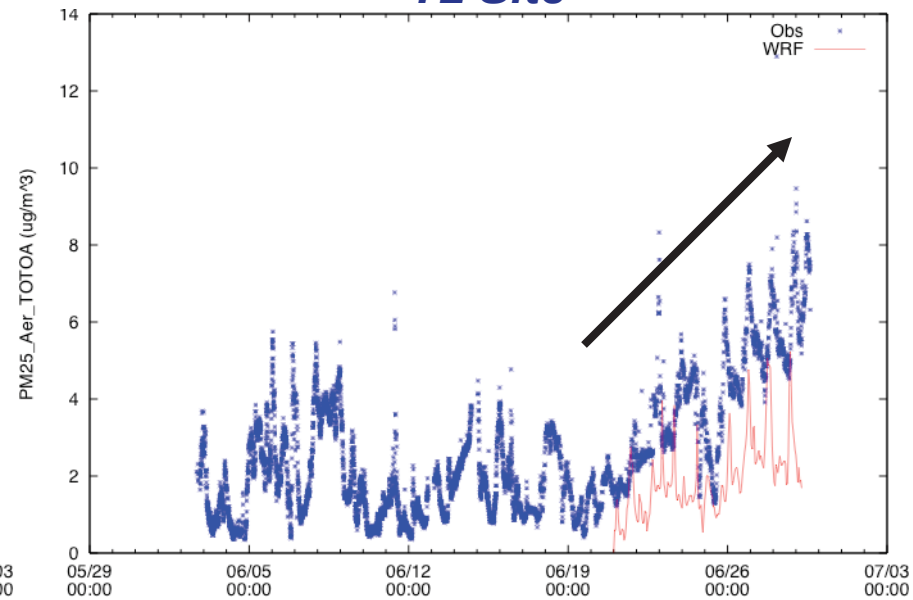
Comparison with Surface Sites

Aerosols Not Predicted as Well as CO, NO, NO_2, and Ozone

T0 Site



T1 Site



- OM better predicted in the city at T0 than at the rural T1 sites

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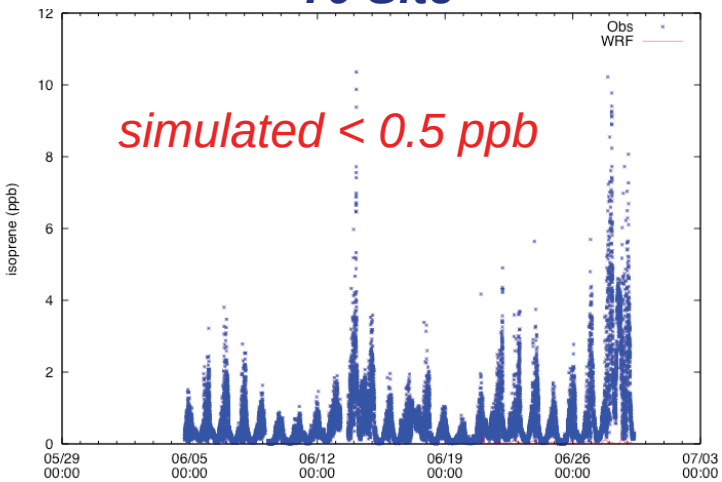
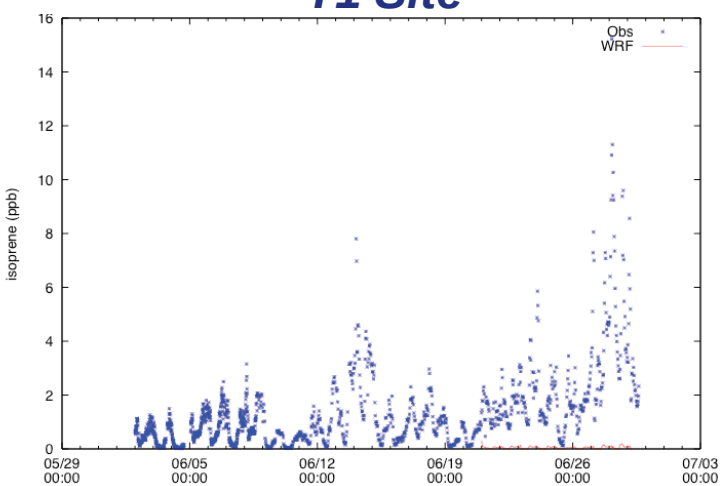
Biogenic Species

