Dynamic Evaluation of Long-Term Air Quality Model Simulations Over the Northeastern U.S.

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Abstract Dynamic model evaluation assesses a modeling system's ability to reproduce changes in air quality induced by changes in meteorology and/or emissions. In this paper, we illustrate various approaches to dynamic model evaluation utilizing 18 years of air quality simulations performed with the regional-scale MM5/SMOKE/CMAQ modeling system over the Northeastern U.S. for the time period 1988 - 2005. A comparison of observed and simulated weekly cycles in elemental carbon (EC) and organic carbon (OC) concentrations shows significant differences, indicating potential problems with the magnitude and temporal allocation of traffic-related emissions and the split between primary and secondary organic aerosols. A comparison of the observed and simulated interrelationships between temperature and ozone over the 18-year simulation period reveals that the high end of the modeled ozone concentration distribution is less influenced by interannual variability in the high end of the temperature distribution as compared to the observations.

Introduction

Regional-scale photochemical modelling systems are routinely used to support air quality planning activities. Often, model evaluation focuses on comparing predictions from the base case scenario against observations. While such comparisons can help build confidence in the performance of the modelling system, they can leave several key questions unanswered: how well does the modelling system capture the impacts of projected changes in emissions? How well does the modelling system capture the effects of meteorological variability on pollutant concentrations, a question of particular importance when using regional-scale models to assess the effects of climate change? These questions are at the core of "dynamic model evaluation", a concept defined by Gilliland et al. (2008) and integrated into an overall model evaluation framework by Dennis et al. (2010). In this paper, we present some illustrative examples for dynamic model evaluation using results from air quality simulations over the Northeastern U.S. covering an 18 year period from 1988 to 2005.

Modeling System, Observations, and Method of Analysis

The model simulations analyzed here have been described in greater detail in Hogrefe et al. (2009; 2010) and Pierce et al. (2010). The following is a brief summary of the model set-up used for the simulations analyzed in this study. The MM5 meteorological model was used to simulate meteorological conditions over the Northeastern U.S. for the time period from January 1, 1988 to December 31, 2005 using two-way nested grids with 36km and 12km grid cell sizes. Emission inventories were compiled from a variety of sources as described in Hogrefe et al. (2009) and processed by the SMOKE system. Air quality simulations were performed with the Community Multiscale Air Quality (CMAQ) model, version 4.6. As described in Hogrefe et al. (2010), chemical boundary conditions for the 36km grid were extracted from archived monthly-mean fields of global chemistry simulations performed for the 1988-2005 time period with the ECHAM5-MOZART modelling system as part of the RETRO project (RETRO, 2007).

Hourly ozone (O_3) observations from 1988 to 2005 were obtained from the U.S. EPA Air Quality System (AQS). Only sites located within the 12 km CMAQ modelling domain were included in the analysis. After screening for data completeness, 90 O_3 monitors were selected for the analysis. Hourly temperature observations for 1988 – 2005 were obtained from the Data Support Section at the National Center for Atmospheric Research (NCAR-DSS). To analyze the observed and simulated relationships between temperature and O_3, the closest temperature monitor was selected for each of the 90 O_3 sites described above. To analyze 2000 – 2005 CMAQ predictions of Elemental Carbon (EC) and organic carbon (OC), filter-based 24-hr average concentrations were obtained from AQS for 27 Chemical Speciation Network (CSN) monitors located in the 12 km CMAQ domain.

Results and Discussion

As pointed out by Pierce et al. (2010), the pronounced differences in anthropogenic emissions between weekdays and weekends offer an excellent opportunity for the dynamic evaluation. While Pierce et al. (2010) examined weekend/weekday (WEWD) differences in observed and simulated concentrations of

O_3 and its precursors, here we focus on WEWD differences in concentrations of carbonaceous fine particles. Figure 1 presents averaged weekly cycles of observed and simulated concentrations of EC and OC based on all available data at the 27 CSN sites from 2000 to 2005. The observed EC concentrations show a marked decline on weekends, decreasing from a weekday average of about 0.7 $\mu g/m^3$ to a weekend average of about 0.55 $\mu g/m^3$, a reduction of more than 20%. A majority of this reduction likely is due to reduced diesel truck traffic on weekends. The CMAQ predictions also show a decrease of EC concentrations on weekends, but the magnitude of this decrease (from about 0.85 $\mu g/m^3$ to about 0.8 $\mu g/m^3$) is much smaller than that observed. This underestimation may be indicative of problems with either the magnitude or the temporal allocation of diesel truck emissions. The differences between observed and simulated weekly cycles are even more pronounced for OC. While the observations display little systematic WEWD differences, the weekly cycle of the simulated OC concentrations does show a decrease on weekends, closely resembling the weekly cycle of the simulated EC concentrations. A possible explanation for the discrepancies could be a different split between primary and secondary OC. Specifically, the observed total OC concentrations may contain a larger portion of secondary OC than the simulated total OC concentrations. Since biogenic emissions can be a significant contributor to secondary OC and are not expected to exhibit a regular weekly cycle, the absence of a pronounced WEWD differences in the observed OC concentrations supports this hypothesis. Further support comes from the model's underestimation of observed total OC concentrations and from the fact that the model simulated weekly cycle of OC closely resembles that of EC, a purely primary component. In summary, this comparison of the observed and simulated weekly cycles of EC and OC provides an illustration where dynamic evaluation can provide a starting point for further diagnostic studies aimed at improving the model's response to emission changes.

