Steven E. Peckham^{1*}, Georg A. Grell¹, Stuart A. McKeen², and James M. Wilczak³

¹Cooperative Institute for Research in Environmental Sciences (CIRES), University of Colorado/NOAA Research – Forecast Systems Laboratory, Boulder, Colorado ²Cooperative Institute for Research in Environmental Sciences (CIRES), University of Colorado/NOAA Research – Aeronomy Laboratory, Boulder, Colorado ³NOAA – Environmental Technology Laboratory, Boulder, Colorado

1. INTRODUCTION

The 2004 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 several research aircraft. Although many of the ground stations routinely collect data year-round, the period of most intensive measurements was from 1 July through 16 August 2004.

Real-time numerical weather and air quality forecasts during NEAQS 2004 were provided by several university and government institutions including the NOAA Forecast Systems Laboratory (FSL). The numerical model used to produce weather and air quality forecasts at FSL is the Weather Research and Forecast model with chemistry (WRF-Chem) (Grell et al., 2004). The WRF-Chem model is designed to integrate the meteorology and atmospheric 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 WRF-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. In addition, atmospheric aerosols have been

*Corresponding author address: Steven E. Peckham, NOAA/FSL, R/FS1, DSRC, 325 Broadway, Boulder, CO 80305

E-mail: steven.peckham@noaa.gov.

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 (0000 and 1200 UTC) are available online (http://www.wrf-model.org/WG11).

For the purpose of diagnostic evaluation, retrospective simulations of the 2004 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 forecasts. In addition, several high-pollution events will be compared in order to evaluate the overall performance of the WRF-Chem numerical model.

2. METHODOLOGY

A series of 36-h 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 3000 m at the domain top.

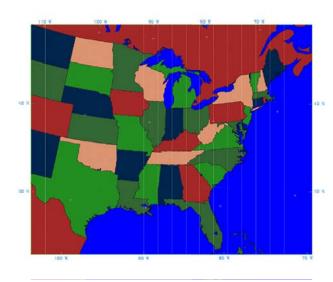


Fig. 1. Regional coverage of the 27-km horizontal grid spacing domain used for the WRF-Chem simulations.

Simulations were conducted every 12 h (0000Z and 1200Z) starting from 5 July 2002 and ending on 20 August 2002. Information about the model configuration is provided in Table 1.

Meteorological initial conditions are 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. Atmospheric chemical constituents are initialized from the previous 12-h forecast with the exception of the 0000Z simulation for 1 July 2002 that used an idealized atmospheric chemistry profile.

Table 1. WRF-Chem Configuration options

5th horizontal /3rd vertical Advection scheme Microphysics NCEP 3-class simple ice Longwave radiation RRTM Shortwave radiation Dudhia Surface layer Monin-Obukhov (Janjic Eta) Land-surface model Boundary layer scheme Mellor-Yamada-Janjic TKE Betts-Miller-Janjic Cumulus parameterization 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. The anthropogenic surface and point source emissions used in the simulations were obtained from the EPA Net-99 emission database. Biogenic emissions include surface emissions of isoprene, monoterpenes, volatile organic compounds, and soil emissions of nitrogen and are obtained from the EPA biogenic emissions inventory system (BEIS) version 3.11 dataset.

3. SIMULATION RESULTS

The presentation will include some of the forecast results from the NEAQS2004 field program. In addition, results from the ongoing forecast evaluation study will be shown. Preliminary findings suggest that the WRF-Chem model performance is comparable to, or slightly better than, the other forecast models used during the 2004 NEAQS field program.

4. References

- Ackermann, I. J., H. Hass, M. Memmesheimer, A. Ebel, F. S. Binkowski, and U. Shankar, 1998: Modal aerosol dynamics model for Europe: Development and first applications, *Atmos. Environ.*, **32**, No.17, 2981-2999.
- Binkowski, F. S. and U. Shankar, 1995: The regional particulate matter model, 1. Model description and preliminary results, *J. Geophys. Res.*, **100**, 26191-26209.
- Byun, D. W. and J. K. S. Ching, ed., 1999: Science algorithms of the EPA Models-3 Community Multi-scale Air Quality (CMAQ) modeling system, *EPA Report, EPA/600/R-99/030*, NERL, Research Triangle Park, NC.
- Grell, G. A., S. E. Peckham, R. Schmitz, S. A. McKeen, J. Wilczak, B. Eder, and W. Skamarack 2004: Fully coupled "online" chemistry within the WRF model: *Atmos. Environ.* (paper accepted)
- Koch, S. E., S. G. Benjamin, J. A. McGinley, J. M. Brown, P. Schultz, E. J. Szoke, T. G. Smirnova, B. L. Shaw, D. L. Birkenheuer, S. Albers, S. E. Peckham, and G. A. Grell, 2004: Real-time applications of the WRF model at the Forecast Systems Laboratory, *Preprints, 20th Conference on Weather Analysis and Forecasting/16th Conference on Numerical Weather Prediction,* Seattle, WA, Amer. Meteor. Soc.
- Schell B., I. J. Ackermann, H. Hass, F. S. Binkowski, and A. Ebel, 2001: Modeling the formation of secondary organic aerosol within a comprehensive air quality model system, *J. Geophys. Res.*, **106**, 28275-28293.
- Stockwell, W. R., P. Middleton, J. S. Chang, and X. Tang, 1990: The second generation regional acid deposition model chemical mechanism for regional air quality modeling. *J. Geophys. Res.*, **95**, 16343-16367.