P163 Assessing Multi-year Changes in Modeled and Observed Maximum 8-hour Ozone With a Dynamic Evaluation Approach

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1. INTRODUCTION

Model evaluation results provide valuable quantitative information to help guide research efforts for model improvement and to establish a model's credibility for particular regulatory applications. To advance model evaluation, an evaluation framework composed of four approaches has been designed to promote comprehensive model evaluation (Dennis et al., 2010). One of the emerging new approaches is referred to as dynamic evaluation. As part of dynamic evaluation, air quality model's pollutant response to changes in emissions and/or meteorology is assessed against changes found in observed concentrations.

Dynamic evaluation requires historical case study periods when a sufficient emissions change or meteorological variability has occurred that could be confidently determined to have had an impact on observed air quality. In this study, a dynamic evaluation effort was undertaken with the Community Multiscale Air Quality (CMAQ) model to assess it's ability to reproduce changes in maximum 8-hour ozone (O_3) concentrations in the eastern United States over five consecutive summer periods (2002-2006) during which substantial NO_X emission reductions took place (USEPA, 2005). The results presented herein focus on relative (%) changes in modeled concentrations against observed changes at CASTNet (Clean Air Status and Trends Network) measurement sites over this multi-year period.

2. STUDY DESCRIPTION

2.1 Modeling Details and Simulations

The CMAQv4.7 chemical transport model using the CB05 (Carbon Bond 2005) chemical mechanism (Byun and Schere, 2006) was applied in this study. The various process modules employed in the model configuration are described in Appel et al. (2009). A large regional modeling domain that encompassed the eastern two-thirds of the US and southern Canada was designed with a 12-km horizontal grid cell size. The vertical structure contained 24 layers and the thickness of layer 1 was ≈40 m. Boundary concentrations were provided by CMAQ simulation results from a continental (36-km grid cell size) domain. Although annual simulations were performed, model results from June 1 through August 31 period were analyzed in this study for 2002 to 2006.

Meteorological fields were generated by the Penn State/NCAR fifth generation mesoscale model (MM5; Grell et al., 1994). The MM5 v3.6.3 was applied in a non-hydrostatic mode and included the FDDA (four-dimensional data assimilation) technique using available observed winds, temperature, and moisture analysis fields, which has been shown to provide more accurate 3-D modeled fields for air quality simulations (Otte, 2008). The MCIP (Meteorology-Chemistry Interface Processor) program was exercised to create compatible input data files of hourly meteorological fields to drive CMAQ.

Emissions data sets were developed by the Sparse Matrix Operator Kernel Emissions (SMOKEv2.2) processing system. Anthropogenic emissions from the US EPA NEI (National Emissions Inventory) 2002 and 2005 data bases were used to generate surface area and minor point source emissions. Emissions for other years were projected based on these NEI datasets. For many major elevated point sources, the Continuous Emissions Monitoring Systems (CEMS) hourly pollutant emissions measurements were utilized and plume rise was performed on-line in CMAQ to specify these emission rates within the proper model layers. The MOBILE6 model was applied to develop hourly gridded on-road vehicle emissions using VMT and fleet emission factors along with county-specific control program information. BEISv3.14 was applied to compute biogenic emissions of NO_X, isoprene and other natural VOC species.

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2.2 Observations

Ozone measurements from the summer periods spanning June 1 to August 31 during 2002-2006 were extracted from the CASTNet (http://www.epa.gov/castnet) on-line data sets. The maximum daily 8-hour (MDA8) O_3 concentration was computed from hourly data at each site. Specifically, the MDA8 value for each day was determined by selecting the maximum value from forward running 8-h average O_3 concentrations calculated for each hour at each site. This procedure was also applied to determine the modeled MDA8 values from CMAQ hourly O_3 concentrations in the grid cell where each monitoring site was located.

3. ANALYSES AND RESULTS

The O_3 metric adopted for analysis was the average MDA8 concentration computed from values equal to and above the 95th percentile (hereafter referred to as ≥95th%ile) of the cumulative frequency distribution (CFD) composed of observed and model results from the 92 days of each 3-month period. It represents the upper part of the CFD and is similar to the regularity metric of the O_3 design value. It was also utilized by Gilliland et al. (2008) in the prototype dynamic evaluation application. The relative (%) changes in the observations and model results were computed from $(C_{YY}–C_{02})$ x 100. / C_{02} where C_{02} serves as the summer 2002 reference MDA8 (≥95th%ile) values and C_{YY} represents values determined from successive summer periods.

