5.4 Dynamic model evaluation of NO_x emissions reductions on ozone concentrations in the presence of uncertain emission inventories

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Abstract The Community Multiscale Air Quality (CMAQ) model was evaluated for its ability to reproduce observed changes in ambient concentrations of ozone (O_3) for two seasons: the summer of 2002 and the summer of 2005 covering the eastern United States. These two summer periods were distinguished by large emissions reductions stemming from controls mandated by the NO_x State Implementation Plan (SIP) after 2002. CMAQ was evaluated for the robustness of its response in ambient O_3 levels to changes in NO_x emissions. Furthermore, uncertainties in the NO_x emissions inventory were propagated through the model using a direct sensitivity approach. Considering a 50% uncertainty in the area and mobile source NO_x emissions, the model was able to replicate changes in O_3 concentrations between 2002 and 2005 at most observation sites.

1. Introduction

Previous dynamic evaluation of regional air quality models have focused on comparing the absolute change predicted by the CMAQ model with the absolute change seen in the O_3 observations (Gilliland et al. 2008). For example, the measurements might have registered a -10.6 ppb change in O_3 according to some metric, while the modeling results for the same time period might have shown a -5.1 ppb change in the same metric. While much has been learned from such model evaluations, it is difficult to assess the overall ability of the model to respond robustly to changes in emissions inputs since model input, mainly emissions, is known to be uncertain.

Consideration of uncertainty in the inputs enables us to better evaluate model's response to emission changes.

2. Method

All modeling was performed on a 12 km horizontal resolution grid covering the Eastern United States for the periods of 1 May – 31 August 2002, and 1 May – 31 August 2005. CMAQ version 4.7.1, instrumented with DDM-3D (Napelenok et al. 2008), was used to calculate O_3 concentrations and sensitivities to three emission sectors for NO_x: area sources, mobile source, and point sources. Meteorology was calculated using MM5 with standard physics options, and emissions were developed using SMOKE based on temporally and spatially resolved fire, electricity generating units, and mobile sources. Ozone observations from the AQS and CASTNET networks were used to evaluate the model predictions of ozone.

Calculated DDM-3D sensitivities were used to provide responses to the perturbations in the inputs of the three NO_x emissions categories outlined above through Taylor series expansion (Hakami et al. 2003). Generally, pollutant concentration as a function of any one perturbation can be reconstructed using the following:

$$C_j(\bar{\mathbf{x}},t) = C_0(\bar{\mathbf{x}},t) + \Delta\varepsilon_j S_j^{(1)}(\bar{\mathbf{x}},t) + \frac{1}{2}\Delta\varepsilon_j^2 S_{j,j}^{(2)}(\bar{\mathbf{x}},t) + (h.o.t),$$

where $C_j(\bar{\mathbf{x}},t)$ is the concentration due to a specific perturbation j; $C_0(\bar{\mathbf{x}},t)$ is base simulation concentration; $\Delta\varepsilon_j$ is the fractional perturbation of the parameter j; $S_j^{(1)}(\bar{\mathbf{x}},t)$ and $S_{j,j}^{(2)}(\bar{\mathbf{x}},t)$ are the first and second order sensitivity coefficients, and *h.o.t* are higher order terms with little impact on the approximation. More than one perturbation to the base case would simply require additional terms in the Taylor series expansion.

Various estimates of uncertainty from each NO_x emissions sector were used in the analysis, ranging from ±30-70% for ground-level area and mobile sources and ±3-5% for elevated point sources. The source of uncertainty in point sources was due mainly to measurement error in the Continuous Emissions Monitoring (CEM) technology and, hence, was set to low values.

For each uncertainty scenario evaluated, e.g. ±50% area sources, ±50% mobile sources, and ±3% point sources, a perturbation parameter, $\Delta\varepsilon_j$, was randomly chosen from a normal distribution spanning the uncertainty range using Monte-Carlo sampling. Combined with the DDM-3D calculated sensitivity coefficients, the resulting sets of uncertainty estimates were used in the Taylor Series to generate an ensemble of ozone predictions at each location in the domain during each simulation period.

In an effort to remove some of the influences of meteorology, observed and modeled data were analyzed in terms of cumulative frequency distribution at each

location. The dynamic signal in ozone air quality between the two episodes (2002 and 2005) in the observations was calculated simply as the difference between the distributions for each year. Modeling results were treated similarly, but accounting for the ensemble of possible outcomes at each location. The model was then evaluated for its ability to respond to large changes in emissions inputs.

