Plume Chemistry Modeling with SCICHEM and CMAQ: Cumberland Power Plant on 6 July 1999

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Motivation

• A need exists for single-source modeling that accurately simulates secondary PM$_{2.5}$ and ozone formation

• The SCICHEM reactive plume model could potentially play a role in single-source applications for secondary pollutants

• However, tools for processing SCICHEM inputs/outputs must be developed and predictions thoroughly evaluated

• This study is a preliminary evaluation of a “pre-release” version of SCICHEM using in-plume observations
  – Information presented here is considered preliminary by the U.S. EPA and is provided to describe and illustrate potential approaches
  – Results could change due to improvements in the modeling tools through our ongoing development work
SCICHEM: Second-order Closure Integrated puff model with CHEMistry

- Plume represented by numerous puffs that are advected and dispersed independently according to local meteorology
- Second-order closure for integrating turbulent diffusion equation
  - Dispersion rate is related to velocity fluctuation statistics
- Puff merging/splitting to represent inhomogeneous meteorology
  - Puffs split when grow to value related to grid resolution
  - Puffs merge when overlap is significant
- Simulates chemical processes in gas, aerosol, and aqueous phases
TVA Cumberland Power Plant

- Located ~80 km NW of Nashville
  - Lat: 36°23'29" N, Lon: 87°39'17" W
- Consumes ~20,000 tons of coal per day
- Two coal-fired generating units with summer net capability of 2,386 MW
- Observations available from helicopter plume transects in July 1999

Emissions (tons):

<table>
<thead>
<tr>
<th>Species</th>
<th>1999</th>
<th>2010</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO\textsubscript{x}</td>
<td>80,900</td>
<td>4,890</td>
</tr>
<tr>
<td>SO\textsubscript{2}</td>
<td>15,920</td>
<td>11,430</td>
</tr>
</tbody>
</table>

Source: http://www.tva.com/environment/air/cumb.htm

Source: Steven Greenwood (Feb 2004)
SCICHEM Modeling

- **SCICHEMv2.1 configuration**
  - Carbon Bond-IV gas-phase chemistry
  - MADRID aerosols w/ ISORROPIA inorganic thermodynamics
- **Period**
  - 1999 Nashville/Middle Tennessee Southern Oxidants Study
  - 6 July 1999 for hour 0-18 LST
- **Cases**
  1) **SCICHEM-WRF**
     - **Meteorology**: WRFv3.3 output converted to MEDOC format with MMIFv2.1
     - **Background concentration**: Time-varying based on CMAQ output
  2) **SCICHEM-DIAG**
     - **Meteorology**: Interpolated field based on observations from four stations provided in SCICHEM “pre-release” test-case files
     - **Background concentration**: Constant values from SCICHEM “pre-release” test-case files with \( O_3 = 60 \) ppb and \( SO_2 = 0.5 \) ppb
- **Emissions**
  - Hourly emissions of NO, NO\(_2\), SO\(_2\), etc. based on CEM data (see next slide)
CMAQ Modeling

- Community Multiscale Air Quality (CMAQ) model version 4.7.1
- 2001 National Emissions Inventory anthropogenic emissions
- 1999 hour-specific biogenic emissions estimated with BEIS model
- 1999 hour-specific CEM data for TVA Cumberland plant emissions
  - http://camddataandmaps.epa.gov/gdm/index.cfm?fuseaction=emissions.wizard

![Emissions for Cumberland Power Plant, 6 July 1999](image)

![Modeling Domains](image)
Comparison of Absolute Concentrations: CMAQ and SCICHEM-WRF

– Overlay SCICHEM-WRF predictions at receptor rings onto CMAQ spatial concentration fields
SO₂ Concentration: CMAQ and SCICHEM-WRF

Preliminary results; subject to change
NO$_x$ Concentration: CMAQ and SCICHEM-WRF

Preliminary results; subject to change
Comparison of Plume Concentrations: CMAQ, SCICHEM-WRF, SCICHEM-DIAG

- Estimate plume concentrations for CMAQ and SCICHEM by subtracting zero-out predictions from base-case predictions
- Overlay SCICHEM plume concentrations at receptor rings onto CMAQ plume-concentration fields
SO₂ Difference (Base - Zero out):
CMAQ, SCICHEM-WRF, SCICHEM-DIAG

Preliminary results; subject to change
NO$_x$ Difference (Base - Zero out):
CMAQ, SCICHEM-WRF, SCICHEM-DIAG

Preliminary results; subject to change
O₃ Difference (Base - Zero Out): CMAQ, SCICHEM-WRF, SCICHEM-DIAG

Ozone production: NO + O₃ → NO₂ + O

Preliminary results; subject to change
Surface Tracer Concentration:
SCICHEM-WRF and SCICHEM-DIAG

Preliminary results; subject to change
TVA Bell 205 Helicopter Observations

- 12 traverses of plume downwind of the TVA power plant on 6 July 1999 at an average altitude of 500 m
  - Clear day with light winds from west/northwest
- Observed species include $O_3$, NO, NO$_2$, and SO$_2$
SO₂ for Plume Transects on July 6th

Preliminary results; subject to change
NO$_x$ for Plume Transects on July 6$^{th}$
O₃ for Plume Transects on July 6ᵗʰ

Preliminary results; subject to change
Comparison of Centered Profiles: Observed, SCICHEM-WRF, SCICHEM-DIAG

- Find max/min in concentration along plume transect or receptor arc
- Center concentrations to max/min value
- Compare centered profiles for model and observations
SO$_2$ Centered Profiles
Observations, SCICHEM-WRF, SCICHEM-DIAG

6 July 1999 TVA Plume Transects: Sulfur Dioxide

Radius: 11 km

Radius: 31 km

Radius: 65 km

Preliminary results; subject to change
NO$_x$ Centered Profiles
Observations, SCICHEM-WRF, SCICHEM-DIAG

6 July 1999 TVA Plume Transects: NO$_x$

Preliminary results; subject to change
O$_3$ Centered Profiles
Observations, SCICHEM-WRF, SCICHEM-DIAG

Preliminary results; subject to change
Summary of Preliminary Work

- Preliminary tools were developed for using SCICHEM
  - Process model inputs/outputs
  - Compare SCICHEM results with CMAQ results and observations
- SCICHEMv2.1 and CMAQv4.7.1 simulations were conducted for 6 July 1999 TVA Cumberland Plant case
- Reasonable model behavior was observed, e.g.,
  - Elevated SO$_2$ and NO$_x$ concentration in plume
  - SO$_2$ and NO$_x$ concentration profiles broaden and have lower peaks in afternoon and further from source due to dilution
  - O$_3$ titration in NO$_x$-rich, VOC-poor plume; O$_3$ production far from source
  - SCICHEM and CMAQ predictions are qualitatively similar
Next Steps

• Explore the impact of different treatments of ambient background concentrations in SCICHEM
• Extend the study to consider NO\textsubscript{x} oxidation products (i.e., NO\textsubscript{z}), PM\textsubscript{2.5}, and vertical profiles
• Consider additional plume observation studies
• Compare with CMAQ-APT (Advanced Plume Treatment) when available
• Simulate longer periods and larger domains
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