ADAPTATION AND APPLICATION OF THE COMMUNITY MULTISCALE AIR QUALITY (CMAQ) MODELING SYSTEM FOR REAL-TIME AIR QUALITY FORECASTING DURING THE SUMMER OF 2004

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1. INTRODUCTION

The ability to forecast local and regional air pollution events is challenging since the processes governing the production and sustenance of atmospheric pollutants are complex and often non-linear. Comprehensive atmospheric models, by representing in as much detail as possible the various dynamical, physical, and chemical processes regulating the atmospheric fate of pollutants, provide a scientifically sound tool for air quality forecasting. The availability of increased computational power coupled with advances in the computational structure of the models has now enabled their use in real-time air quality forecasting. In recent years, such efforts have been used to provide daily guidance to state and local air quality forecasters (e.g., McHenry et al., 2004) as well as to aid in design of field experiments (e.g., Flatoy et al., 2000; Uno et al., 2003; Lawrence et al., 2003).

Recently, the National Oceanic and Atmospheric Administration (NOAA), and the U.S. Environmental Protection Agency (EPA) partnered to develop a real-time air-quality forecasting (AQF) system that is based on the National Weather Service (NWS) National Centers for Environmental Prediction's (NCEP's) Eta model (Black, 1994) and the U.S. EPA's Community Multiscale Air Quality (CMAQ) Modeling System (Byun and Ching, 1999). An initial version of the system was deployed to forecast surface-level O_3 pollution over the northeast U.S. during the summer of 2003 (Davidson et al., 2003). In this paper we summarize further enhancements to the AQF modeling system as well as initial results from its forecast applications during the summer of 2004.

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2. THE ETA-CMAQ AQF SYSTEM

The Eta-CMAQ AQF system consists of three primary components: (1) the Eta meteorological model that simulates the atmospheric dynamic conditions for the forecast period; (2) the CMAQ model which simulates the transport, chemical evolution, and deposition of atmospheric pollutants; and (3) an interface component, PREMAQ, that facilitates the transformation of Eta derived meteorological fields to conform with the CMAQ grid structure, coordinate system, and input data format. Since both the Eta and CMAQ models use significantly different coordinate systems and grid structures, the interface component has been carefully designed to minimize effects associated with horizontal and vertical interpolation of dynamical fields in this initial implementation. Details on the methods employed and impacts of assumptions invoked can be found in Otte et al. (2004).

The emission inventories used by the AQF system were updated to represent the 2004 forecast period. NO_x emissions from point sources were projected to 2004 (relative to a 2001 base inventory) using estimates derived from the annual energy outlook by the Department of Energy (http: //www.eia.doe.gov/oiaf/aeo/index. html). Since MOBILE6 is computationally expensive and inefficient for real-time applications, mobile source emissions were estimated using approximations to the MOBILE6 model. In this approach SMOKE/MOBILE6 was used to create retrospective emissions over an eight-week period over the AQF grid using the 1999 Vehicle Miles Traveled (VMT) data and 2004 vehicle fleet information. Least squares regressions relating the emissions to variations in temperature were then developed for each grid cell at each hour of the week and for each emitted species. Consequently, mobile emissions could then be readily estimated in the forecast system using the temperature fields from the Eta model (Pouliot et al., 2003). Area source emissions were based on the 2001 National Emissions Inventory, version 3, while BEIS3.12 (Pierce et al., 2002) was used to estimate the biogenic emissions.

During the summer of 2004, the AQF system was exercised in three streams: (1) experimental production of O_3 forecasts over the northeast U.S. (1x domain) for dissemination to the general public; (2) developmental forecasts of O_3 over an expanded eastern U.S. domain (3x domain) for dissemination to a focus group of forecasters; and (3) developmental forecasts of both O_3 and particulate matter (PM) concentrations over the 3x domain for initial assessments of PM forecast capabilities. In the first two applications, aerosols were not simulated by CMAQ. In all applications the CB4 mechanism was used, the horizontal grid resolution was 12km while the vertical extent from the surface to 100 mb, was discretized using 22 layers of variable thickness.

The turbulent mixing scheme in CMAQ was enhanced to allow the minimum value of the surface layer vertical eddy diffusivity (K_z) to vary spatially depending on the fraction of urban area (f_{urban}) in each grid cell. In this formulation, the minimum K_z varies linearly between 0.1 m^2/s (f_{urban}= 0) and 2 m^2/s (f_{urban}= 1) depending on f_{urban}. The approach allows for K_z in rural regions to fall off to lower a value than predominantly urban regions, and effectively: (1) prevents simulated nighttime precursor concentrations in urban areas from becoming too large; and (2) increases night time O_3 titration which consequently reduces the modeled O_3 over-predictions.

Two approaches for specifying lateral boundary conditions (LBCs) to CMAQ were investigated: (1) based on typical “clean” tropospheric background values; and (2) based on seasonal averages derived from prior CMAQ simulations over the continental U.S. for the summer of 2001. The default clean profiles were used for the 1x domain, while the seasonal LBC profiles were used in the developmental 3x forecast applications. To improve the representation of O_3 in the free troposphere, additional modifications of the O_3 LBCs using forecast results from NCEP’s Global Forecast System (GFS) were explored. In the GFS, O_3 is initialized using the Solar Backscatter Ultra Violet (SBUV-2) satellite observations. The evolution of the 3-D O_3 fields in the GFS is then simulated by its transport schemes and a zonally averaged production and depletion scheme.

