Meteorology, Emissions, and Grid Resolution: Effects on Discrete and Probabilistic Model Performance

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Abstract In this study, we analyze the impacts of perturbations in meteorology and emissions and variations in grid resolution on air quality forecast simulations. The meteorological perturbations considered in this study introduce a typical variability of ~1°C, 250 - 500 m, 1 m/s, and 15 - 30° for temperature, PBL height, wind speed, and wind direction, respectively. The effects of grid resolution are typically smaller and more localized. Results of the air quality simulations show that the perturbations in meteorology tend to have a larger impact on pollutant concentrations than emission perturbations and grid resolution effects. Operational model evaluation results show that the meteorological and grid resolution ensembles impact a wider range of model performance metrics than emission perturbations. Probabilistic model performance was found to vary with exceedance thresholds. The results of this study suggest that meteorological perturbations introduced through ensemble weather forecasts are the most important factor in constructing a model-based O_3 and $PM_{2.5}$ ensemble forecasting system.

Keywords: Ensemble Modeling, Model Evaluation, Direct Decoupled Method

Introduction

The development of ensemble forecast systems is a promising avenue for improving air quality forecast guidance and to develop probabilistic forecast products. The goal of this study is to quantify and compare the impacts of perturbations in meteorology, emissions, and grid resolution on predictions of O_3, NO_2, CO, Elemental Carbon (EC), and total $PM_{2.5}$ over the Northeastern U.S. and to evaluate these ensembles with operational and probabilistic metrics.

Database and Methods

All simulations analyzed in this study were performed for August 1 – 31, 2010 and January 1- February 15, 2011 over the Northeastern U.S. Air quality fields for the meteorological perturbation ensemble were generated by using twelve different MM5 and WRF weather forecasts from the Stony Brook University ensemble system to drive CMAQ4.7.1 on two nested horizontal domains with a grid spacing of 36 km and 12 km, respectively. The twelve weather forecast ensemble members differ in their choice of initial and boundary conditions as well as different convective parameterization, boundary layer, and microphysical schemes. Members of the grid resolution perturbation ensemble were generated by performing WRF-Urban Canopy Model (UCM)/CMAQ4.7.1 simulations for nested 36 km, 12 km, and 4 km domains and considering the nine 4 km cells within each 12 km cell as perturbations from the 12 km base case. To create the emission perturbation ensemble, we used the Direct Decoupled Method (DDM) (Hakami et al., 2003) implemented in CMAQ. CMAQ-DDM simulations were performed with one MM5 member of the meteorological perturbation ensemble. Following the general approach described in Napelenok et al. (2008) and Pinder et al. (2009), the CMAQ-DDM sensitivity fields were used to develop reduced-form models for O_3, NO_2, EC, and $PM_{2.5}$. For calculating pollutant variations caused by emission uncertainties, we used perturbations in NO_x, VOC, and $PM_{2.5}$ emissions sampled from a uniform distribution representing an uncertainty range of +/-50%. These MM5/CMAQ-DDM simulations were performed on two nested horizontal domains with a grid spacing of 36 km and 12 km, respectively. All analyses were performed for the smallest domain common to all simulations, i.e. the 4 km domain used for the WRF-UCM/CMAQ4.7.1 simulations. The focus of this analysis was on daily maximum 8-hr O_3 and CO, daily maximum 1-hr NO_2, and 24-hr average EC and total $PM_{2.5}$. Observations for model evaluation were obtained from the U.S. EPA's Air Quality System (AQS).

Results and Discussion

To quantify the variability of key meteorological variables (2m temperature, PBL heights, 10m wind speed and 10m wind direction) introduced by the meteorological and grid resolution ensembles, we computed the standard deviation of these variables across all ensemble members at 2pm EST for each day for each grid cell in the analysis domain and then averaged these resulting daily maps for both the summer and winter simulation periods. These seasonally averaged maps of ensemble standard deviations reveal that the meteorological perturbations considered in this study introduce a typical variability of ~1°C, 250 - 500 m, 1 m/s, and 15 - 30° for temperature, PBL height, wind speed, and wind direction, respectively. The effects of grid resolution on meteorological variables are typically smaller and more localized, with the largest effects near land/sea interfaces and in complex terrain.

