Dynamic evaluation of the CMAQv5.0 modeling system: Assessing the model's ability to simulate ozone changes due to NO_x emission reductions

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Abstract

Regional air quality models are frequently used for regulatory applications to predict changes in air quality due to changes in emissions or changes in meteorology. Dynamic model evaluation is thus an important step in establishing credibility in the model predicted pollutant response. Beginning in 2003, the U.S. Environmental Protection Agency required substantial reductions in NO_x emissions from power plants in the eastern U.S. which resulted in a decrease in ozone concentrations at monitoring sites in this region. This observable change in air quality has been used previously as a case study for dynamic evaluation of the Community Multiscale Air Quality (CMAQ) modeling system. Evaluation studies of previous CMAQ versions have shown that the model predicted decrease in ozone from 2002 to 2005 is less than the observed ozone change in this region. In this study, summertime simulations of 2002 and 2005 were conducted using the CMAQ version 5.0 modeling system released in 2012 that included several model updates aimed at improving the model predicted response, including updates to important model inputs. "Cross" simulations were conducted to separate the modeled impact of the emissions changes on ozone concentrations from the changes attributable to differences in meteorology across these years. Results show the change in the upper end of the ozone distribution explained by emission reductions is similar in magnitude to the change in ozone due to changes in meteorology across these years. Overall, the observed ozone decrease in the eastern U.S. continues to be underestimated by the model at both urban and rural monitoring sites.

1 Introduction

EPA's Nitrogen Oxides State Implementation Plan Call (NO_x SIP Call) rule was implemented in 2003 through early 2004. A NO_x Budget Trading program was established that led to reductions in NO_x emissions from large electrical generating units (EGUs) in twenty states and Washington DC. Emission reductions contributed to a thirty percent reduction in observed ozone levels in many parts of the region between the summers of 2002 and 2005 (Gilliland *et al.* 2008). Continuous emissions monitoring data were available for major units, allowing for very accurate quantification of the emission reduction. These features make this an excellent retrospective case for evaluating the ability of models to predict changes in air quality resulting from changes in emissions, referred to as dynamic evaluation (Dennis *et al.*, 2010). Here we build upon the dynamic evaluation of the Community Multiscale Air Quality (CMAQ) modeling system documented by Gilliland *et al.* (2008) and Godowitch *et al.* (2008) using this case study to evaluate a new version

of the modeling system (CMAQv5.0.1) and utilizing novel "cross" simulations to separately quantify the impact on ozone predictions stemming from (a) changes in emissions and (b) changes in meteorology.

2 Methods

CMAQv5.0.1 simulations were performed over the continental U.S. for June 1 through September 30th 2002 and 2005 using a grid with 12km horizontal resolution and 35 vertical layers . Meteorological inputs were based on WRF3.3 with MCIPv4.0. Emissions inputs used SMOKE3.1 with MOVESv2010b for 2002 and 2005 mobile emissions. Emissions inputs included inline NO produced from lightning using year specific data from the National Lightning Detection Network. Boundary conditions were based on 2005 monthly median values from a GEOS-Chem v9-01-02 simulation using v8-02-01 chemistry, GEOS-5 meteorology and ICOADS shipping emissions. Ozone observations from the AQS and CASTNET networks were used to evaluate model predicted daily maximum 8-hour average ozone (MDA8 O_3), the model metric used for attainment demonstrations. In addition, AQS NO_2 monitors are used to diagnose errors in emission inputs.

In addition to the 2002 and 2005 simulations (Sim02e02m, Sim05e05m), two "cross" sensitivity simulations are used to simulate air quality under 2005 emissions with 2002 meteorology (Sim05e02m) and 2002 emissions with 2005 meteorology (Sim02e05m). The processing of emissions from EGUs with available continuous emission monitoring systems (CEM) data for these simulations is based on unit specific adjustments of the emissions to account for the impact of different meteorological influences in a different year. Summertime 2005 NO_x emissions are generally lower than 2002 emissions, but the temporal fluctuations are different due to differences in electricity demand which is heavily influenced by year-specific meteorology. To estimate 2002 emissions with 2005 meteorological patterns ($EMIS_{02e05m}$) we scale the hourly 2005 CEM emissions (CEM_{2005}) based on the ratio of summer total CEM emissions (S_{Y1}/S_{Y2}) for a particular EGU unit in 2002 versus 2005:

$$EMIS_{02e05m} = CEM_{2005} \times (S_{2002}/S_{2005}) \quad (1)$$

An analogous calculation is made to estimate 2005 emissions with 2002 meteorological patterns.

