Dynamic analysis: assessing CMAQ’s ability to capture air quality trends over a time period of changing emissions

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Air Pollution Accountability

- Seeks to quantify impacts of regulations on outcomes of interest
- Confounding variables obscure signal at each link
- Goal: Assess CMAQ’s ability to capture air quality changes over period of changing emissions

Henneman et al. (2016), JAWMA
Substantial emissions reductions in multiple species from mobile and EGU sources

Utility Emissions:
90% decrease in NO\textsubscript{X} & SO\textsubscript{2} in southeastern U.S.

EPA Air Markets Program Data (2016)

On-road Mobile Emissions:
60-90% decrease in multiple pollutants* in Atlanta, GA

*NO\textsubscript{X}, SO\textsubscript{2}, PM\textsubscript{2.5}, CO, VOC, EC, OC

Henneman et al. (in review)
CMAQ/SMOKE/WRF modeling system

Chemical Transport Model:
- Community Multiscale Air Quality Model with the Decoupled Direct Method (CMAQ-DDM, v5.0.2) and CB05tucl_ae6 mechanism

Emissions Model:
- Sparse Matrix Operator Kernel Emissions (SMOKE, v3.5.1) Modeling System
- 2002 & 2011 NEIs

Meteorology Model:
- Weather Research and Forecasting (WRF, v3.6.1) Model

Domain:
- Eastern US, 12km
- 201x162 horizontal grid
- 13 Vertical Layers
CMAQ/SMOKE/WRF modeling system

<table>
<thead>
<tr>
<th></th>
<th>Operational Evaluation</th>
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<tbody>
<tr>
<td></td>
<td>01E•01M</td>
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<tr>
<td>Emissions</td>
<td>2001</td>
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<td>Meteorology</td>
<td>2001</td>
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How well does CMAQ capture observed air quality changes?

What caused the air quality changes?

CMAQ-DDM/3D

1. Concentration
2. Sensitivity
CMAQ-modeled changes 2001 vs. 2011: Summertime $O_3$ decreases, Wintertime $O_3$ increases

Model Evaluation

<table>
<thead>
<tr>
<th>NMB</th>
<th>NME</th>
<th>MB</th>
<th>ME</th>
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<tbody>
<tr>
<td>18 ppb</td>
<td>16 ppb</td>
<td>14 ppb</td>
<td>12 ppb</td>
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<tr>
<td>10 ppb</td>
<td>8 ppb</td>
<td>6 ppb</td>
<td>4 ppb</td>
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<tr>
<td>-6 ppb</td>
<td>-10%</td>
<td>-20%</td>
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Ranges (typical) from Simon et al. (2012)

Evaluation based on AQS (EPA)
CMAQ-modeled changes 2001 vs. 2011: PM$_{2.5}$ decreases in summer and winter

Model Evaluation

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<th>NMB</th>
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<tbody>
<tr>
<td>70%</td>
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Ranges (typical) from Simon et al. (2012)

Evaluation based on AQS (EPA)
How well does CMAQ capture observed changes between 2001 and 2011?

Dynamic evaluation of PM$_{2.5}$ for Southeast: (AL, FL, GA, MS, NC, SC, TN)

<table>
<thead>
<tr>
<th></th>
<th>Observed</th>
<th>CMAQ</th>
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<tbody>
<tr>
<td>2001</td>
<td>13.9</td>
<td>10.7</td>
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<tr>
<td>2011</td>
<td>10.4</td>
<td>7.9</td>
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<tr>
<td>Difference</td>
<td>3.5</td>
<td>2.8</td>
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- CMAQ biased low in both years
- Slight under-prediction of change across years
- Negative bias in the summertime, positive in the winter
- Model performs similarly in 2001 and 2011
Which species contribute most to bias?

Mean Bias (MB) can help answer: 

$$MB = \frac{1}{N} \sum_{i=1}^{N} (C_m - C_o)$$

- **2001**
  - Main contributors for Jun-Aug (-): sulfate and OC
  - Main contributors for Dec-Feb (+): EC and OC

- **2011**
  - Main contributors for Jun-Aug (-): sulfate and OC
  - Main contributors for Dec-Feb (+): EC and OC
Aerosol pH conventional wisdom: decreased sulfate should lead to increased pH

\[ \text{SO}_2/\text{SO}_4^{2-} \quad \text{(driver of aerosol pH)} \]
\[ \text{NH}_3/\text{NH}_4^+ \quad \text{(neutralizer)} \]

- Conventional wisdom: aerosols are neutralized, pH should go up
- ISORROPIA used to calculate aerosol pH by using CMAQ modeled ion concentrations as inputs
Aerosol acidity: pH remains low across period of changing emissions

- CMAQ results consistent with observed changes in pH
- Nationwide, increases estimated at 0-5% yr\(^{-1}\)

Guan et al., in preparation
Dynamic evaluation: separating impacts of emissions and meteorology using CDFs

- Change in median ozone (5 ppb) attributable to emissions changes
- Meteorology effects on 95th percentile larger than emissions: implications on compliance

Emissions: \(11 \times 10^1 \) – \(01 \times 10^1\)
Meteorological: \(11 \times 10^{11} \) – \(11 \times 10^1\)

- Impacts of emissions changes increase at higher percentiles
Sensitivity: 1\textsuperscript{st}-order response of concentration to emission

\text{CMAQ-DDM/3D}

1. Concentration  
2. Sensitivity  
slope of the tangent line at \( E_A \)
Ozone sensitivities to EGU and on-road sources decrease

**EGU sensitivities**

- Sensitivities in both seasons trend to zero
- Summertime sensitivities around power plants remain important

**On-road sensitivities**

- Sensitivities in both seasons trend to zero
- Hot-spot remains in southeast
PM$_{2.5}$ sensitivities to EGU and on-road sources decrease

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<thead>
<tr>
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<th>2011</th>
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<td><strong>EGU sensitivities</strong></td>
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<td>January</td>
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- Sensitivities in both seasons decrease (larger change in winter)
- Ohio River Valley and point sources remain important

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- Sensitivities decrease across seasons
- In 2011, winter sensitivities larger than summer sensitivities
Meteorology has little effect on sensitivities

- Little change attributable to meteorology

**Ozone – On-road sensitivities**

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- Some differences in southeastern U.S.

**PM$_{2.5}$ – EGU sensitivities**

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Conclusions

• Operational Evaluation
  – CMAQ captures $O_3$ and PM$_{2.5}$ concentration changes, with different species dominating bias in different seasons
  – Sulfate and OC are the main contributors to bias in summer, and EC and OC in winter
  – Aerosols remain highly acidic, despite of significant reduction of SO$_2$ emissions
  – Sensitivity decreases from 2001 to 2011

• Dynamic Evaluation
  – Emissions drives concentration changes, though meteorology has larger effect on high $O_3$ days
  – Meteorology has little effect on sensitivity
  – Corroborates empirical evidence (Henneman et al., 2015)