P653   Using Dynamic Evaluation to Assess Changes in Modeled and Observed Maximum 8-hour Ozone Concentrations in Response to NO$_X$ Emission Reductions

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1. INTRODUCTION

An emerging innovative model evaluation approach is referred to as dynamic evaluation. The focus of dynamic evaluation is to investigate an air quality model's predicted change in concentration due to changes in emissions and/or meteorological parameters, which are key inputs to a photochemical grid model.   Therefore, changes in modeled concentrations are compared to changes in observations. In order to undertake a dynamic evaluation study, historical case study periods are required that exhibit sufficient emissions change or meteorological variability that could have a detectable impact on observed air quality. In this study, a dynamic evaluation study was undertaken with the Community Multiscale Air Quality (CMAQ) modeling system to assess its ability to reproduce changes in maximum 8-hour ozone (O$_3$) concentrations with emphasis on the eastern United States. The summer periods of 2002 and 2006 were selected because substantial NO$_X$ emission reductions had taken place between these particular years due to controls associated with the NO$_X$ State Implementation Plan (SIP) Call Rule program (USEPA, 2005). The selected results of analyses presented herein focus on an investigation of the relative (%) changes in maximum 8-h O$_3$ between summer periods in 2002 and 2006 from model simulations and in the rural-based CASTNET (Clean Air Status and Trends Network) measurements.

2. STUDY DESCRIPTION

2.1 Modeling Details and Simulations

The current CMAQv5.0 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

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are described in Appel et al. (2009). A modeling domain encompassing the entire continental US, southern Canada and portions of Mexico was applied with a 12 x 12 km horizontal grid cell size. The vertical structure contained 35 layers and the thickness of layer 1 was close to 20 m. The same boundary conditions from a GEOS-Chem global model simulation of 2006 were supplied for both periods. Model simulations were performed for the 3-month period spanning June 1 through August 31 in both 2002 and 2006 for this study with a 10-day spin-up period prior to June 1 of each period to eliminate the influence of initial conditions.

Meteorological fields were generated by the Weather Research & Forecast (WRFv3.3) model. The WRF simulations included an updated FDDA (four-dimensional data assimilation) technique using all available observed winds, temperature, and moisture analysis fields, which has been shown to provide more accurate 3-D modeled wind fields (Gilliam et al., 2012). The MCIP (Meteorology-Chemistry Interface Processor) program was exercised to create compatible input data files of hourly meteorological fields to drive CMAQ.

Emission data sets were developed by the Sparse Matrix Operator Kernel Emissions (SMOKEv3.1) processing system. Anthropogenic emissions from the US EPA NEI (National Emissions Inventory) 2002 and 2005 data bases were used to generate gridded surface emissions of various sectors. For major elevated point sources, the Continuous Emissions Monitoring Systems (CEMS) hourly pollutant emission measurements were utilized and plume rise was performed on-line within 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 vehicle miles traveled (VMT) and fleet emission factors along with county-specific control program information. BEISv3.14 was used to compute biogenic emissions of NO$_X$, isoprene, and other naturally emitted VOC species.   NO$_X$ generated by lightning was also included in model simulations.

2.2 Observations

Ozone measurements from the summer periods spanning June 1 to August 31 for 2002 and 2006 were extracted from the CASTNET (www.epa.gov/castnet) data sets available on-line. The maximum daily average 8-hour (MDA8) O_3 concentration was determined from hourly data at each site. Specifically, the MDA8 value for each day was obtained by selecting the maximum value from the 8-h running average O_3 concentrations calculated starting at each hour for each site. This procedure was also applied to determine the modeled MDA8 values from CMAQ hourly O_3 concentrations from the grid cells where each monitoring site was located. In addition, the observed and modeled MDA8 values were not necessarily selected from the same 8 hour interval of each day.

3. ANALYSES AND RESULTS

The composite cumulative distribution functions (CDFs) of observed and modeled MDA8 O_3 values over all days from all CASTNET site locations are shown in Figure 1a and 1b, respectively. The observed and modeled distributions of MDA8 O_3 exhibit the familiar S-shape with considerable curvature at the lower and upper tails. A notable result is a distinctive shift toward lower MDA8 O_3 values from 2002 to 2006 over a rather broad portion of the observed and modeled distributions. At the median (50th percentile), the decrease from 2002 to 2006 in the both observed and modeled results is quite comparable. However, there appears to be greater decreases (i.e. more change) at higher MDA8 O_3 concentrations from 2002 to 2006 in the observed results than exists in the upper portions of the modeled distributions. Similar features were found in the observed and model CDFs for individual sites and the extent of O_3 change was site-specific, which will be explored further herein.