3. INITIAL RESULTS

The 2004 O_3 forecast season was atypical in that it was characterized by cool and wet conditions and very few O_3 exceedances in the north east U.S. Figure 1 presents example regional distributions of model forecasts for surface O_3 on two typical days characterized by high and low O_3 levels, respectively. Figure 2 summarizes the model performance in predicting surface O_3 levels for the June-August, 2004 period. Illustrated in the figure is the variation in the mean bias in predicted daily maximum O_3 at 612 surface monitoring sites from the AIRNOW network. Also shown is the variation in the observed domain mean daily maximum O_3. As can be seen, the 2004 ozone season has been characterized by relatively few days with regionally high O_3. Additionally, it can be noted that the days on which the forecasts exhibit high mean bias are typically characterized by low observed regional O_3. These high biases in turn arise from over-predictions at the low ozone range (see for example bottom panel of Figure 1).

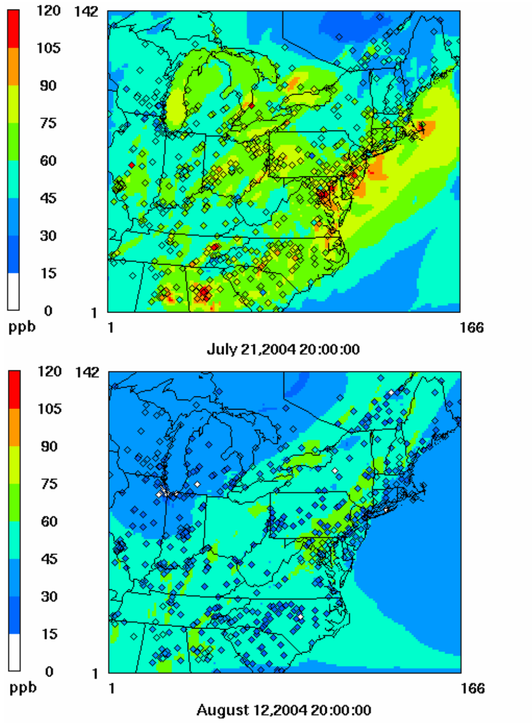

Figure 1: Forecast surface level O_3 distributions at 2000 GMT over the 1x domain on July 21, 2004 (top) and August 12, 2004 (bottom). Color-coded diamonds indicate observed values.

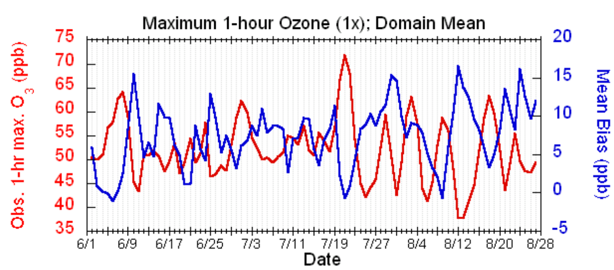

Figure 2: Variations in observed domain mean maximum O_3 and mean bias over the 1x domain.

The median observed hourly O_3 concentrations for the June-August, 2004 period were <40 ppb at a majority of the sites in the northeast U.S. Given that the model LBCs for O_3 are specified between 40-45 ppb through the depth of the boundary layer, the over-predictions at the low observed range can be attributed, in part, to the LBC specification.

In general, the over-predictions at the low observed ozone range are also found to be spatially correlated with regions of cloud cover and precipitation. Typically, under conditions of widespread cloudiness and precipitation, relatively low O_3 was observed regionally with values in the 15-30 ppb range or less; the modeled O_3 concentrations under such conditions were often in the 45-60 ppb range (cf. Figure 1, bottom panel). To better understand the role of modeled cloud processes and their formulation in influencing these over-predictions, a variety of diagnostic simulations have been conducted to test existing and alternate formulations. These include:

(1) Examination of the CMAQ cloud mixing formulation, especially the representation of the effects of downdrafts and their role in top-down mixing;

(2) Limiting the CMAQ-diagnosed cloud-tops to below the GFS tropopause to study the combined effect of the use of GFS-derived O_3 and cloud mixing processes;

(3) Specification of cloud fraction fields and their effect on photolysis;

(4) Use of modeled and clear sky radiation fields to estimate below-cloud photolysis attenuation factors.

Initial results from these diagnostic simulations indicate that both the representation of cloud mixing and the effects of clouds on the attenuation of photolysis rates play significant roles in dictating the extent of modeled over-predictions. In particular, under conditions characterized by significant convective and frontal activity, relatively high artificial levels of O_3 within the boundary layer in CMAQ can arise from downward mixing in deep clouds that extend up to the tropopause. Limiting the influence of the downdrafts as well as the cloud tops to below the tropopause can help alleviate these problems. Initial tests also suggest that using the modeled radiation fields from the Eta model to derive the below-cloud attenuation factors could provide a more spatially consistent and accurate representation of the effects of clouds on regulating the photochemistry.

4. SUMMARY

Results from the 2004 forecast applications highlight the importance of lateral boundary condition specification in dictating simulated background O_3 levels. The accurate simulation of the background levels becomes particularly important in dictating model performance for conditions characterized by low regional O_3 as in this summer. The over predictions at the low O_3 concentration range were found to arise from a combination of effects related to lateral boundary condition specification, representation of cloud mixing, and effects of clouds on attenuation of photolysis rates. Initial tests with alternate formulations of the cloud mixing and photolysis attenuation schemes in CMAQ show improvements in model performance over the limited periods tested. Additional evaluation of these alternate formulations is currently underway to test their robustness over a wider range of conditions.

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