Modeling the Formation of Secondary Organic Aerosols from Semi-Volatile Organic Vapors in the Mexico City Region

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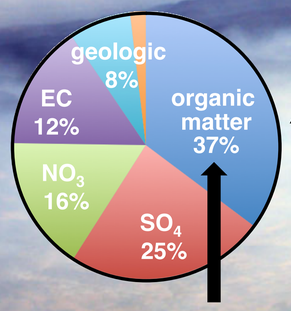
Importance of Secondary Organic Aerosols (SOA)

MILAGRO — Megacity Initiative: Local and Global Research Observations

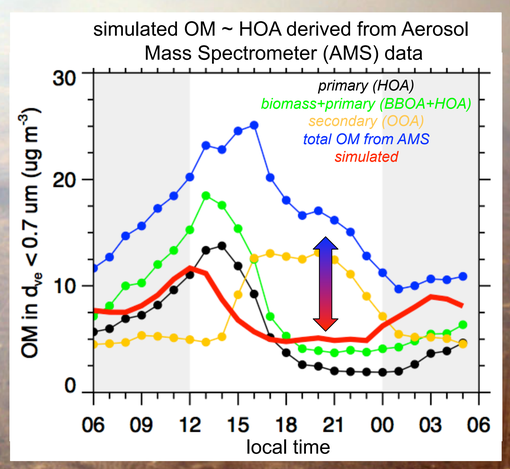
Megacity Initiative: Local and Global and Local Research Observations

Field Campaign during March 2006



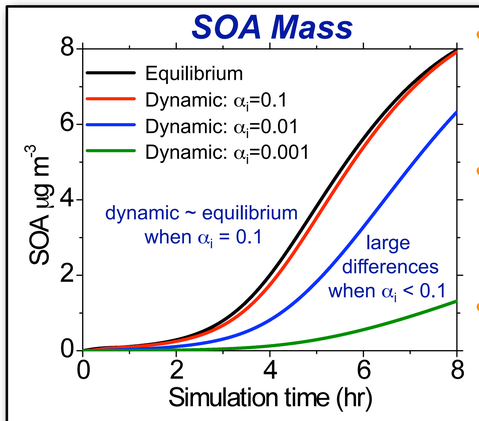
Average Observed Composition in Mexico City

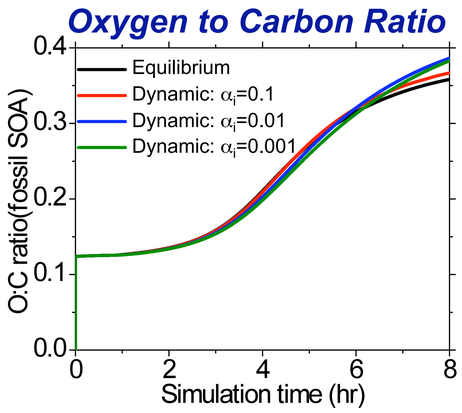
- SOA is a large fraction of the total mass of organic matter (OM) in many regions
- SOA severely under-predicted – a major problem for climate models [e.g. *de Gouw et al*. 2005]
- SOA contributes to direct radiative forcing and organics may play a role in cloud-aerosol interactions

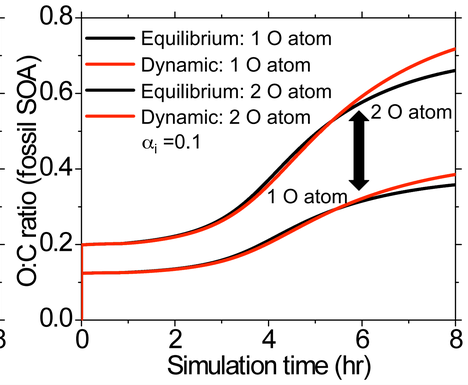


from Fast et al. [2009]

0-D Box Modeling





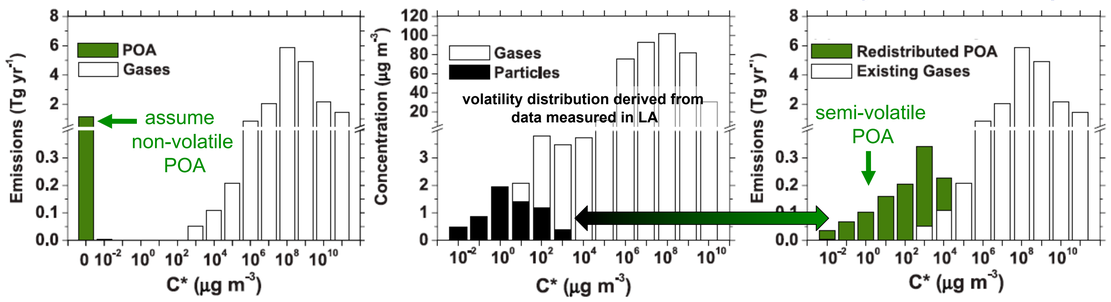


- While most models assume thermodynamic equilibrium for gas-particle SOA partitioning, SOA formation may be limited by mass transfer ➡ useful to test dynamic approach in MOSAIC
- Dynamic approach: the mass accommodation coefficient, α_i, used to compute gas-particle mass transfer rate often assumed to be 0.1 (may be smaller)
- In addition to producing sufficient mass, SOA treatments must also represent the oxidation state of aerosols (represented by O:C ratios) such as those obtained from recent AMS measurement techniques