Simulated Isoprene Far too Low

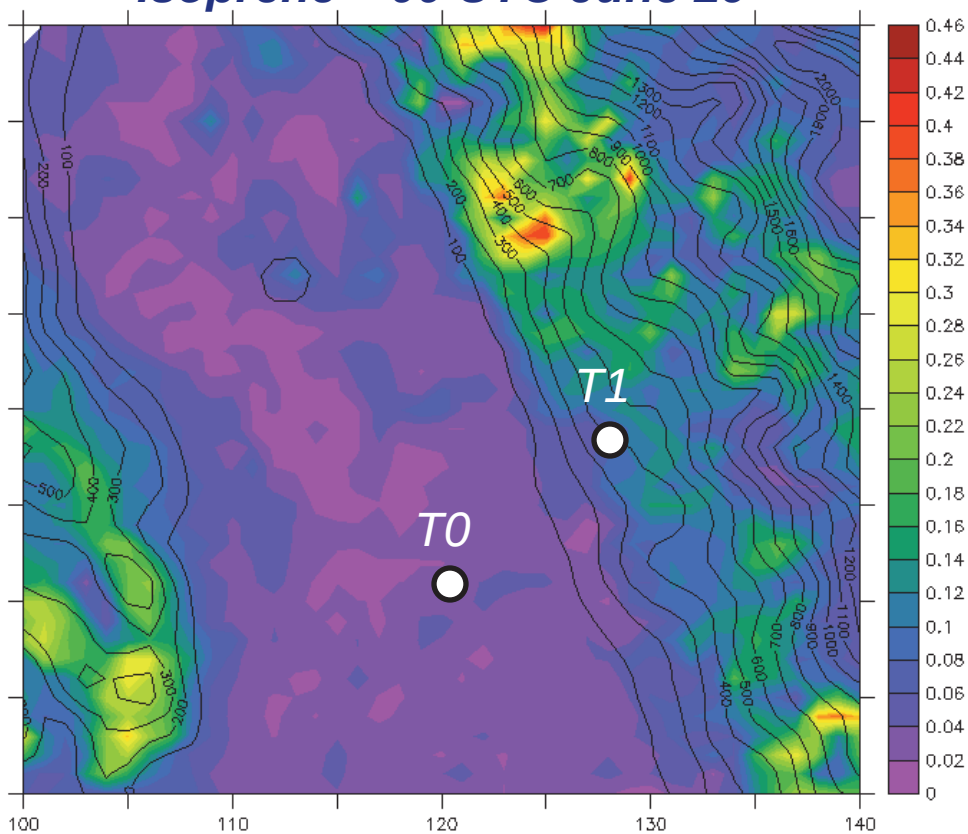
T0 Site



T1 Site



Isoprene – 00 UTC June 29



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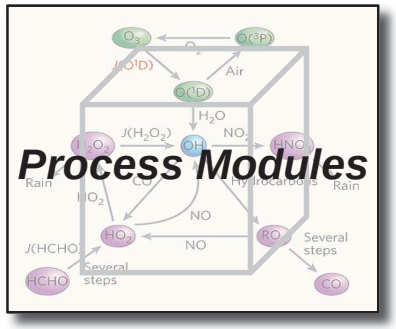
Next Steps

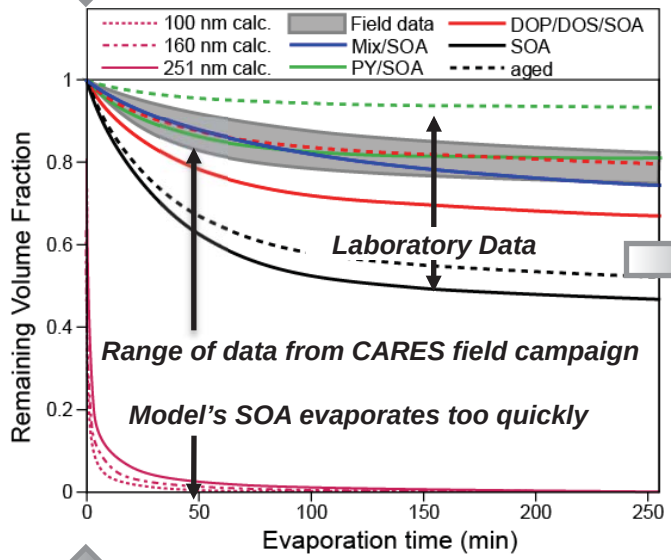
- Emissions
  - *Check problem with biogenic emissions*
  - *Missing local SO_2 sources?*
  - *Compare NEI 2005 and CARB 2008 anthropogenic emissions*
- Need to ensure gas phase chemistry is reasonably simulated before further assessments of aerosols and SOA
- Then, perform SOA simulations, with and without biogenic emission
  - *Currently difference on OM is ~ 0.2 $\mu g\ m^{-3}$, but isoprene far too low*
  - *Determine whether current SOA parameterization reasonable represents anthropogenic-biogenic interactions, if no then tests alternative formations*
  - *Employ recent findings on SOA formation and evaporation from laboratory / field / theory*
- Evaluate simulated optical properties (employ O:C ratio for organics) and quantify impact of SOA on regional aerosol radiative forcing

Collaborate with ASR Investigators

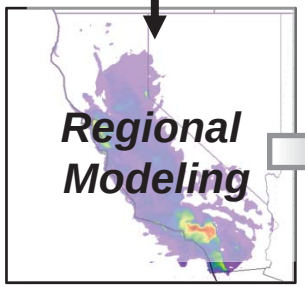
Utilize Aerosol Modeling Testbed Framework

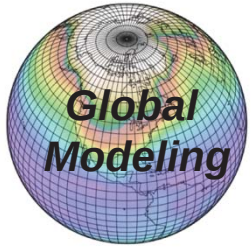


Perform new experiments to define physical relationships



Revise process model of SOA based on new data





Does new SOA treatment compare better with field data than exiting treatments?

If so, make recommendations for use in global model.

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