Using Dynamic Evaluation to Assess CMAQ Model Response Induced by Emissions Changes and Meteorological Variability

James Godowitch, Alice Gilliland, Robert Pinder, Kristen Foley, S.T. Rao

2009 AMAD Peer Review: Session 2
Model Evaluation: Establishing Model's Credibility

Environmental Issue

Ground-level ozone (O_3) continues to be a pervasive criteria pollutant with maximum 8-hour O_3 exceeding acceptable levels in the United States. Exposure to elevated ozone levels can strongly impact both human health and ecosystems. In an effort to reduce maximum O_3 levels, recent control programs have been implemented in a concerted effort to reduce emissions of nitrogen oxides (NO_X), the key precursor species involved in photo-chemical ozone production. Air quality management decisions rely in part upon air quality grid model simulation results from proposed emission reduction scenarios to demonstrate attainment of the federal O_3 standard. Model performance evaluations, generally conducted during regulatory applications, that compare predicted concentrations to measurements for a base case period do not establish that a model will respond correctly to emissions changes. An air quality model's ability to accurately capture changes in concentrations related to emission changes is crucial for the development of meaningful and cost-effective control strategies. AMAD has conducted model evaluation research to advance the development and application of innovative evaluation methods to better understand the strengths and weaknesses of the Community Multiscale Air Quality (CMAQ) model and to increase its scientific credibility. Selected results from the dynamic evaluation approach are presented to demonstrate how well CMAQ produces changes in air quality.

Research Objectives

Design and conduct a modeling study and an evaluation effort of a regional air quality model using the CMAQ modeling system to;

- Investigate magnitudes and changes in NO_X emissions due to control programs for selection of modeling periods
- Assess the model's ability to simulate changes in observed daily maximum 8-h O_3 from real-world NO_X emission reductions and meteorological variability
- Investigate model response for different chemical mechanisms
- Identify model inputs/ processes needing improvement

Modeling Approach

The retrospective period for the initial application of dynamic evaluation involved selected summer seasons between 2002 and 2005 spanning the EPA's NO_X SIP Call program implementation from 2003 through May 2004. The key modeling scenarios in Table 1 were designed to investigate model response to changing emissions and / or meteorological differences for the summer periods of 2002 (pre-NO_X SIP Call period) and the summers of 2004 and 2005 (post-NO_X SIP Call periods). The dynamic evaluation compared observed ozone changes against modeled changes generated from scenarios M02E02, M04E04, and M05E05.

Table 1. Matrix of modeling scenarios

	Summer (J-J-A) Meteorology		
Emissions	**2002**	**2004**	**2005**
2002	**M02E02**[abc]	M04E02[a]	------
2004	M02E04[a]	**M04E04**[ab]	-------
2005	------	------	**M05E05**[abc]

Chemical mechanisms: a - CB4, b - SAPRC99, c - CB05 used NEI 2002 and 2005 county-specific control program information and NMIM model to apply MOBILE6; simulations for a,b applied a reference county and NEI 2001 (adjusted) emissions

Results and Discussion

- Large point source NO_X emission reductions (≈-40%) occurred due to the NO_X SIP Call program and a gradual decline in mobile source emissions (≈ -17 to -20%) occurred from 2002 to 2005

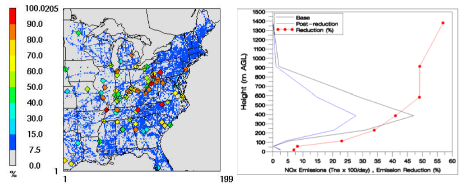
Table 2. NO_X emissions budgets for summer periods

Projections from 2001 National Emission Inventory (NEI)	NO_X Emissions (ktons) EGUs	Non-EGUs	Mobile	Non-road	Total*
Summer 2002	858	466	1423	770	3517
Summer 2004	507	466	1257	770	3000
Difference (2004-2002)	-41%		-12%		-15%
Summer 2005	513	466	1172	770	2921
Difference (2005-2002)	-40%		-18%		-17%
2002 and 2005 NEI					
Summer 2002 NEI	853	373	1148	734	3108
Summer 2005 NEI	493	370	911	722	2496
Difference (2005-2002)	-42%		-21%		-20%

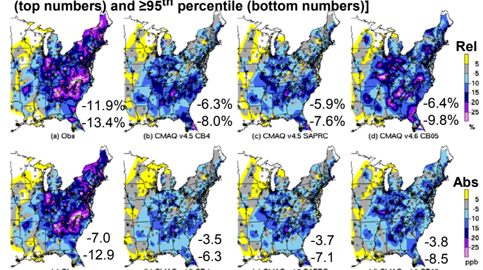
* These sums only include the major emission sectors listed above. Other sectors that are less than 5% of the total emissions are included in the emission inputs to CMAQ but not in this table.

Spatial (horizontal) and vertical changes in NO_X emissions:

- Substantial emission reductions occurred aloft at major power plants in the Ohio River Valley and at isolated point sources across the region causing less NO_X transport downwind especially during the nocturnal period when the elevated plumes.
- Mobile emissions exhibit decreases in urban areas and along roadways causing a gradual decline in surface NO_X concentrations.