An O_3 metric adopted for analysis of concentration changes was the MDA8 concentration obtained by averaging values equal to and above the 95th percentile (hereafter referred to as ≥95th percentile) of the CDF. This MDA8 ozone value derived from the upper five percentiles of the CDF is similar to the regulatory metric of the O_3 design value.

The MDA8 (≥95th percentile) was also utilized by Gilliland et al. (2008) in their prototype
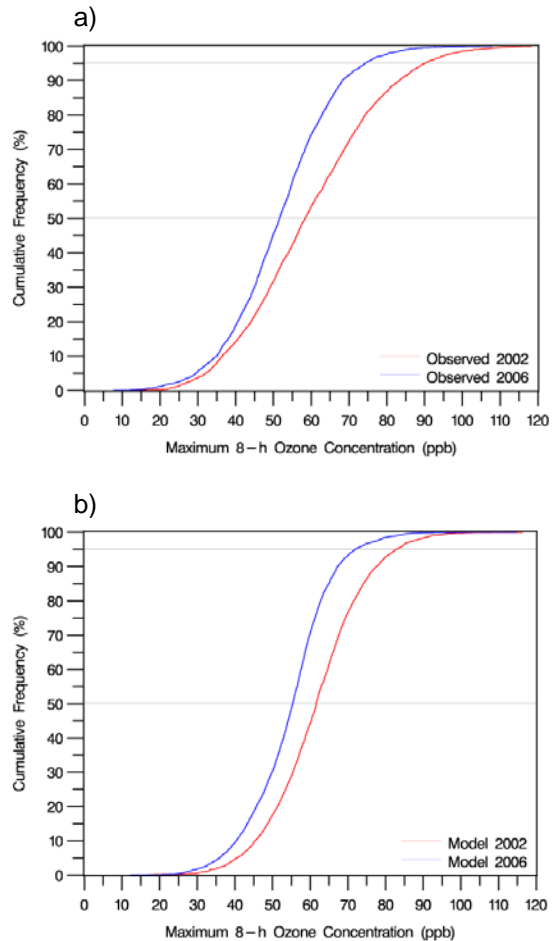

Figure 1. Cumulative distribution functions of MDA8 O_3 values from summer 2002 and 2006 periods from a) CASTNET sites and b) modeled results.

dynamic evaluation effort.

The modeled and observed results of the MDA8 (≥95th percentile) O_3 from summer 2002 and 2006 are displayed in Figure 2 to demonstrate the impact of NO_X emission reductions occurring between these years on ambient ozone levels. In particular, major elevated point source emissions had decreased by about 40% during 2003-04 in conjunction with the EPA's NO_X SIP Call program (Godowitch et al., 2008). The estimated decline in on-road NO_X emissions from the MOBILE6 model was more gradual at about 6% per year during this period. Very similar meteorological conditions conducive to ozone formation occurred during the summer 2002 and 2006 months. Summer 2002 was a particularly active ozone season with several notable multi-day episodes exhibiting high O_3

levels. During summer 2002, high MDA8 O_3 concentrations are evident in the CMAQ results and at CASTNET sites along the northeast urban corridor, mid-Atlantic states, and Ohio River Valley region (Figure 2a). It is also apparent that the model tended to underestimate several observed CASTNET site values during this particular summer period. Results from summer 2006 (Figure 2b) are noticeably lower than summer 2002 in most of the eastern US, reflecting the impact of the NO_X emission reductions on the MDA8 ozone concentrations. Additionally, modeled values exhibit much better agreement at the CASTNET sites during the 2006 period.

Relative changes in percentage terms for the observations and model results were computed from $(C_{06}–C_{02})$ x 100. / C_{02} where C_{02} and C_{06} represent MDA8 O_3 (≥95th percentile) values for summer 2002 and 2006, respectively. Figure 3 displays the relative differences between results in Figures 2a and 2b in the form of the percentage change in the MDA8 (≥95th percentile) concentrations between these two summer periods. Although there is considerable spatial variability, 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 in the MDA8 O_3 metric, however, the percentage decreases in observed values at many of the CASTNET rural locations appear to be more negative than those in the model's gridded results between these two summer periods.

