On the Use of Model Evaluation Approaches to Investigate the Impact of Recent Emission Changes and Meteorological Variability on Tropospheric Ozone Concentrations in the Eastern U.S.

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Comprehensive Approach to Model Evaluation

Overview: Evaluation can be envisioned as a four-pronged activity, with overlap and interactions between each activity. The goal is to ensure the integrity of the modeling system from a scientific and policy perspective.

Model Evaluation Framework

- **Model-predicted concentration and deposition**
  - **Model Inputs**: meteorology and emissions
  - **Chemical transformation**: gas, aerosol, and aqueous phases
  - **Transport**: advection and diffusion
  - **Removal**: dry and wet deposition

- **Operational Evaluation**
  - How do the model predicted concentrations compare to observed concentration data?
  - What are the overall temporal or spatial prediction errors or biases?

- **Dynamic Evaluation**
  - Can the model capture changes related to meteorological events or variations?
  - Can the model capture changes related to emission reductions?

- **Diagnostic Evaluation**
  - Are model errors or biases caused by model inputs or by modeled processes?
  - Can we identify the specific modeled process(es) responsible?

- **Probabilistic Evaluation**
  - What is our confidence in the model-predicted values?
  - How do observed concentrations compare within an uncertainty range of model predictions?
Analysis Tool For Operational Evaluation

- Development of the Atmospheric Model Evaluation Tool (AMETv1.1)

- AMET is a comprehensive software package that is used to pair observations with gridded model data for meteorological and air quality related applications.

- AMET performs statistical calculations and creates a variety of output products to enable researchers to better understand and evaluate model predictions and improve the science within the models.

- AMET output includes tabular statistics, graphical representations of statistics, and spatial plots. AMET is built entirely on open-source software, and while currently set-up to work with MM5, WRF and CMAQ model data, the software could easily be extended to work with other models.

- Downloadable from www.cmascenter.org

The AMET Flow Chart

Observations
• Meteorological
• Air Quality

Model Output
• MM5/WRF (MET)
• CMAQ (AQ)

Model Evaluation Database
MySQL relational database stores all model-observation pairs in tables that can then accessed by the R scripts (and many other programs as well) for analysis.

Observation-Model Synchronization
Match observations with model predictions in time and space (Fortran)

Generate database records (Fortran)

Populate Database (Perl)

Other, User-developed tools
The MySQL database is a standard, widely used and easily connectable database that allows users to extract data using other software (Excel, Matlab, Perl, SAS, etc.)

R Scripts
Domain Statistics
Diurnal Statistics
Time Series Plots
Spatial Plots
Box Plots
Scatter Plots
Bar Plots
“Soccer Goal” Plots
“Bugle” Plots
Histograms
Time-Height Plots
Examples of AMET Evaluation Results for Ozone
(taken from Appel et al., 2011)
About Dynamic Evaluation:

- Characterizes a model’s ability to reproduce observed changes in air quality induced by changes in emissions and/or meteorology (i.e. comparisons of $\Delta C$ in relative or absolute terms over extended time periods in the observations and modeled values)

- Need for sufficient emission reductions to have a discernable signal on ambient concentration levels

- Initial study – assessment of model response to NO$_x$ SIP Call point source emission reductions and decline in mobile emissions on maximum 8-hour O$_3$ concentrations (summers 2002, 2004, 2005) (Gilliland et al., 2008; Atmos. Environ. paper)
## NO\textsubscript{x} Emissions in Modeling Domain

<table>
<thead>
<tr>
<th></th>
<th>EGUs</th>
<th>Mobile</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Eastern U.S. Emissions (12-km domain)</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Summer 2002</td>
<td>858</td>
<td>1423</td>
<td>3517</td>
</tr>
<tr>
<td>Summer 2004</td>
<td>507</td>
<td>1257</td>
<td>3000</td>
</tr>
<tr>
<td><strong>Summers 2004-2002 % Change</strong></td>
<td>-41%</td>
<td>-12%</td>
<td>-13%</td>
</tr>
<tr>
<td>Summer 2005</td>
<td>513</td>
<td>1172</td>
<td>2921</td>
</tr>
<tr>
<td><strong>Summers 2005-2002 % Change</strong></td>
<td>-40%</td>
<td>-18%</td>
<td>-17%</td>
</tr>
</tbody>
</table>
Example of major point source NOx emission reductions between 2002 and 2004 due to NOx SIP Call (based on CEMS data)
Vertical distribution of major point source NO$_X$ emissions and emission reduction aloft in the modeling domain

- Notable NO$_X$ emission reductions occurred at levels aloft from 2002 to 2004
MOBILE6 model on-road NOx emissions exhibited a steady decrease over this multi-summer period.

