J2.16 Development and Evaluation of the NOAA/EPA Prototype Air Quality Model Prediction System

Jeff McQueen*, Pius Lee, Marina Tsidulko, Geoff DiMego
Mesoscale Modeling Branch
NOAA/NWS/NCEP/Environmental Modeling Center

Tanya Otte, Jon Pleim, Jeff Young, George Pouliot, Brian Eder, Daiwen Kang and Ken Schere
NOAA/ARL/Atmospheric Sciences Modeling Division
(On assignment to the EPA/National Exposure Research Laboratory)

Jerry Gorline, Michael Schenk, Paul Dallavalle and Wilson Shaffer
NOAA/NWS/Meteorological Development Laboratory

Paula Davidson and Nelson Seaman
NOAA/NWS/Office of Science and Technology

1. INTRODUCTION

During 2003, NOAA and the U.S. EPA signed a Memorandum of Agreement to work together to develop a National air quality forecasting capability. To meet this goal, NOAA's National Weather Service (NWS), the Office of Atmospheric Research (OAR) and the U.S. EPA developed and evaluated a prototype ozone forecast capability for the Eastern U.S. (Davidson et al. 2004) The NWS/ National Centers for Environmental Prediction (NCEP) Eta model at 12 km was used to provide meteorological predictions for the EPA Community Multi-scale Air Quality (CMAQ) model to produce up to 48 h ozone predictions. The CMAQ system simulates various chemical and physical processes that are important for modeling atmospheric trace gas transformations and distributions. CMAQ includes chemical mechanisms to simulate various air quality constituents including tropospheric ozone, fine particles, toxics, acidic deposition, and visibility degradation.

Dabberdt et al. (2003) summarized meteorological research needs in order to improve air quality forecasting. Improvements are needed in the observing, understanding and predicting the boundary-layer structure and wind fields. Also, high resolution and consistent modeling databases should be computed (e.g.: databases for land-use, vegetation, terrain). In 2003, much of the NOAA/EPA development emphasized the proper coupling of the Eta land-surface, boundary layer, and wind fields with the CMAQ coordinate system and physical and chemical processes. Another focus in 2003 was the creation of emissions input suitable for an air quality forecasting system. A final focus was on optimizing CMAQ for the operational systems.

For this study, CMAQ predictions were evaluated against monitoring data collected with EPA's surface ozone network. This paper summarizes the prediction model system developments (Section 2) and presents preliminary quantitative results from the surface ozone evaluation system (Section 3). Verification of the surface ozone predictions included both mean absolute and root mean square errors of the hourly average and maximum daily 1 hourly ozone values. Comparisons were also made on model performance in urban versus rural areas and during episodes when high ozone was observed.

A companion study (Wilzcak et al. 2004) evaluated the Eta model with special emphasis on key meteorological predictions (for example, vertical boundary layer mixing, clouds and radiation, and land surface) that influence air quality. The results of this study will be reviewed here to help diagnose Eta model errors that may have contributed to ozone prediction errors.

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*Corresponding Author Address: Jeff McQueen, NCEP/EMC, W/NP22 Room 207, 5200 Auth Road, Camp Springs, MD 20746-4304; jeff.mcqueen@noaa.gov

2. NOAA-EPA AQ PREDICTION SYSTEM

Beginning in June 2003, NCEP ran the coupled Eta-CMAQ air quality prediction system to provide predictions of surface ozone for up to 48 hours for the Northeastern U.S.