Mobile emissions for the cross runs are based on MOVES simulations using the designated emissions year and meteorology year (e.g. 2002 emissions with 2005 meteorology). Emissions from nonroad (e.g. construction), industrial point and large marine sectors are based on the emissions year but shifted to match the day-of-the week of the meteorology year. Emissions from fertilizer application, biogenic sources, NO_x from lightning, fires and dust are tied to the meteorological year. All other sectors have the same inventory for all scenarios except modified for the day-of-the-week of the meteorology year.

3 Results and Discussion

Figure 1 shows the 2005 – 2002 difference in the average of the top ten summer MDA8 ozone values. The model predicts large ozone decreases in NC and VA, but not as large as what is seen in the observations. In addition, the model misses the region of 15-25ppb observed decreases along the east coast and Ohio River Valley. In order to diagnose this model error we evaluate the change in NO_2 mixing ratios at AQS sites within NO_x SIP call states. Analysis by Godowitch *et al.* (2010) indicates that morning NO_x concentrations are strongly related to ground level NO_x emissions levels. An evaluation of the change in 2005-2002 weekday NO_2 mixing ratios showed

that the decrease in morning (5am-9am) NO_x levels from 2002 to 2005 is underestimated by the model (observed median decrease of 15% verses modeled decrease of 6%), suggesting an underestimation of the decrease in surface NO_2 emissions across these years (Zhou *et al.* 2013, Kang *et al.* 2013).

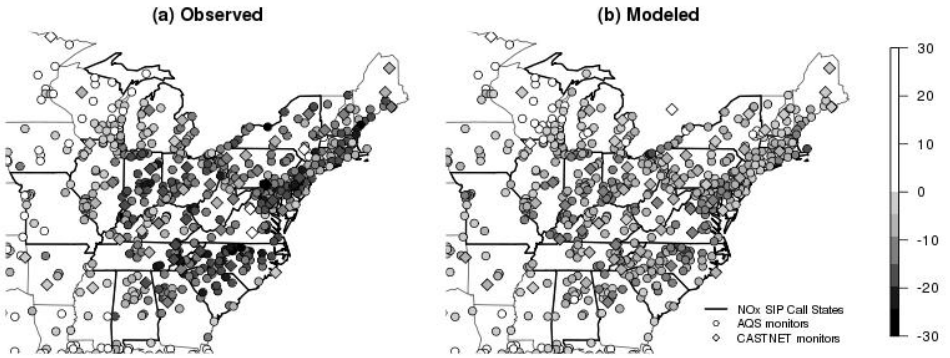

Figure 1. 2005-2002 difference in the average of the top ten summer MDA8 ozone values (ppb) at AQS sites (circles) and CASTNET sites (diamonds).

