CMAQ Aerosol Module

Current Research and Future Plans

Prakash V. Bhave*
Atmospheric Sciences Modeling Division
NOAA - Air Resources Laboratory
Research Triangle Park, NC

* On assignment to the National Exposure Research Laboratory, U.S. EPA.

CMAQ Model Peer Review Meeting
R.T.P., NC
December 17, 2003

Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.
Overview

• Current Research
  ▪ Secondary Organic Aerosols
  ▪ Source Apportionment

• Future Plans
  ▪ Coarse PM Chemistry & Physics
  ▪ Aerosol Thermodynamics
  ▪ Source-Oriented Multimodal Mixture
Secondary Organic Aerosols

Gas Phase

- ROG’s
- Oxidation
- SVOC’s

Aerosol Phase

- Cond. / Evap.
- Organic Material
- Inorganics, H₂O

Emissions

Organic Material
Secondary Organic Aerosols

• Chemical Species
  ▪ 6 ROG’s (5 anthropogenic, 1 biogenic)
  ▪ 10 SVOC products (8 anthro. & 2 bio.)
    • Temperature dependant saturation vapor pressure ($\Delta H = 156$ 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/m³
- Biogenic: 0 – 3.8 μg/m³
- 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
## Source Apportionment

<table>
<thead>
<tr>
<th>Receptor-Oriented</th>
<th>Source-Oriented</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Input Requirements</strong></td>
<td></td>
</tr>
<tr>
<td>• Atmospheric aerosol measurements</td>
<td></td>
</tr>
<tr>
<td>• Source profiles</td>
<td></td>
</tr>
<tr>
<td><strong>Output</strong></td>
<td></td>
</tr>
<tr>
<td>• Contribution of each source to atmospheric sample</td>
<td></td>
</tr>
<tr>
<td><strong>Input Requirements</strong></td>
<td></td>
</tr>
<tr>
<td>• Emission inventory</td>
<td></td>
</tr>
<tr>
<td>• Meteorology data</td>
<td></td>
</tr>
<tr>
<td>• Reaction mechanisms</td>
<td></td>
</tr>
<tr>
<td><strong>Output</strong></td>
<td></td>
</tr>
<tr>
<td>• Particle composition, size, concentration, and source</td>
<td></td>
</tr>
</tbody>
</table>
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., \( \text{POA}_1 = \text{diesel exhaust POA} \); \( \text{POA}_2 = \text{gasoline exhaust POA} \); etc.)
  ▪ Apply same equations to source-specific species (e.g., growth, coagulation, deposition)
Source Apportionment

- Model Results

**POA – Diesel Exhaust**
July 15, 1999 – 1100 GMT

**POA – Food Cooking**
July 15, 1999 – 1100 GMT
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 HNO₃ to be added
  - Interactions of crustal material with HNO₃ and H₂SO₄ 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
Future Plans (3-5yr): Source-Oriented Multimodal Mixture

Present Configuration

Future Configuration

Nucleation  Combustion  Sea Salt  Soil,Dust
Fine Mixture  Coarse Mixture
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)