J2.15 COMPARISONS BETWEEN OBSERVATIONS MADE DURING NEAQS AND AIR QUALITY FORECASTS FROM MM5 AND WRF CHEMISTRY MODELS

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1. INTRODUCTION

The 2002 New England Air Quality Study (NEAQS) was an intensive effort to investigate the chemical and meteorological factors that contribute to poor air quality in the New England region. The campaign combined efforts of numerous educational institutions as well as federal, state, and local agencies. Observational data were collected from an extensive network of ground sites, from the NOAA research vessel Ronald H. Brown, and from the DOE G-1 aircraft. Although many of the ground stations routinely collect data year-round, the period of most intensive measurements was from July 12 through August 10, 2002.

Real-time numerical weather and air quality forecasts during NEAQS 2002 were provided by the National Center for Environmental Prediction (NCEP) and the NOAA Forecast Systems Laboratory (FSL). The numerical model used to produce weather and air quality forecasts at FSL is the PSU-NCAR mesoscale model (MM5) chemistry model (Grell et al. 2000). The MM5/Chem model is designed to integrate the meteorology and atmospheric chemistry simultaneously ("online") as opposed to previous air quality models (e.g., CMAQ; Byun and Ching, 1999) that integrate the meteorology and atmospheric chemistry separately (“offline”). The MM5/Chem model incorporates an air chemistry mechanism package based on RADM2 (Stockwell et al., 1990), biogenic emissions, surface deposition, tracer transport by convection, turbulence, photolysis, and advective transport.

Starting in 2002, air chemistry was implemented in the nonhydrostatic, eulerian-mass coordinate version of the Weather Research and Forecast (WRF) weather model (Grell et al. 2004). The WRF/Chem model is similar in its physical and chemical concepts to MM5/Chem but it uses the WRF model as the meteorological component. Likewise, the WRF/Chem model has incorporated the RADM2 air chemistry mechanism package, biogenic emissions, surface deposition, tracer transport by convection, turbulence, photolysis, and advective transport. In addition, atmospheric aerosols have been incorporated using the Modal Aerosol Dynamics Model for Europe (MADE) (Ackermann *et al.*, 1998) which itself is a modification of the Regional Particulate Model (Binkowski and Shankar, 1995). Secondary organic aerosols (SOA) have been incorporated into MADE by Schell *et al.*, (2001), by means of the Secondary Organic Aerosol Model (SORGAM).

Real-time forecasts are being made with the WRF/Chem model for the eastern half of the U. S.. This model configuration is one of several real-time simulations being conducted at NOAA/FSL (Koch et al. 2004). Select fields from the forecasts (00 and 12 UTC) are available online (http://www.wrf-model.org/WG11).

For the purpose of diagnostic evaluation, retrospective simulations of the 2002 NEAQS forecasts were conducted using the WRF/Chem model. Comparisons are made between the meteorological and chemical species observations and the numerical simulation results in order to evaluate the WRF/Chem simulations. The presentation will briefly discuss the model configuration used in real-time and retrospective simulations. In addition, several high- pollution events will be compared in order to evaluate the overall performance of MM5/Chem and WRF/Chem.

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2. METHODOLOGY

A series of 24-hour simulations were performed on a roughly 3600 km x 3000 km numerical grid having 27-km horizontal resolution and centered at 86°W longitude and 34.5°N latitude (Fig. 1). The domain extends vertically to 18 km with a vertical mesh interval smoothly increasing from 7 m near the surface to approximately 500 meters at the domain top. Simulations were conducted every 12 hours (00Z and 12Z) starting from 5 July 2002 and ending on 20 August 2002. Information about configuration of each model is provided in Tables 1 and 2.