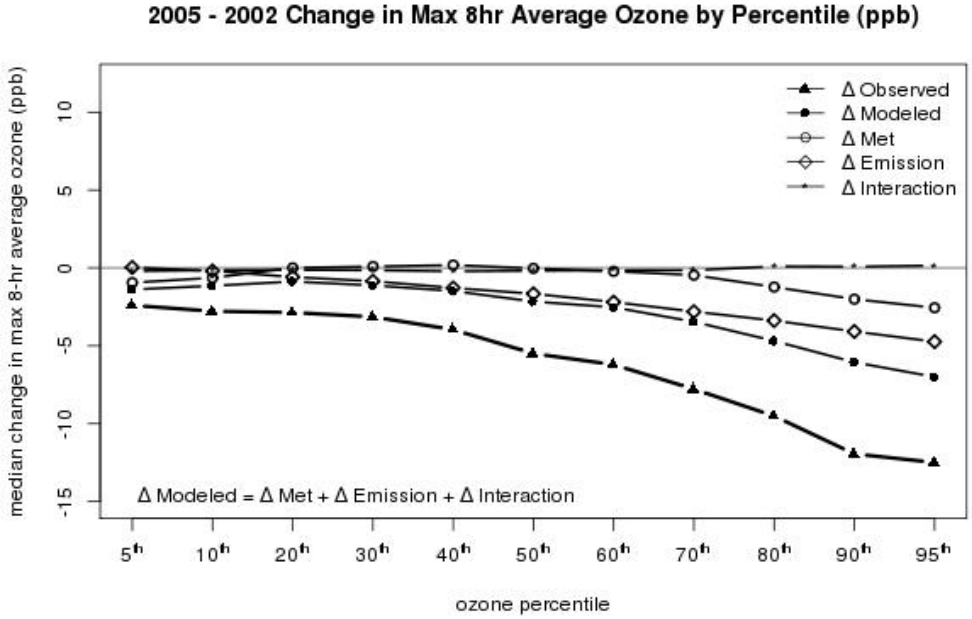

Figure 2. The median change in ozone across AQS sites within NOx SIP Call states at different percentiles of max 8hr average ozone (ppb) based on the 2005-2002 observations (filled triangles), and model simulations: Sim05e05m-Sim02e02m (filled circles; total modeled change), Sim05e02m-Sim02e02m (diamonds; emissions change) and Sim02e05m-Sim02e02m (circles; meteorology change). The remaining interaction term (stars) represents the effect of meteorology on ozone chemistry that is not captured by the cross simulations.

Figure 2 shows the change in modeled and observed ozone at different percentiles (calculated across 122 summer days at each site). For each percentile, the median change across all 444 AQS

sites within NOx SIP Call states is plotted. Utilizing the cross simulations, the change in the modeled ozone at each percentile is decomposed into the change due to emissions, the change due to meteorology and the interaction between emissions and meteorology. Changes in the upper end of the ozone distribution are driven by both emissions and meteorology. The change in the lower end of the ozone distribution is driven almost entirely by meteorological changes.

The methodology presented here is able to account for the effect of meteorology on emissions as well as the meteorological impact on air quality through advection and dispersion. As a result we are able to isolate and quantify the impact of the emission controls across these years. Understanding the specific emissions or meteorological-driven causes of the remaining difference between the observed and modeled change in high summertime ozone levels will require additional diagnostic evaluation. Ongoing work includes decomposing the change in NO_x and CO to compare the meteorology-based changes to what we see in ozone. We also plan to evaluate the predicted change in meteorological parameters (e.g. temperature, wind speed) during "high" and "low" ozone days.

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Questions and Answers

Q: Are you distinguishing between two effects of meteorology: (a) an advection and dispersion effect, and (b) an emission-related effect, e.g. temperature on evaporative emissions? Do you think we need new terms in order to discriminate clearly between these two effects, e.g. for discussions with policy makers? Do you think such "meteorological normalization" will be important for regulatory modeling in the future?

A: You are exactly correct. When we talk about changes due to meteorology in this paper, this includes both the (a) and (b) effects that you describe. For example, we found a small (± 0.5%) change in state wide total NO_x emissions from mobile sources due to changes in meteorology from 2002 to 2005, which could have a slight impact on the modeled ozone predictions. With an additional set of sensitivity simulations it would be possible to further decompose the meteorological effects into these categories in order to quantify the impact from each effect on the final ozone levels. In this application, we suspect the advection and dispersion effect would dominate the ozone signal, but we agree that this would be interesting to explore. We agree that quantifying the impact of a retrospective emission control by removing the impacts of meteorology during the control period is a very valuable approach for communicating to policy makers the net benefit of expensive control measures.

Q: How many alternative meteorological fields did you use to determine the influence of meteorology on ozone concentration? In which way did you evaluate the meteorological fields?

A: The simulations described here rely on meteorological inputs from WRF3.3 simulations for 2002 and 2005. The WRF simulations are considered the state-of-the-art for air quality applications in terms of the parameterizations and data assimilation methods used. The meteorological fields were evaluated against surface measurements for 2 meter temperature, wind speed, wind direction and mixing ratio and the evaluation metrics were found to be similar or better than previous simulations for these time periods. We agree that it would be valuable to repeat these simulations using alternative meteorological inputs to identify if the impacts on ozone are consistent under different scientifically valid input fields.

Q: Given that health effects assessments are sensitive to "average" ozone (the entire distribution), not just the 8-hr max statistics, how well did the model capture the change in median ozone levels (both over the whole year and the ozone season)?

A: We looked at a plot similar to Figure 2 based on June – September daily median ozone levels rather than daily maximum 8hr average ozone. As expected, the change in the daily median ozone levels is smaller than the change in the max 8-hr metric across all percentiles for both the modeled and observed values. Similar to Figure 2, the difference between the modeled and observed change in the median increases with increasing percentiles. Overall, the model performs slightly better at capturing the change in the median ozone, compared to results for the max 8-hr statistic. We have not looked at the change over the entire year but agree that this would be very relevant for health effect assessment applications.