3. Results and Discussion

Ensembles of model predictions allowed for more informative comparisons of model results with the observed data. The standard CMAQ model underestimated the maximum 8hr O_3 concentrations in 2002 and overestimated in 2005 for middle to high ozone events, leading to the dampening of the observed $O_{3\text{-}2002} - O_{3\text{-}2005}$ signal (Fig.1). Accounting for even a modest degree of emissions uncertainty, in the same scenario, showed that model estimates were closer to observed values.

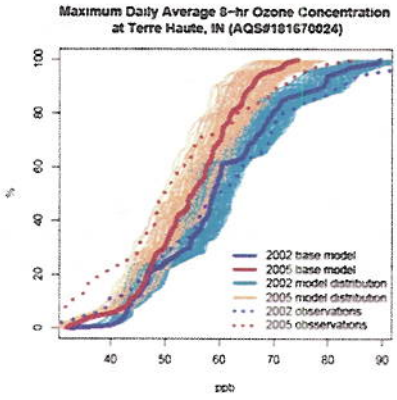

Fig. 1. Modeled and observed maximum 8hr O_3 concentrations in 2002 and 2005 as well as possible NO_x emissions uncertainty ensemble members under relatively low estimates of uncertainty. Results are shown for a monitoring site in Terre Haute, IN.

Concentration ensembles allowed for comparison of whether or not the observed $O_{3\text{-}2002} - O_{3\text{-}2005}$ signal was within the ensemble of modeled signal. It was found that with 50% uncertainty in NO_x emissions from mobile and area sources, the model-predicted signal in ozone encompassed that in the observations at 441 out of 684 total measurement sites (Fig.2). As expected, higher levels of uncertainty corresponded to higher number of sites where predictions were correct.

In summary, a method for dynamical evaluation of maximum 8hr O_3 predictions considering emissions uncertainty was applied to the large emissions reductions of NO_x that occurred in accordance with the NO_x SIP Call. Due to the uncertainties in inputs, the model was unable to reproduce the signal in an absolute sense. However, accounting for some of these uncertainties in the emission inventory enabled us to better assess model's response to reductions in NO_x emissions.

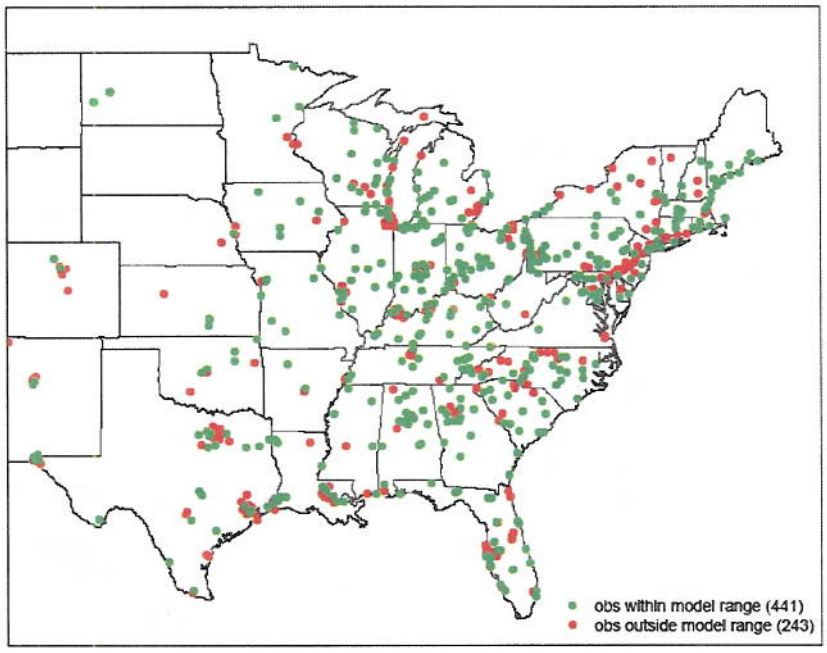

Fig. 2. Measure of success of the model in predicting the measured signal of ozone change between 2002 and 2005 for the 95th percentile of data. At the majority of the sites (441), the signal was predicted correctly considering 50% uncertainty in NO_x emissions.

References

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Discussion

V. Nochvai:

1) What is the influence of the second order sensitivity terms on prognosis accuracy?

The importance of second order sensitivity terms is varies in space. For NO_x emissions sensitivity, second order terms are typically large near model grid cells with high emissions.

2) How can you justify 3% accuracy for point sources emission data?

Emission rates for the NO_x point source inventory used in this study were collected by measurements from continuous emission monitoring (CEM) system outfitted on the units at the point of emissions. The error on CEMs is primarily measurement error and is very low.