> Note: All surface NOx emissions and non-mobile (i.e., area, minor point, and nonroad sources) NOx emissions are for summer 2002 only.
CMAQ multi-year simulation details:

- CMAQ v4.7 with CB05 chemical mechanism

- Consistent annual simulations from 2002 - 2006
  > 36-km CONUS domain and nested 12-km Eastern U.S. domain (240 X 279)

- Meteorology – MM5v3.7.4 + MCIPv4.3 (MM5 34L → CMAQ 24L)
  > Pleim-Xiu LSM (Land surface module), ACM2
  > Four-dimensional data assimilation (FDDA); Analysis nudging
    3-hourly 3-D Objective Analysis (OA) fields (winds, T, and q)
    Base case method - nudging above PBL, surface nudging of winds

- SMOKEv2.2 - Emissions based on 2002 NEI
  > Year-specific updates to fires, MOBILE6 and EGU point (CEMS data) emissions

- GEOS-CHEM boundary conditions prescribed for 36-km CONUS domain
  > Based on 2002 GEOS-CHEM simulation
  > Vary monthly/spatially, but same set of monthly values used for each year
Temporal Behavior in Weekday Urban Surface NOₓ Concentrations

- Highest values exist in the 6-9 AM “rush” period in model and observations, so focus on change over this time period.
- Decrease exhibited in concentrations from summer 2002 to summer 2006

* 42 sites in EUS urban areas
Greater decline is evident in mobile (light gray) NO\textsubscript{X} emissions than in total (dark gray - all sectors) modeled emissions over this period (based on modeled and observed results at 42 major EUS urban sites. Bars represent inner quartiles (25\textsuperscript{th}-75\textsuperscript{th} percentiles), Whiskers extend from 10\textsuperscript{th}-90\textsuperscript{th} percentiles. Lines connect median values.
Percentage Change in Modeled (gray) and Observed (white) weekday morning NO$_X$ (6-9 AM) concentrations at urban sites

> Modeled NO$_X$ concentrations controlled by change in total emissions, so decline somewhat less than observed
Weekday morning median NO$_x$ concentrations under various ventilation (U x Zi) conditions for different summers

- Both model and observed concentration decrease with increasing ventilation (higher U and/or greater Zi) conditions.
- Both modeled and observed concentrations declined from 2002 to 2006 for all ventilation conditions.
CMAQ/CB05 Results for Summers 2002 and 2005:
A decline in ozone levels is evident across the region due to lower NO$_X$ emissions, but dynamic evaluation examines how modeled and observed changes compare.

Lower max 8-h O$_3$ in 2005, especially in areas where higher levels existed during 2002 (i.e., ORV, SE, and NE corridor)
Example CFDs* of Modeled and Observed Max 8-h O₃ Concentrations for summer 2002 and 2006

- Greater decreases often exhibited at the higher O₃ levels in both modeled and observed results

* Change assessed at values ≥ 95th percentiles of cumulative frequency distributions (CFDs)
Modeled and Observed Maximum 8-h $O_3$ Results*
over five summer (JJA) periods

- Substantial overlap between model and obs for most periods; model results generally track the observed changes and concentrations over this period
- Largest drop in summer 2004; significant meteorological effect (cooler / wetter period)

* Based on CASTNET sites
Change in obs somewhat greater than in model during daytime period between summer 2002 and 2006: associated with model underestimates of highest ozone levels during 2002 episodes.
Regarding Diagnostic Model Evaluation:

> Designed to probe a particular modeled process (i.e. chemical or physical processes) in order to gain a better understanding of the reasons for poor or good model agreement with observations.

> Need for process-oriented measurements to compare with modeled values, which are often not routinely available (ex; precursor & secondary species obs to examine O₃ chemistry, meteorological transport or deposition); process evaluation requires a variety of parameter obs often only available from special field studies).

> Important potential benefits to model performance from improvements in a modeled process representation.
Average Daily Maximum 8-h Ozone: Modeled and CASTNET results during 5 summer (JJA) periods

- Model captures day-to-day variation associated with the synoptic cycle (i.e. FDDA adjusts met model over the course of a 5-day simulation period)
Modeled and observed daily average maximum 8-hour ozone and 95th percentile concentrations from the rural CASTNET sites in the eastern US during summer 2002

Aug. 10-15 episode examined in more detail
Diurnal Cycle of the PBL

Boundary Layer Mixing Heights and The Residual Layer (after Stull, 1988)

- Photochemical \( \text{O}_3 \) production
- Nocturnal LLJ transport
- \( \text{O}_3 \) mixed down in AM
Evolution (build-up) of Modeled Ozone Along a Backtrajectory Path Spanning 3+ Episode Days