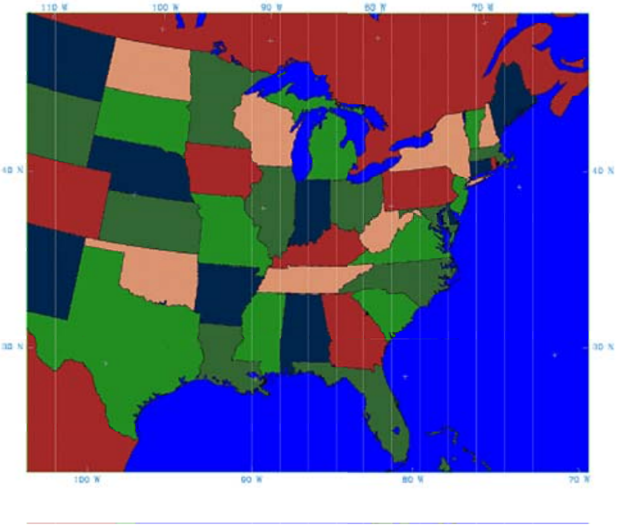


Fig. 1. Regional coverage of the 27-km horizontal grid spacing domain used for the MM5/Chem and WRF/Chem simulations.

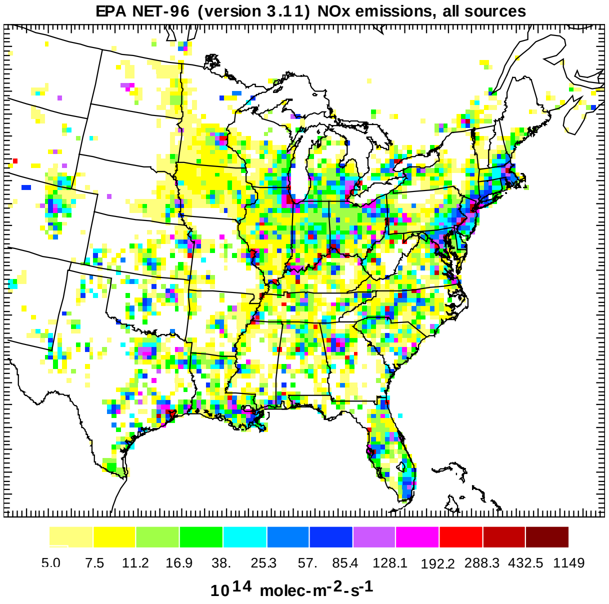


Fig. 2. Surface emissions of NOx (molec. m^{-2} s^{-1}) derived for a numerical mesh using 27-km grid spacing from the Net-96 EPA emissions database.

Meteorological initial conditions were obtained from the Rapid Update Cycle (RUC) model analysis fields generated at FSL and lateral boundary conditions are derived from the NCEP ETA-model forecast. MM5/Chem forecasts were initialized 12-hr prior to the forecast start time and nudged toward the current analysis fields. Nudging is not currently available in the WRF model so the simulations were started at the initialization time. Atmospheric chemical constituents were initialized from the previous 12-hour forecast with the exception of the 00Z simulation for 5 July 2002 that used an idealized atmospheric chemistry profile.

Table 1. MM5/Chem Configuration options

Microphysics	Mixed phase (Reisner)
Longwave radiation	RRTM
Shortwave radiation	Dudhia
Land-surface model	Smirnova
Boundary layer scheme	Mellor-Yamada 2.5 TKE
Cumulus parameterization	Improved Grell
Photolysis scheme	Madronich (1987)
Chemistry option	RADM2
Aerosol option	None

Table 2. WRF/Chem Configuration options

Advection scheme	5th horizontal /3rd vertical
Microphysics	NCEP 3-class simple ice
Longwave radiation	RRTM
Shortwave radiation	Dudhia
Surface layer	Monin-Obukhov (Janjic Eta)
Land-surface model	OSU
Boundary layer scheme	Mellor-Yamada-Janjic TKE
Cumulus parameterization	Betts-Miller-Janjic
Photolysis scheme	Madronich (1987)
Chemistry option	RADM2
Aerosol option	MADE/SORGAM

Anthropogenic emissions were interpolated to the three-dimensional model grid and were updated hourly (e.g., Fig.2). The anthropogenic surface and point source emissions used in the simulations were obtained from the EPA Net-96 emission database. Biogenic emissions include surface emissions of isoprene, monoterpenes, VOCs and soil emissions of nitrogen (Simpson et al. 1995).

3. SIMULATION RESULTS

High pollution events in northern New England often result from transport of pollutants from urban, industrial, and power-plant sources to the south and west. Hence, forecasting such events requires the numerical models to correctly forecast the temperature/moisture profile as well as the wind direction and strength in the lower few kilometers of the troposphere. During the nighttime portion of the diurnal cycle, the flow in this lower-troposphere is often dominated by a low-level jet. When the low-level jet over New England is from the southwesterly direction, it can transport minimally diluted pollutants from urban areas into the Gulf of Maine.

