CMAQ Aerosol Module
Current Research and Future Plans

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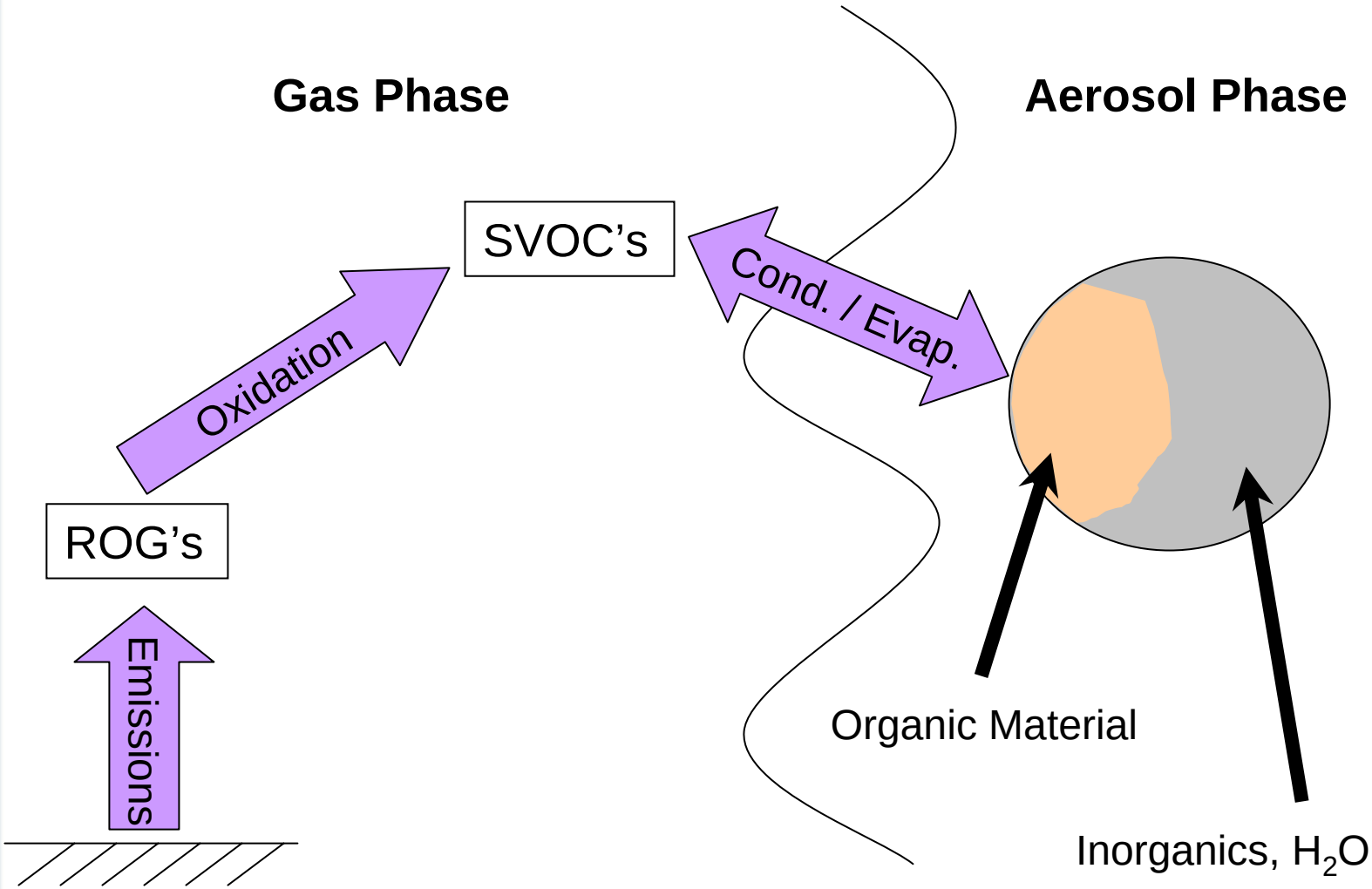
Overview

- Current Research
  - Secondary Organic Aerosols
  - Source Apportionment
- Future Plans
  - Coarse PM Chemistry & Physics
  - Aerosol Thermodynamics
  - Source-Oriented Multimodal Mixture