Release location and release height of 500 m near Albany, NY
Modeled and Observed Ozone Profiles at the Trajectory Release Time and Location (Aug 12 ; 17 UTC ; near Albany, NY )

Modeled < Observed $O_3$ within the PBL in this case
Ozone aloft ~ 60-70 ppb prior to PBL growth period

> Study underway to investigate cause(s) for underestimated O$_3$ aloft

* Summer 2002 experiment days
Mean Modeled and Observed (UMD aircraft) O₃ Profiles (Mid-afternoon period during Summer 2002)
Examine net ozone chemical production against observations from aircraft measurements

Net OPEs* from Different Afternoon Cases
(Results in mid-PBL from Summer 2002)

<table>
<thead>
<tr>
<th>Date</th>
<th>Observed</th>
<th>Model</th>
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<tbody>
<tr>
<td>July 12</td>
<td>7.1</td>
<td>6.5</td>
</tr>
<tr>
<td>July 13</td>
<td>6.2</td>
<td>6.0</td>
</tr>
<tr>
<td>July 14</td>
<td>3.4</td>
<td>4.3</td>
</tr>
<tr>
<td>July 16</td>
<td>8.1</td>
<td>6.4</td>
</tr>
<tr>
<td>July 17</td>
<td>7.4</td>
<td>7.2</td>
</tr>
<tr>
<td>July 21</td>
<td>6.6</td>
<td>4.9</td>
</tr>
<tr>
<td>July 22</td>
<td>6.4</td>
<td>5.4</td>
</tr>
</tbody>
</table>

* Ozone production efficiency (OPE) derived from slope of $O_3$ vs $NO_2$ relationship
Corr. Coefficients $\approx 0.98$
Chemical Age and Net Ozone Production Efficiency (OPE)
(July 2002 afternoons in mid-PBL)
(Based on all cases: BNL aircraft data and CMAQ Results)
Spatial distribution of CMAQ modeled and observed $O_3$ along an aircraft flight pattern during a summer afternoon.

Evidence of spatial displacements in modeled $O_3$ patterns?
Spatial displacement of modeled high O₃ aloft from locations of observed profiles

Modeled speeds < profiler winds during a nighttime hour

CMAQ (black) and observed (green) profiles of O₃ near Richmond, VA at mid-morning on June 11, 2002
CAP* Sites during Summer 2002

* Cooperative Agency Profiler

http://madis-data.noaa.gov/cap
Vertical time section of average wind speed difference over the entire summer period using all profiler sites

(model – observed)

Evidence that model base case underestimates speeds in nocturnal LLJ
Modeled and Profiler Wind Speeds
(August 11, 2002, 0400 CDT at ~ 450 m AGL)
In base case simulation:

- Modeled speeds < observed in LLJ and within residual layer
- Height of maximum speed of jet at lower level in model
- Modeled directions exhibit slight bias (more southerly)
- Very similar results found at other mid-Atlantic profiler sites
WRF model has replaced MM5 as the meteorological driver for CMAQ applications. WRFv3.0 model evaluation results exhibited as good or better performance than MM5 (Gilliam and Pleim; J. Appl. Met. & Clim., 2010). Effort underway with a series of sensitivity runs using WRF with different FDDA options and observational data sets to investigate impact on transport and whether improvements are possible, especially at night. Evaluation of modeled winds against independent data sets. Identify strategy for applying FDDA with 3-D OA fields, supplemented with available input measurements (i.e., NOAA/NPN and CAP Profilers, Doppler VAD, Rawinsonde data sets) which produces most accurate wind fields.

* Four dimensional data assimilation

Example wind speed field at a nocturnal hour from WRF.
Base case FDDA using coarse NAM (ETA) OA fields

Model Wind Fields (≈ 500 m) at 0800 UTC on August 11, 2002

No FDDA < 2 km
(i.e. below layer 13)

Model dynamics generated higher speeds in mid-ATL jet and elsewhere in the region
Preliminary Results from Selected Runs with Different FDDA Options and Input data

- Wind speeds in LLJ at FME are impacted by the FDDA option applied in the model run
Preliminary Results of Different WRF/FDDA Sensitivity Runs for Hourly Wind Speed and Wind Direction versus Profiler Winds at 450 m

Results with all available upper air data sets provided closest comparisons to independent profiler winds at this level.
In Summary:

Our efforts will continue to pursue a comprehensive evaluation framework which includes: operational / dynamic / diagnostic / probabilistic approaches to more thoroughly assess CMAQ model performance and to guide further scientific improvements in the CMAQ modeling system.