From the dynamic model evaluation perspective, it is also of interest how well the model can capture the interrelationships between meteorological and air quality variables. As an illustration, we compared the relationship between summer-

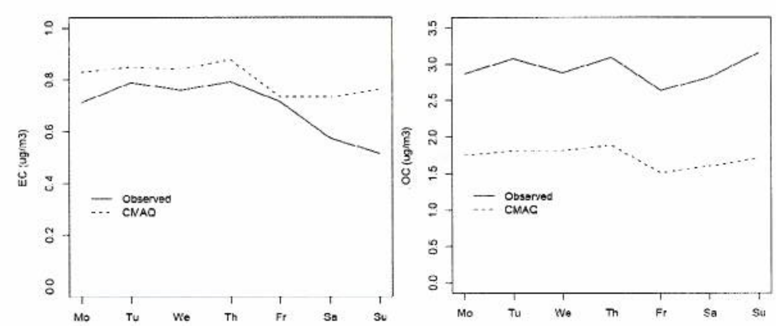

Fig. 1 Average weekly cycle of observed and simulated EC (left) and OC (right) concentrations.

time temperature and O_3 anomalies for both observations and model simulations. To this end, anomalies for each variable were computed by first rank-ordering each year's May-September distribution of daily maximum temperature and daily maximum 8-hr O_3 at each site and then, for each given percentile and each site, subtracting the site- and percentile-specific 18-year mean value from the value for a given year. Figure 2 displays a comparison of the observed and simulated relationship between summertime temperature and O_3 anomalies. The figure depicts box-whisker plots of the anomalies in the 95^{th} percentile of summertime 8-hr daily maximum O_3 concentrations as a function of the anomalies in the 95^{th} percentile of summertime daily maximum temperature. The figure illustrates that for summers when the observed anomaly of the 95^{th} temperature percentile is greater than +3 °C, the distribution of anomalies of the 95^{th} O_3 percentile has a median value of +22 ppb. Conversely, for summers when the observed anomaly of the 95^{th} temperature percentile is less than -3 °C, the distribution of anomalies of the 95^{th} O_3 percentile has a median value of -8 ppb. The corresponding modeled values are +17 ppb and -5 ppb, respectively, indicating that the high end of the modeled O_3 distribution appears to be less influenced by interannual variability in the high end of the temperature distribution than the high end of the observed O_3 distribution.

Summary and Outlook

The dynamic evaluation examples presented in this study indicate potential problems with the magnitude and temporal allocation of traffic emissions and the split between primary and secondary organic aerosols in the 1988 – 2005 MM5/CMAQ simulations analyzed here. Also, the modeling system did not fully capture the relationship between the high end of the summertime temperature and O_3 distributions. As discussed by Hogrefe et al. (2010), key uncertainties affecting the long-term regional-scale simulations, such as the ones analyzed in this study, are estimates of sector-specific, spatially-resolved long-term emission trends and the spe-

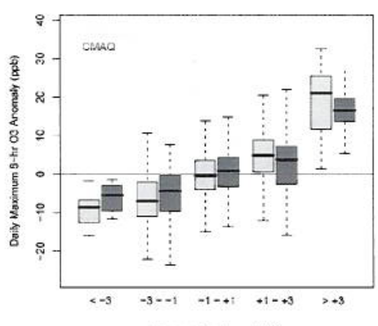

Fig. 2 Relationship between ozone and temperature anomalies for observations and simulations calculated as described in the text.

cification of lateral boundary conditions. The examples presented in this study also highlight opportunities for further dynamic evaluation, such as examining potential changes in photochemical regime over time and additional analyses of the interrelationships between climate and air quality variables. Finally, long-term simulations, such as the one presented here, have a number of potential applications, including tracking the effects of emission reductions, health impact studies, investigating the interactions between climate change and air quality, and testing assumptions about emissions and boundary conditions.

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Question and Answer

Volker Matthias: Was the model nudged with respect to temperature also on the inner grid and in the boundary layer? Did you investigate the effect of grid resolution on the ozone variability?

Answer: Temperature, wind speed, and moisture values were nudged on both grids, but no nudging for temperature and moisture was performed within the boundary layer. To date we have not yet performed a detailed analysis of the impact of grid resolution on the simulated ozone variability.