Secondary Organic Aerosols



Secondary Organic Aerosols

- Chemical Species
  - 6 ROG's (5 anthropogenic, 1 biogenic)
  - 10 SVOC products (8 anthro. & 2 bio.)
    - Temperature dependant saturation vapor pressure (ΔH = 156 kJ/mol)
  - Secondary Organic Aerosol
    - Anthropogenic and biogenic SOA contributions are explicitly tracked

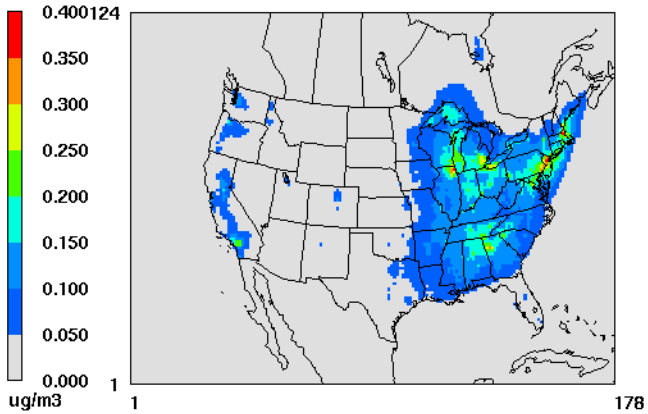
- References
  - Pankow, J.F. [*AtmEnv*, 1994]
  - Odum, et al. [*ES&T*, 1997]
  - Schell, et al. [*JGR*, 2001]

Secondary Organic Aerosols

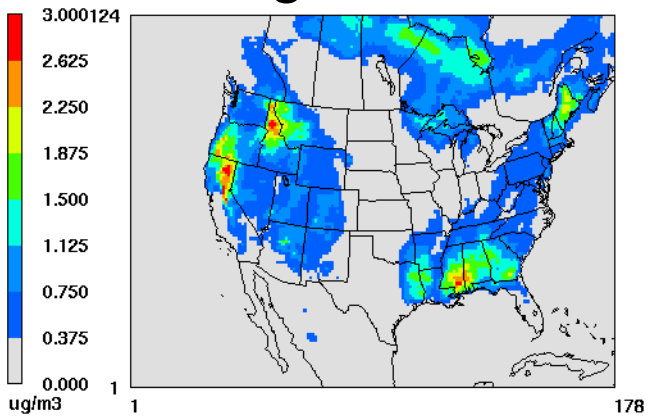
Model Results
June 16-23,1999 Avg.

- Anthro: 0 – 0.4 μg/m^3
- Biogenic: 0 – 3.8 μg/m^3
- Comparable with model results in literature
  Pun et al. [*ES&T*, 2003]
- Comparing with ambient estimates of total SOA
- Comparing with radiocarbon and biogenic SOA tracers
- Future model developments:
  - Acid-catalyzed reactions
  - Fog/cloud processing

Anthropogenic SOA



Biogenic SOA



Source Apportionment

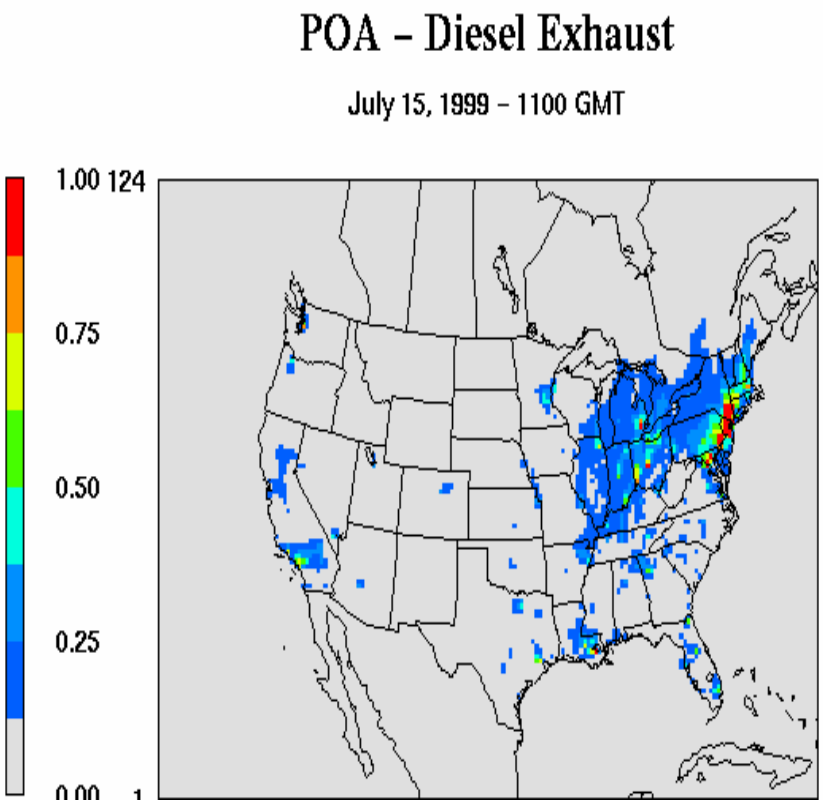
Receptor-Oriented	Source-Oriented
Input Requirements • Atmospheric aerosol measurements • Source profiles Output • Contribution of each source to atmospheric sample	Input Requirements • Emission inventory • Meteorology data • Reaction mechanisms Output • Particle composition, size, concentration, and source