After sunset on 4 Aug. 2002, light southerly flow accelerated as a LLJ developed with maximum speeds of 11-13 m/s at an elevation of 300-400 m MSL. A layer of enhanced ozone is observed off of the New England coast by an ozone-profiling lidar aboard the R/V Ron Brown (Fig 3). Trajectory analysis indicates that the pollution developed over the urban and industrial sources to the southwest in Southern New England.

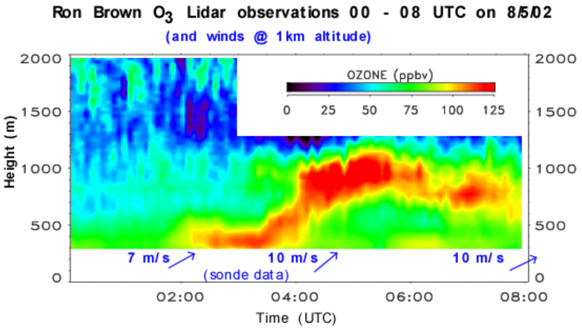


Fig. 3. Ozone concentration (ppb) observed aboard the *R/V Ron Brown* in the Gulf of Maine on 5 Aug 2002 between the hours of 00 and 8 UTC. The ozone concentration (ppb) scale is provided by the color bar.

The MM5/Chem forecast and the WRF/Chem retrospective simulation starting at 12 UTC on 4 August 2002 reveal that both models performed adequately in forecasting the ozone evolution observed in the Gulf of Maine by the *R/V Ron Brown* (Fig. 4). Both models, probably due to the coarse horizontal resolution, over-predict the early evening (00 UTC) ozone concentration. In addition, neither model produce a shallow layer of high ozone along the surface that was observed between 00 UTC and 4 UTC. However, both models produce a layer of enhanced ozone near 1 km MSL between 4 UTC and 6 UTC (Fig. 5).

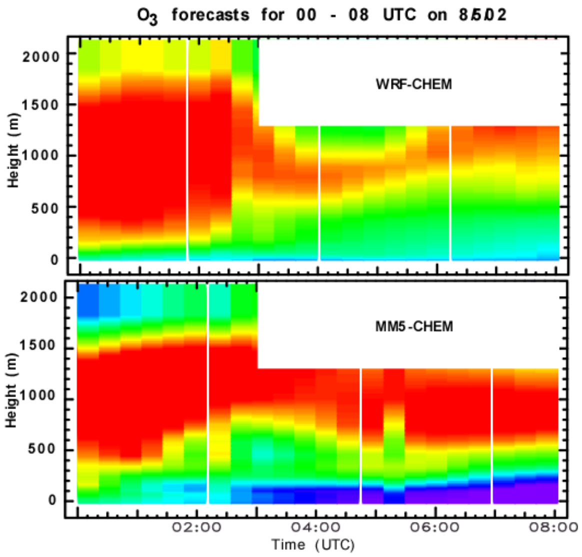
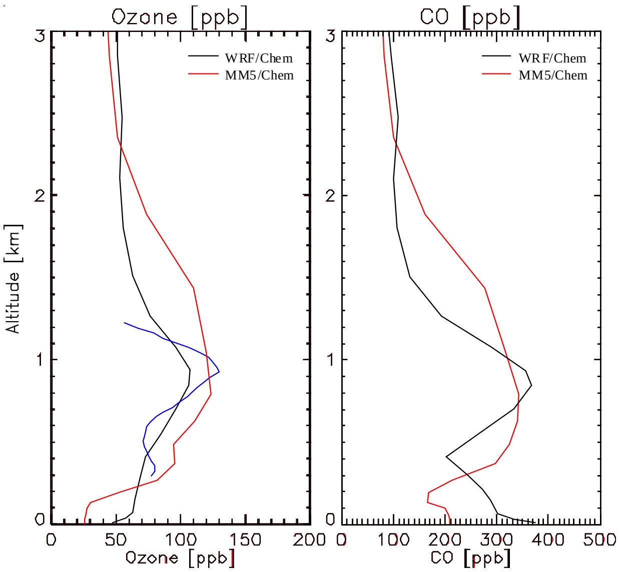


Fig. 4. Ozone concentration (ppb) simulated by the WRF/Chem and MM5/Chem models between the hours of 00 z and 8 z on 5 August 2002. The ozone concentration (ppb) scale is provided by the color bar in Figure 3.