assumed addition of oxygen per generation of aging significantly affects O:C ratio and increases SOA mass somewhat (not shown)

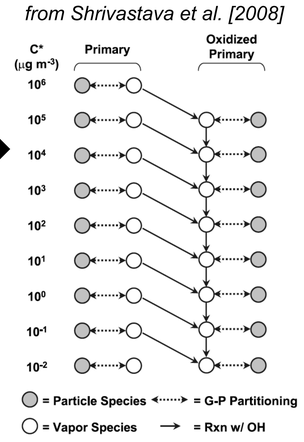
Modeling Strategy

Most Current Models ***Observations*** ***Volatility Basis Set (VBS)***



- Implemented VBS approach in MOSAIC, both in the 0-D box model and 3-D WRF-Chem model framework
  - *Species with similar volatility lumped into effective saturation concentration (C*) bins*
  - *# of volatility bins: 9 for fresh and 8 for aged*
  - *Separate VBS species for fossil and biomass burning sources*
  - *Predict both oxygen and carbon mass for each SOA species to obtain O:C ratios*
  - *Prognostic SOA species: 380 for 4 size bins, 684 for 8 size bins*
- Utilize MILAGRO and CARES data in the Aerosol Modeling Testbed to assess performance and computational cost of VBS approach when compared to other approaches
- Develop simplified approach suitable for climate models

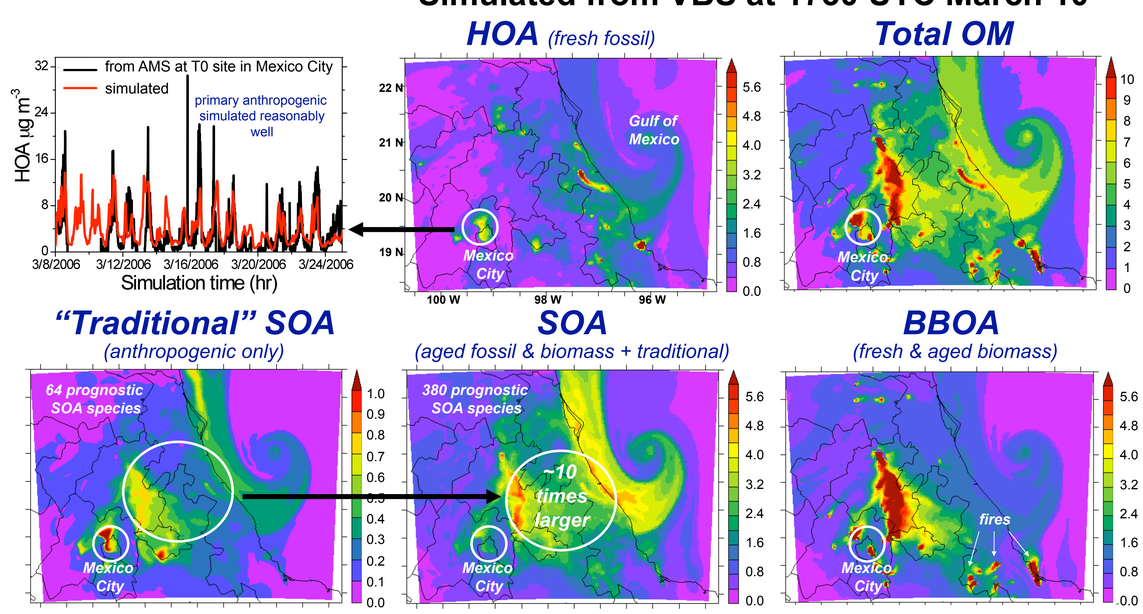
from Shrivastava et al. [2008]



3-D Modeling

- Preliminary simulation for MILAGRO performed with 4 size bins and equilibrium approach; currently revising VBS and evaluating it with several AMS data sets
- SOA from biogenic sources likely to be very important [*Hodzic et al*. 2009] and not yet included in the present results
- ~16 min per simulation hour using 120 processors, ~2 times more expensive than 'traditional' SOA approach

Simulated from VBS at 1730 UTC March 10



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