A closer examination of the model and observed changes at the CASTNET sites is displayed in Figure 4 for the median (50th percentile) and ≥95th percentile MDA8 concentration levels. The spread in the box/whisker results reveals the variations across the measurement network spanning the eastern US. Although the model results show declines in MDA8 O_3 that agree rather closely with observed changes at the median MDA8 level (Fig. 4b), modeled changes in the ≥95th percentile values exhibit less overlap with the observed results and are less negative in the model results at this upper level, as anticipated from the percentage changes displayed in Figure 3. Nevertheless, Figure 4 also indicates that more decrease in MDA8 O_3 occurred at the ≥95th percentile than at the median value in both modeled and observed results.

a)

b)

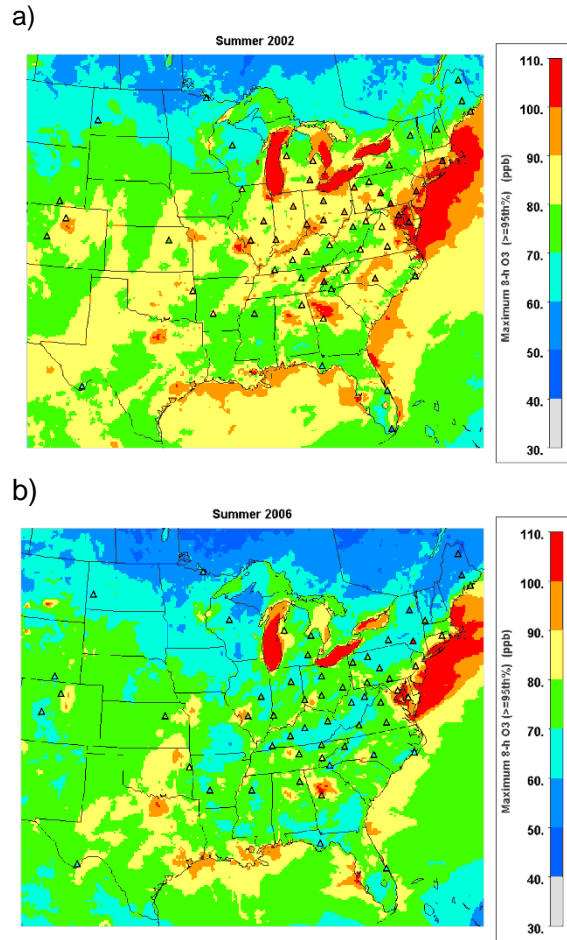Figure 2. MDA8 O_3 (≥95th percentile) concentrations from CMAQ and from CASTNET sites from summer (a) 2002 and (b) 2006.

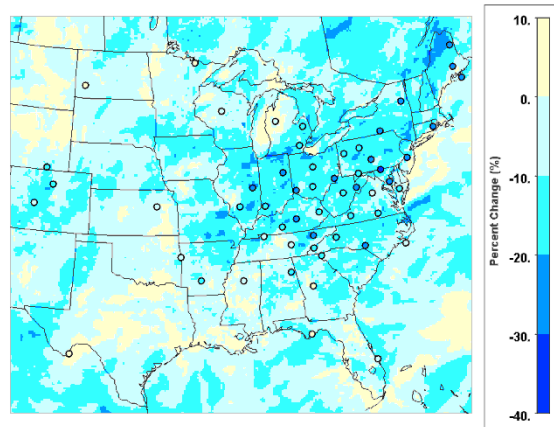Figure 3. Modeled and observed change (%) in MDA8 O_3 (≥95th percentile) between summer of 2002 and 2006. CASTNET site results (open circles) are displayed.
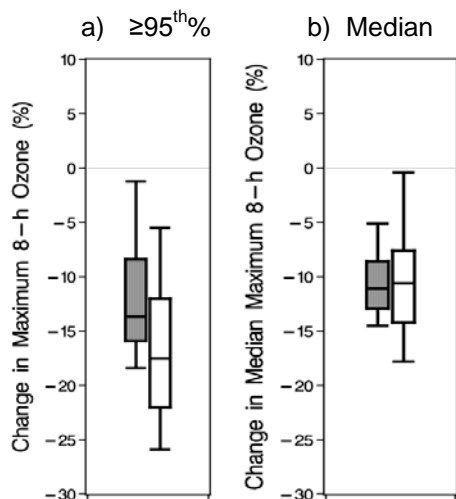
a) ≥95th%   b) Median

Figure 4. Percentage changes in a) MDA8 O_3 (≥95th percentile) concentrations and in the b) median (50th%) value of the modeled (gray) and observed CASTNET site results. Boxes span the 25th-75th percentiles and whiskers extend to the 10th/90th percentiles of the CDF. Horizontal line in each box indicates the median of all values.

4. SUMMARY

A dynamic evaluation of the CMAQv5.0 chemical transport model was conducted to investigate its ability to reproduce changes in maximum 8-h O_3 from summers 2002 to 2006 that are attributable to notable declines in surface and elevated NO_X emissions. At maximum 8-h ozone levels (≥95th percentile), model results exhibited considerable spatial agreement with the observed change of MDA8 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, which also occurred in the Gilland et al (2008) results with a previous version of CMAQ. However, better agreement was found between the modeled and observed changes at the median (50th%) in our results compared to the previous study. Analysis of emission rates is currently being pursued to ascertain whether insufficient change in total NO_X emissions also contributed to the reduced model response.

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