As stated in the previous section, in addition to meteorological perturbation and grid resolution effects, we also considered the effects of emission perturbations for the analysis of variability in O_3, CO, NO_2, EC, and $PM_{2.5}$ concentrations simulated by CMAQ. The analysis was performed in the same way as described above for the meteorological variables except that the ensemble standard deviation was divided by the ensemble mean to compute the coefficient of variation (CV), which can then be compared between different pollutants. In general, results showed that the impact of meteorological perturbations, grid resolution and emission perturbations on CMAQ air quality simulations varies by time, location, and species. CV for NO_2, EC, and $PM_{2.5}$ are generally larger than CV for CO and O_3. For O_3 and $PM_{2.5}$, the meteorological ensemble caused larger variability than the emission and grid resolution ensembles. For NO_2 and EC, the variability caused by the emission and meteorological ensembles are comparable. Grid resolution effects are largest in urban and coastal grid cells but generally cause less variability than the meteorological and emission ensembles.

Operational evaluation results for O_3, CO, NO_2, and total $PM_{2.5}$ showed that emission perturbations can have a pronounced impact on model bias, especially in urban areas for species with a large primary component (NO_2, wintertime $PM_{2.5}$); this is consistent with the previous finding that the CV for the emission ensemble is largest in urban areas. However, with the exception of NO_2, meteorological perturbations still were found to have a larger effect on model bias than grid resolution effects even at urban locations, again consistent with the CV discussed above. When considering model performance in a Taylor diagram representation that simultaneously depicts correlation coefficient, ratio of modeled to observed standard deviation, and centered root mean square error (RMSE), the results show that the members of the meteorological and grid resolution ensembles span a wider range of "model performance space" (i.e. they have an impact on all three model performance metrics depicted in the Taylor diagram) while the main effect of emission perturbations is on the ratio of modeled-to-observed standard deviations with little impact on correlations and centered RMSE. Two examples of this analysis are shown in Figure 1.

Probabilistic model performance for O_3 and $PM_{2.5}$ was assessed through Talagrand diagrams and reliability diagrams. Results showed that all ensemble predictions were underdispersed. This was especially true for the grid resolution and emission perturbation ensembles, consistent with the finding above that these two ensembles introduced less variability than the meteorological ensemble. Probabilistic model performance, as measured by Brier Skill Scores (BSS) with respect to climatology, was found to vary with exceedance thresholds. For O_3, ensembles showed improvement with respect to climatology for exceedance thresholds up to about 70 ppb while this threshold was about 15 µg/m^3 for $PM_{2.5}$. Overall, the results of this study suggest that, at least for the region and ensemble

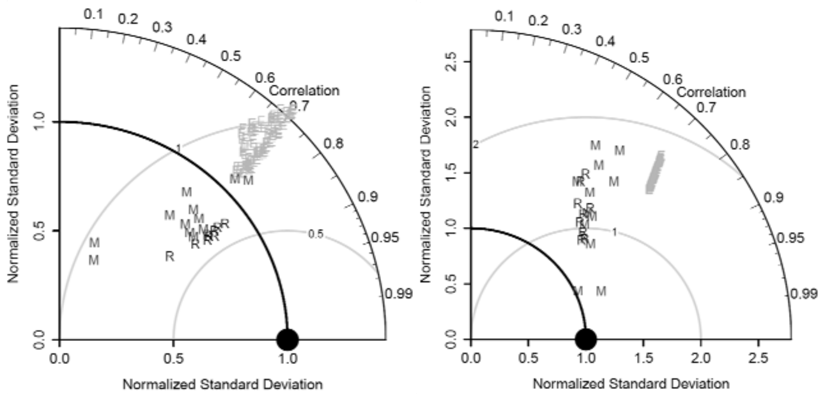

Figure 1. Taylor diagram for daily maximum O_3 (left) and 24-hr average $PM_{2.5}$ (right) at a monitor in Queens, NY during August 2010. "M" (medium grey), "R" (dark grey), and "E" (light grey) denote the meteorological, grid resolution, and emission perturbation ensemble members, respectively.

configurations considered here, meteorological perturbations introduced through ensemble weather forecasts are the most important factor in constructing a model-based O_3 and $PM_{2.5}$ ensemble forecasting system.

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