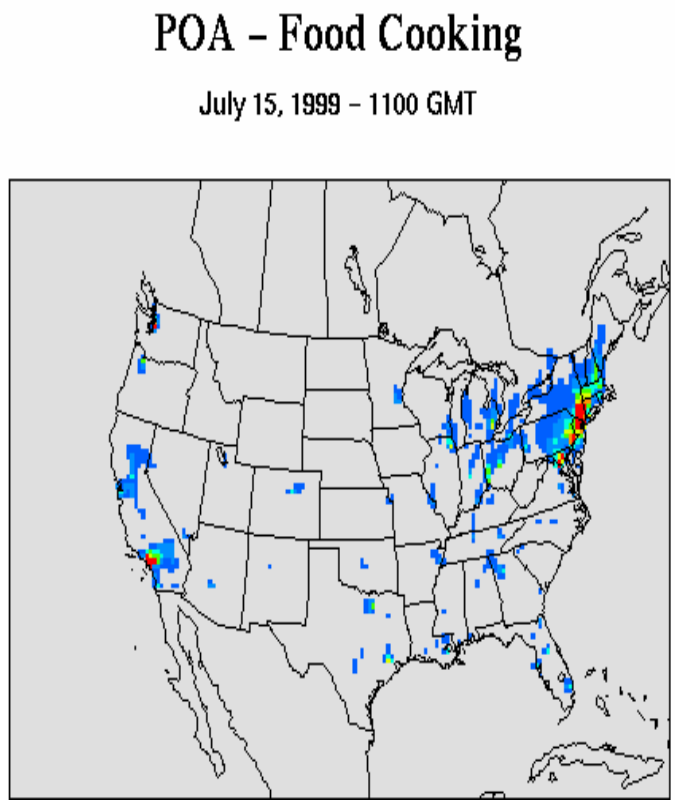
Source Apportionment

- Model Formulation
  - Construct source-segregated emission inventory for POA and EC
  - 9 source categories + 1 miscellaneous
  - Treat the contributions from different sources as different chemical species (e.g., POA_1 = diesel exhaust POA; POA_2 = gasoline exhaust POA; etc.)
  - Apply same equations to source-specific species (e.g., growth, coagulation, deposition)

Source Apportionment

- Model Results





Source Apportionment

- Model Evaluation
  - Speciate CMAQ output using emissions source profiles of individual organic compounds
  - Evaluate speciated CMAQ outputs against individual organic compound measurements
  - Compare source apportionment results with receptor-oriented model results
  - Identify and quantify inventory deficiencies

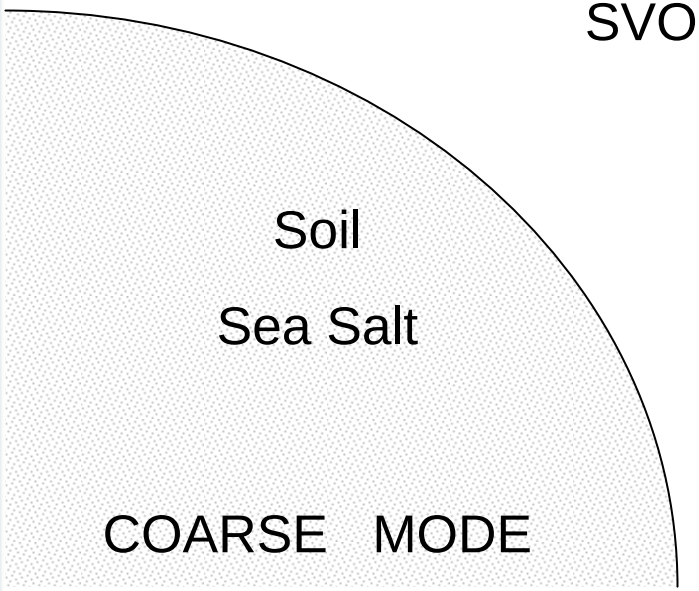
  - Organic compound measurements and receptor-oriented model results available at 8 sites in Southeast U.S., 1 month per season, April, July, August 1999, and January 2000.
  - Zheng et al. [*ES&T*, 2002]