The initial test domain is shown in Fig. 1. The system consisted of the following components outlined in Fig. 2:

Figure 1. CMAQ North East U.S. Domain

- *The NCEP/EMC North American Eta 12 km 60 level prediction system* provides gridded meteorological model predictions at hourly intervals. (Rogers et al. 1996, 2001). Recent improvements to the Eta system are described by Ferrier et al. (2003). These changes included improved grid-scale cloud microphysics and interactions with short and long-wave radiation. Direct analysis of the WSR-88D radar radial velocities and use of NOAA-17 satellite radiances were incorporated into the EDAS 3DVAR assimilation system.
- *The modified Eta product generator, AQM-PRDGEN,* interpolates Eta native grid model outputs(rotated lat-lon Arakawa E grid) to an intermediate grid with 22 terrain-following sigma vertical layers that were prepared by the Eta postprocessor. Additional Eta fields were also output for use in the emissions processing, chemical transport and air-surface interactions (Table 1).
- *The CMAQ preprocessor, PREMAQ,* prepares the CMAQ-ready meteorological and emissions files. PREMAQ converts the Eta output from the intermediate grid to the Arakawa C grid and computes the atmospheric state variables required by CMAQ. PREMAQ then prepares the biogenic, area, and point and mobile source emissions for the forecast. Table 2 summarizes the PREMAQ configuration used for the summer 2003 test period.
- *The CMAQ atmospheric chemistry model* (Byun and Ching, 1999) provides the ozone forecasts. The CMAQ configuration is described in Table 3. The configuration was optimized to allow the availability of predictions in real-time (e.g.: reduced chemical species, aerosols effects omitted).
- *Boundary conditions*: For the summer 2003, a climatological chemical profile was assumed for the lateral boundary conditions which were kept constant with time.
- *Initial Conditions*: A 6 hour cycling system was developed and run 4 times per day to initialize CMAQ chemistry and soil fields to reduce spinup of soil and chemical constituents. This system is described in Figure 3.

Table 1. Fields added to the Eta postprocessor which are required by CMAQ. *Some fields (italisized*) were already being computed however, these are now output hourly and on the CMAQ sigma layers.

Variable name	**GRIB Param #**	**GRIB Table #**
Geopotential height^{+}	*7*	*2*
Pressure	*1*	*2*
Temperature	*11*	*2*
Specific humidity	*51*	*2*
U-wind	*33*	*2*
V-wind	*34*	*2*
Vertical velocity	*39*	*2*
TKE	*158*	*2*
Cloud water mixing ratio	153	2
Cloud ice mixing ratio	58	2
Rain mixing ratio	170	2
Snow mixing ratio	*171*	*2*
Total cloud cover	71	2
Vegetation type$^{\%}$	225	2
Soil type$^{\%}$	224	2
Canopy conductance$^{\%}$	181	130
PBL height$^{\%}$	221	2
Plant canopy water$^{\%}$	223	2
Vertical Eddy Heat diffusivity+	182	129

3D variables on half sigma levels except: + denotes 3D arrays defined on full sigma levels, and % denotes 2D.

Ozone concentration model forecasts were run twice per day driven by the 0600 and 1200 UTC Eta forecast cycles. The 0600 UTC CMAQ forecast was run to 30 h while the 1200 UTC forecast was run to 48 h.

More information on coupling Eta and CMAQ modeling systems is provided by Otte, et al. (2004). The CMAQ system was run on the NCEP IBM SP super-computer using 33 processors. A 48 hour CMAQ prediction required 30 minutes of cpu time. The 1200 UTC model guidance was required to be available on the NWS Telecommunications Operations Center server by 1730 UTC, while the 0600 UTC 30 hour guidance was required by 1330 UTC.

Predicted 1-hour and 8 hour average surface ozone concentrations were output on the CMAQ grid in WMO GRiB format for further visualization and evaluation against the data provided by EPA's AIRNOW surface ozone measurement network (Wayland, et al., 2002).

Table 2. PREMAQ Emission Configuration

Point Sources	Precomputed temporal emissions factors with met. dependent plume rise effects calculated each hour.
Area	Precomputed for each day of year.
Mobile	Precomputed emission factors from MOBILE 5b with hourly temperature-dependent effects (Pouliot and Pierce, 2003).
Biogenic	BEIS-3, using Eta temperature and radiation variables (Pierce et al. 2002)