2002-08-05
0500 UTC

Fig. 5. Vertical profiles of Ozone and carbon monoxide concentration (ppb) simulated by the WRF/Chem (black line) and MM5/Chem (red line) at 5 UTC on 5 August 2002. The ozone concentration (ppb) observed aboard the *R/V Ron Brown* is shown with the blue line.

Vertical profiles of ozone extracted from the models at the time and location of the *R/V Ron Brown* reveal that both capture the observed structure as well as the height of the peak ozone concentration. However, the near surface values of carbon monoxide are very high. The apparent over-prediction of anthropogenically-produced pollutants (e.g., carbon oxides and nitrogen oxides) is probably due to the coarse surface emissions resolution combined with a shallow inversion over the ocean (Fig. 6). The southwesterly low-level winds transport the low-level pollutants off shore where they are unable to mix vertically resulting in high near-surface pollution concentrations.

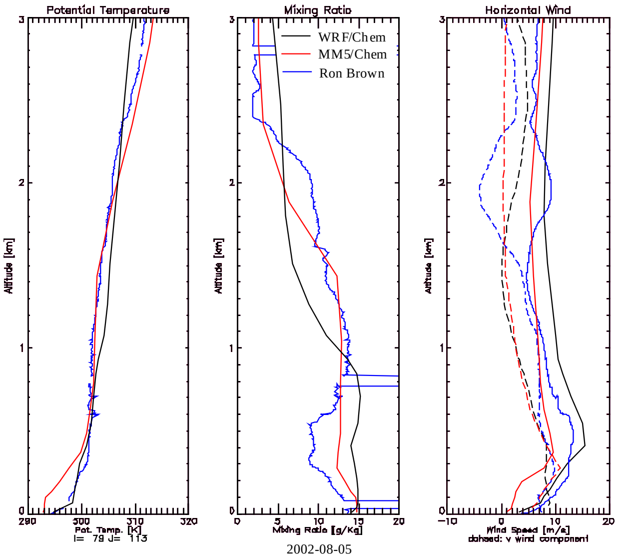


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Fig. 6. Vertical profiles of potential temperature (K), mixing ratio (g kg^{-1}), and u (solid) and v (dashed) wind component simulated by the WRF/Chem (black line) and MM5/Chem (red line) at 5 UTC on 5 August 2002. The potential temperature (K), mixing ratio (g kg^{-1}), and u (solid) and v (dashed) wind components observed aboard the *R/V Ron Brown* are shown with the blue lines.

In addition, the vertical profiles both show a small increase in potential temperature and moisture between 500 m and 1.5 km MSL (the layer containing a high ozone concentration). The nearly uniform structure in potential temperature and mixing ratio (virtual potential temperature) suggests that both models produce a residual boundary layer over the ocean. In the simulated residual boundary layer, the wind is from the southwest indicating that the ozone was probably produced during the daytime over the urban areas of New England and subsequently transported northeastward over the coastal inversion. Observational data also suggests the presence of a residual layer between 600 m and 1.2 km MSL. The model wind direction is in close agreement to the observed southwesterly wind in the residual boundary layer, but the models over predict the wind speed.

4. Summary

Atmospheric chemical forecasts and retrospective simulations have been produced using the MM5/Chem and WRF/Chem numerical models, respectively. The forecasts using MM5/Chem took place between July and August of 2002 and coincided with the New England Air Quality Study. The retrospective simulations using WRF/Chem were conducted for the same region and time period.

Initial analysis of the numerical model results indicates that both models are capable of producing the observed chemical structure of the lower troposphere. Differences between the observations and simulation results appear to be a product of the relatively large grid spacing used in the model as well as the surface emissions data.

Future simulations using WRF/Chem will examine the use of smaller horizontal grid spacing and improved surface emission data. In addition, the impact of including the feedback between aerosols and shortwave radiation will be examined.

5. References

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