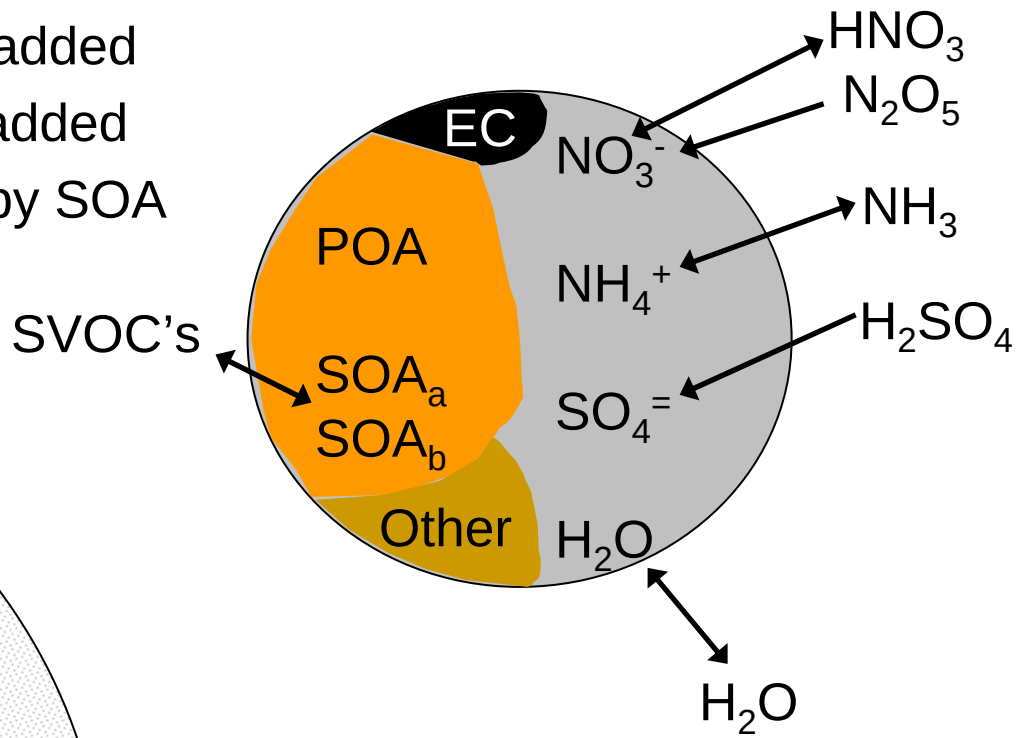
Future Plans (1-2yr): Coarse PM Chemistry

- Current release of CMAQ
  - Coarse mode interacts with neither gas-phase nor fine aerosol
- Future developments
  - Coarse mode coagulation to be added
  - Heterogeneous reactions of sea salt with HNO_3 to be added
  - Interactions of crustal material with HNO_3 and H_2SO_4 to be added
  - Sedimentation of coarse particles to be added

Future Plans (1-2yr): Aerosol Thermodynamics

- Current version assumes gas-finePM equilibrium
- Dynamic and/or hybrid approaches to be added
- Na^+ and Cl^- to be added
- Water absorption by SOA to be added