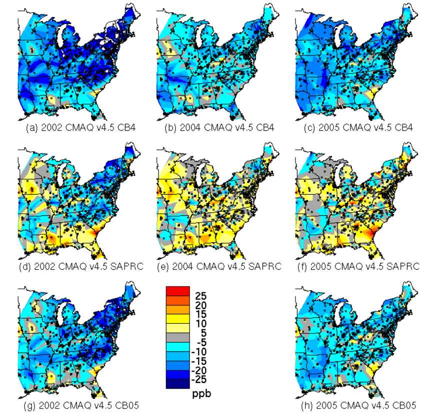
Spatial patterns of observed and modeled relative (Rel, %) change and absolute (Abs, ppb) change in maximum 8-h O_3 at ≥95th percentile: (2005-2002) [Average values shown are at the median (top numbers) and ≥95th percentile (bottom numbers)]



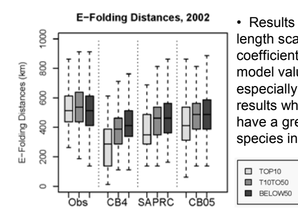
- Declines in maximum O_3 occurred over large portions of the region and were spatially variable between these summer periods exhibiting similar meteorological conditions. Similar patterns with greater declines from 2002-2004 due to cooler/wetter conditions in 2004.
- Differences existed among the chemical mechanisms with the CB05 results closest to observations in the comparison of relative changes
- Most noticeable underestimates in model response were found in the northeastern states
- Observed and modeled values had greater change at ≥95th percentile with complete statistical results given in Gilliland et al. (2008)

Analysis investigating model underestimates of change:

Spatial differences between observations and modeled results for the maximum 8-h O_3 at ≥95th%ile;

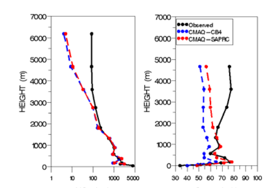


- Although CB4 exhibited a large negative bias (underestimation) during summer 2002, results with SAPRC and CB05 also show underestimates, which strongly contributed to the dampening of the O_3 reduction signal in the comparisons with the post-control summer periods.
- Model underestimates existed during the warmer summers (2002, 2005) with all chemical mechanisms. Less bias was exhibited in the SAPRC results during summers 2004 and 2005, although SAPRC results also displayed notable underestimates along with CB4, CB05 in the northeastern states during summer 2002.



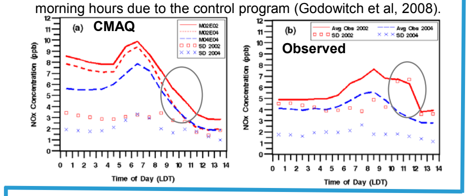
- Results from e-folding distances (a length scale where correlation coefficients drop to 0.37) indicate model values with shorter distances, especially with CB4, than observed results which implies nearby sources have a greater effect than transported species in model results.

Total low-level NO_X emissions grouped by magnitude (highest to lowest emissions)



- Vertical profiles show model results underestimated NO_X and O_3 above about 2 km based on aircraft flights from 2004 experimental studies, although O_3 below 2 km was also underestimated by CB4.

- **Evidence of NO_X concentration change due to NO_X SIP Call**: Notable decreases in surface concentrations between 2002-2004 in both observations (at a western PA site just downwind of the Ohio River Valley) and modeled results with point source NO_X reductions (M02E04 scenario) provide evidence of lower NO_X concentrations in elevated plumes entrained downward at mid-morning hours due to the control program (Godowitch et al, 2008).



Conclusions

- NO_X SIP Call was a unique case study for dynamic evaluation
- Both modeled and observed results showed decreases in maximum 8-h O_3 with greater changes at ≥95th percentile; model underestimated the observed O_3 change between 2002 and two different summers after the NO_X SIP Call emission reductions
- SAPRC mechanism better simulated O_3 changes associated with meteorology differences (2004-2002) than CB4
- CMAQ v4.6 with the CB05 mechanism using recent emission inventories with updated mobile source estimates, showed slight improvements in the modeled O_3 response (2005-2002)
- Spatial correlation analysis (e-folding distances) and measurements aloft suggest model underestimation of the contribution of transported O_3 and precursors, and identify the need for improving photochemical mechanisms

Future Directions

Upcoming research includes:

- Apply dynamic evaluation with results from revised configuration of the current CMAQ (v4.7) model
- Investigate dynamic change during morning rush hour in modeled and observed NO_X concentrations to infer MOBILE6 capability to capture change in mobile emissions signal.
- Apply diagnostic analyses of modeled and observed vertical concentration/wind profiles to assess transport and vertical mixing processes

Impact

- Key findings have been included in the EPA Clean Air Markets Division NO_X budget trading reports available publicly on-line
- Feedback to CMAQ development team impacted selection of chemical mechanisms in the public release of modeling system
- Recognition by the international air quality modeling community of the value and challenges of the dynamic evaluation approach as an essential component of comprehensive model evaluation based on presentations at international conferences and from publications in international journals

Contributors/Collaborators

Christian Hogrefe (SUNY-A/ASRC), Edith Gego, P. Steven Porter (U. Idaho)