Application of a volatility basis set model to secondary organic aerosol simulations across the U.S.

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Outline

• VBS mechanism

• WRF-CHEM evaluation for the eastern U.S., August-September, 2006

• DWH oil spill

• CalNex-2010 simulations – preliminary results
Volatility Basis Set (VBS)

Organic condensable vapors (OCVs)

Faster aging takes place in the gas phase, deposition of these vapors can be significant removal mechanism

\[ Caer_i = \frac{C_{tot,i}}{(1 + c_i^*/M)} \]
SOA yields – RACM mechanism

<table>
<thead>
<tr>
<th>VOC</th>
<th>High NO\textsubscript{x} conditions</th>
<th>Low NO\textsubscript{x} conditions</th>
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<tbody>
<tr>
<td></td>
<td>1</td>
<td>10</td>
</tr>
<tr>
<td>HC5</td>
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<td>HC8</td>
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<tr>
<td>XYL, CSL</td>
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</table>

Updates to Murphy and Pandis (2010)
WRF-CHEM sensitivity runs

- Anthropogenic OCV reaction rate with OH
- Biogenic OCV reaction rate with OH
- Deposition Velocity of OCVs
- Model Horizontal Resolution
- Planetary Boundary Layer Scheme

Optimum Values – Based on Evaluation Statistics

- Both Anthropogenic and Biogenic OCV age
- OCV - OH rx rate = 1. \(10^{-11}\) 1/cm³-s
- Deposition velocity of OCV = 0.25*(HNO3 deposition velocity)
- No additional SVOC or IVOC

Ahmadov et al., submitted
Near surface organic aerosol concentrations, daily averaged during 08/04–09/28, 2006

Ahmadov et al., submitted
## Observation data

<table>
<thead>
<tr>
<th>Network</th>
<th>OC, μgC/m$^3$</th>
<th>EC, μg/m$^3$</th>
<th>Number of sites meeting criteria</th>
<th>Number of valid points</th>
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<tbody>
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</table>
Comparison with the SEARCH data
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Mexican Gulf oil spill from DWH

- NOAA P3 aircraft’s 2 flights on 8th and 10th of June
- High concentrations (10-20 ppb) of aromatics C9-11 were detected
- 10-20 μg/m³ organic particles were observed too!

deGouw J. et al., Science (2011)
Comparison against the surface data: search network

Model shows good overall correlation with observations during June, 2010.

When model shows an impact from the DWH spill, there is a corresponding peak in the observations.

The magnitude and timing of the peaks are not always coincident.
CalNex-2010 domain, 20km resolution domain, topography

4km domain

Bakersfield

Caltech

Caltec
Vertical profile of OA over Caltech, May-16th (weekend)
Evaluation of the organic aerosol simulation, Caltech site, 14/05-15/06, 2010
Concluding remarks

• The new SOA scheme based on the VBS approach, the updated SOA yields and the aging mechanism substantially improves OA simulations by WRF-CHEM

• The new SOA scheme within the MADE module of WRF-CHEM is a computationally efficient and suitable tool for a wide range of air quality modeling applications

• More OA measurements across the U.S. with high spatiotemporal resolution is needed to better constrain the SOA models (e.g. drawback of daily concentrations)

• Additional measurements/variables for better evaluation are necessary: e.g. O:C ratios, PMF analysis, C14...