The modeled and observed results of the MDA8 (≥95th%ile) O_3 from summer 2002 and 2006 are displayed in Figure 1 to demonstrate the impact of large decreases in NO_X emissions spanning these years on ambient ozone levels. On-road mobile and major elevated point source emissions had decreased by nearly 25% and 40%, respectively, over this period. The substantial major point source NO_X emission reductions occurred during 2003-04 in conjunction with the EPA's NO_X SIP Call program (Godowitch et al., 2008), while the estimated decline in on-road NO_X emissions has been more gradual at nearly 6% per year. Relatively similar weather conditions conducive to ozone formation occurred during

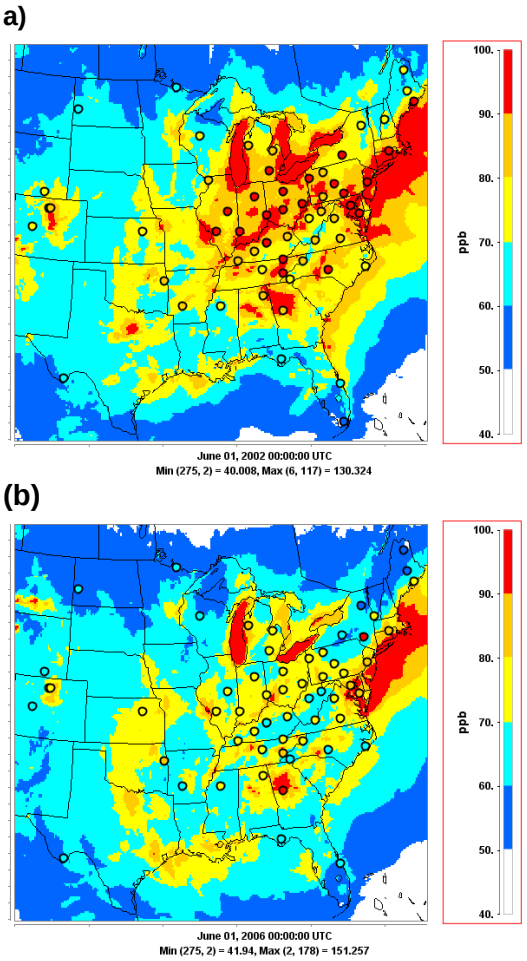

Figure 1. Mean MDA8 O_3 (≥95th%ile) concentrations from CMAQ model results and CASTNet site values from (a) summer 2002 and (b) summer 2006.

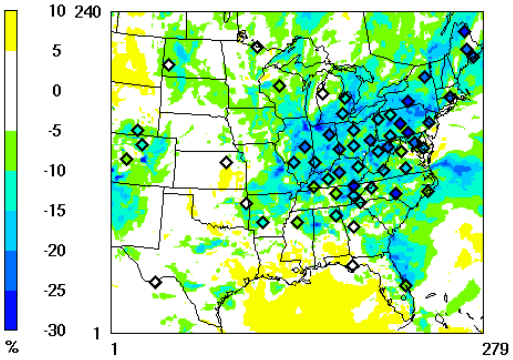

Figure 2. Modeled and observed change (%) in MDA8 O_3 (≥95th%ile) between the summers of 2002 and 2006 [$(C_{06}–C_{02})$ x $100/C_{02}$].

the 2002 and 2006 summer periods. Summer 2002 was an active ozone season with several notable multiple day episodes exhibiting high O_3 levels. High values are evident in the CMAQ results and at CASTNet sites over a large portion of the eastern US (Figure 1a). However, the model underestimated the observed values during this particular summer period. Results from summer 2006 (Figure 1b) are noticeably lower than summer 2002 in most of the eastern US, reflecting the impact of the NO_X emissions reductions. Modeled values appear to be generally closer to observed values at the CASTNet sites.

Figure 2 displays the relative differences between Figures 1a and 1b in the form of the percentage change in the MDA8 (≥95th%ile) concentrations between these two summer periods. Despite considerable spatial variability across the domain, notable decreases in MDA8 O_3 are evident in the Ohio River Valley region as well as portions of the mid-Atlantic and northeast. There is generally good spatial agreement between the modeled and observed change, however, the magnitudes of the decreases in observed changes appear to be somewhat more negative than those in the model's gridded results between these two summer periods.