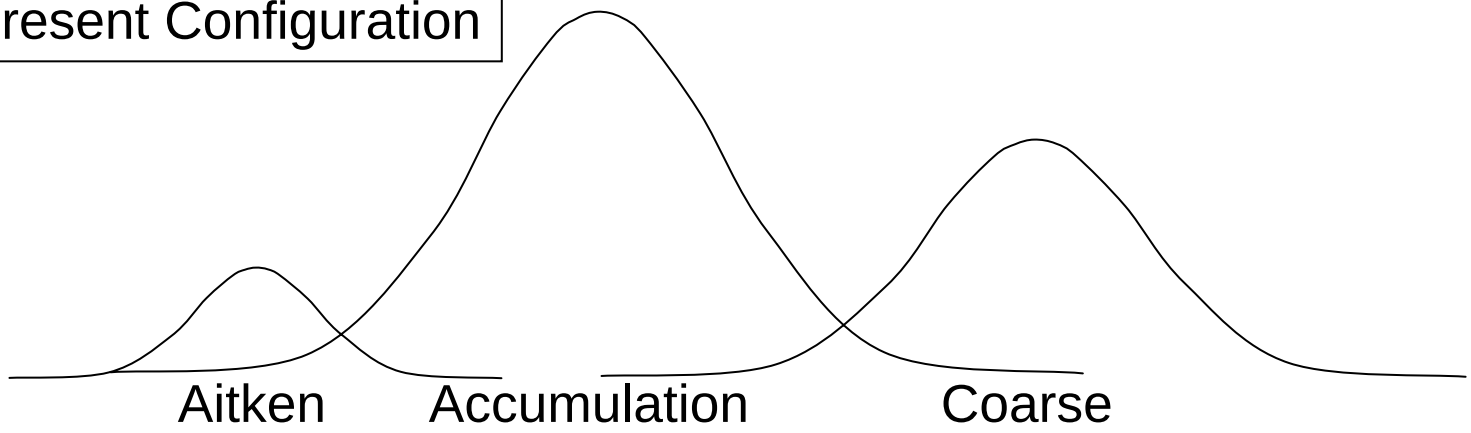


RESEARCH & DEVELOPMENT

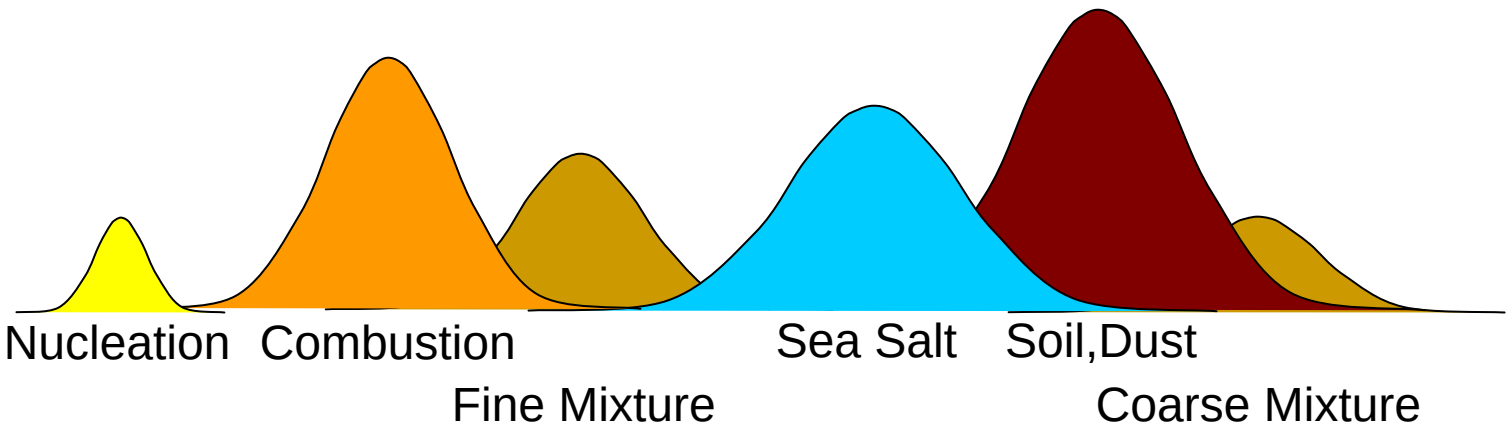
Building a scientific foundation for sound environmental decisions

Future Plans (3-5yr): Source-Oriented Multimodal Mixture

Present Configuration



Future Configuration



Summary

- SOA results match other models
  - Evaluating against state-of-science measurements
- Source apportionment of primary PM can be tracked in CMAQ model
  - Evaluating against organic speciation data and receptor-oriented model results

- Future Plans
  - Coarse PM Chemistry & Physics (1-2 yr)
  - Aerosol Thermodynamics (1-2 yr)
  - Source-Oriented Multimodal Mixture (3-5 yr)