The percentage changes in MDA8 O_3 (≥95th%ile) concentrations for each summer period relative to summer 2002 results were also computed from the site observations and modeled values at the 47 CASTNet locations in the eastern portion of the modeling domain. Figure 3 reveals that overall decreases in both modeled and observed MDA8 (≥95th%ile) O_3 occurred in each summer period after 2002. The more pronounced drop in ozone levels during summer 2004 is attributed to the cooler, wet weather conditions which were unfavorable to ozone formation that predominated during this period across most of the eastern US. Figure 3 also indicates that the modeled results closely tracked the variation in observed changes from summer-to-summer, however, the model changes somewhat underestimated the magnitudes of observed changes. Comparable results were reported by Gilliland et al. (2008) between selected sets of summer periods. Nevertheless, when summer 2002 results are excluded, Figure 3 reveals both the model and observed changes display an increasing downward trend in MDA8 (≥95th%ile) O_3 levels over this period.

As was evident from Figure 1a, the model generally underestimated the high MDA8 O_3 levels in summer 2002, which certainly contributed to the smaller changes obtained in the model results. The model underestimate of ozone levels in summer 2002 is also evident in Figure 4, which shows the observed and modeled MDA8 (≥95th%ile) O_3 concentrations from each summer period. These box/whisker

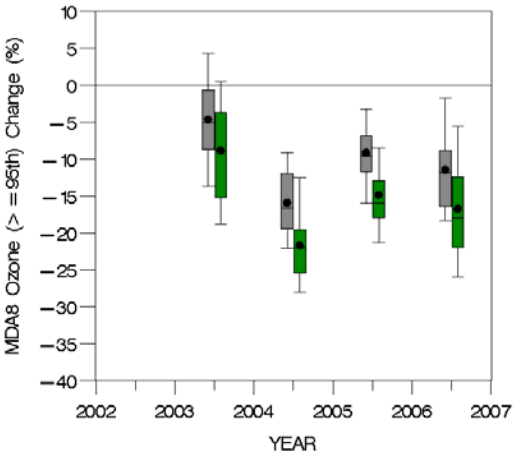

Figure 3. Box/whisker plot of percentage change in the MDA8 O_3 (≥95th%ile) concentration for each summer period with summer 2002 as a reference from observed (green) and modeled (gray) values at CASTNet sites. Boxes span from 25th - 75th percentiles. Whiskers extend to 10th/ 90th percentiles of the CFD. Solid circles are mean values and a horizontal line inside each box represents the median.

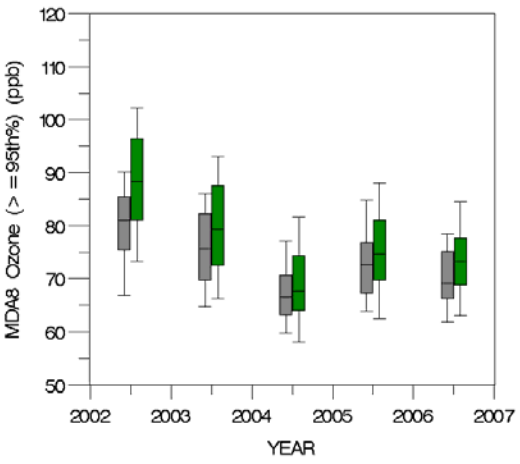

Figure 4. Box/whisker plot of modeled (gray) and observed (green) MDA8 O_3 (≥95th%ile) concentrations from each summer period at CASTNet sites.

results indicate that considerable overlap exists between modeled results and observed values. However, modeled median values tend to be slightly lower than observed medians during most summer periods. Additionally, it is also apparent that greater variability exists in the observed results owing to the greater spread of the 10/90% whiskers than in the model results.

4. SUMMARY

A dynamic evaluation of the CMAQ chemical transport model was conducted to investigate it's ability to reproduce multi-year changes in maximum 8-h O_3 that are attributable to notable declines in surface and elevated NO_X emissions and variations in meteorological conditions over 5-consecutive summer periods from 2002 to 2006. At maximum 8-h ozone levels (≥95th%ile), model results exhibited good spatial agreement with the ozone change in the region and it also demonstrated the capability to track the summer-to-summer differences in the observed change of maximum 8-h O_3 at the CASTNet monitoring sites. However, the modeled change was found to be somewhat less than observed change, which is partially attributed to the model underestimation of the high ozone levels during the summer 2002 reference period. Modeled maximum 8-h O_3 (≥95th%ile) concentrations were lower than observed values and exhibited less variability during each summer period. Further analysis is underway in an attempt to identify the inputs and/or various processes contributing to the model bias at the highest concentration levels.

DISCLAIMER

Although this work was reviewed by the US Environmental Protection Agency and approved for publication, it may not necessarily reflect official Agency policy.

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