Table 3. 2003 CMAQ Configuration

Grid	Lambert-Conformal Arakawa C Centered at 40.5N, 79.5W and true at 36N and 46N.
Nx,Ny	166x142
Grid Spacing	12 km, lower-left corner at: (32.353N, 89.994W)
Vertical levels	22 sigma layers to 100 mb
Transport	Eta u,v winds plus rediagnosed mass-consistent vertical velocities
Vertical diffusion	Bulk PBL Scaling
Dry deposition	Deposition velocities from Pleim and Xiu (1995) Land Surface Model
Cloud processes	Aqueous chemistry w/ RADM sub-grid clouds
Photolysis	Radiation modulated by clouds determined from Eta RH profiles
Chemistry mechanism	Carbon Bond 4(Gery et al. 1989)
Chemistry Solver	Euler backward iterative solver Homogeneous chemistry
Aerosols	Off

3. CMAQ OZONE EVALUATION

The peak 1-h average ozone observations collected by AIRNOW for August 14, 2003 and corresponding CMAQ surface ozone concentrations predictions for 2000 UTC August 14, 2003 are shown in Fig 4. Comparisons from this case reveal an overprediction of ozone around Baltimore-Washington A larger area of concentrations of greater than 100 ppb are forecast by CMAQ there. For this case, CMAQ was rerun with corrected land use and climatologically cleaner lateral boundary conditions than used during the real-time runs. These corrections helped to reduce the positive prediction biases discussed below.

Statistical evaluation for July–Aug, 2003 for ozone monitors in the CMAQ domain (excluding Canadian observations) are shown in Fig. 5 for the 1200 UTC cycle prediction. The RMSE, MAE and Bias for 1-h average predictions all indicate an overprediction of ozone. Biases are highest at night.

Spatial biases are shown in Fig. 6 averaged for 1200 UTC AQ predictions for all model hours during July and August 2003. An overprediction is noted in most areas with strongest biases (greater than 20 ppb) occurring near the Baltimore-Washington corridor on south. Areas of biases greater than 30 ppb are noted near the southern CMAQ domain boundary.

However, some of the overprediction was caused by incorrect specification of land-use parameters input for CMAQ, which resulted in severe under-prediction of dry deposition. The error was corrected on September 8. Rerunning model predictions for a one-week period in August revealed that this error contributed 5-10 ppb to the biases.

4. ETA METEOROLOGICAL EVALUATION

Eta predictions were also evaluated for the Northeastern U.S. during the Summer 2003 NEHRT program (Wilzcak et al. 2004). Boundary layer profilers and surface radiation budget stations deployed for the New England High Resolution Temperature Program (NEHRTP) were used to further diagnose errors in the Eta-CMAQ prediction system. The NEHRTP was a targeted program to investigate methods to improve meteorological forecasts for the energy sector. New observational platforms were deployed to diagnose meteorological model error. Biases in the meteorological forecast model winds, temperature and solar insolation field can strongly impact the accuracies of the air quality prediction. During the Summer 2003, Eta surface temperature predictions were slightly higher than observed in the daytime in New England. Incoming solar insolation was also over-predicted on average by as much as 50-100 W/m2. For the 2003 AQ system, overpredicted solar insolation would affect only the biogenic emissions because predicted photolysis rates were affected primarily by cloud coverage, in turn derived from Eta forecasted RH. More direct coupling of Eta radiation with CMAQ photolysis rate calculations are planned in the future. Some of the errors analyzed for this system (5-10 ppb of the bias) was attributed to incorrect post-processing of the Eta land use parameters for CMAQ.

5. SUMMARY

This paper summarized an experimental air quality prediction system that coupled the NWS operational Eta-12 meteorological model with the CMAQ model to produce twice-daily ozone guidance. Care was taken in coupling the two models to reduce interpolation errors caused by converting Eta meteorological fields to the CMAQ grids. In addition, CMAQ was optimized to run efficiently in a forecast mode.

Overprediction of ozone was noted in most areas. Some of this error was explained by incorrect landuse coupling. Future upgrades include improved coupling with the Eta boundary layer and radiation parameter predictions, improving CMAQ chemical boundary conditions, and use of an expanded grid to incorporate more pollutant source areas.

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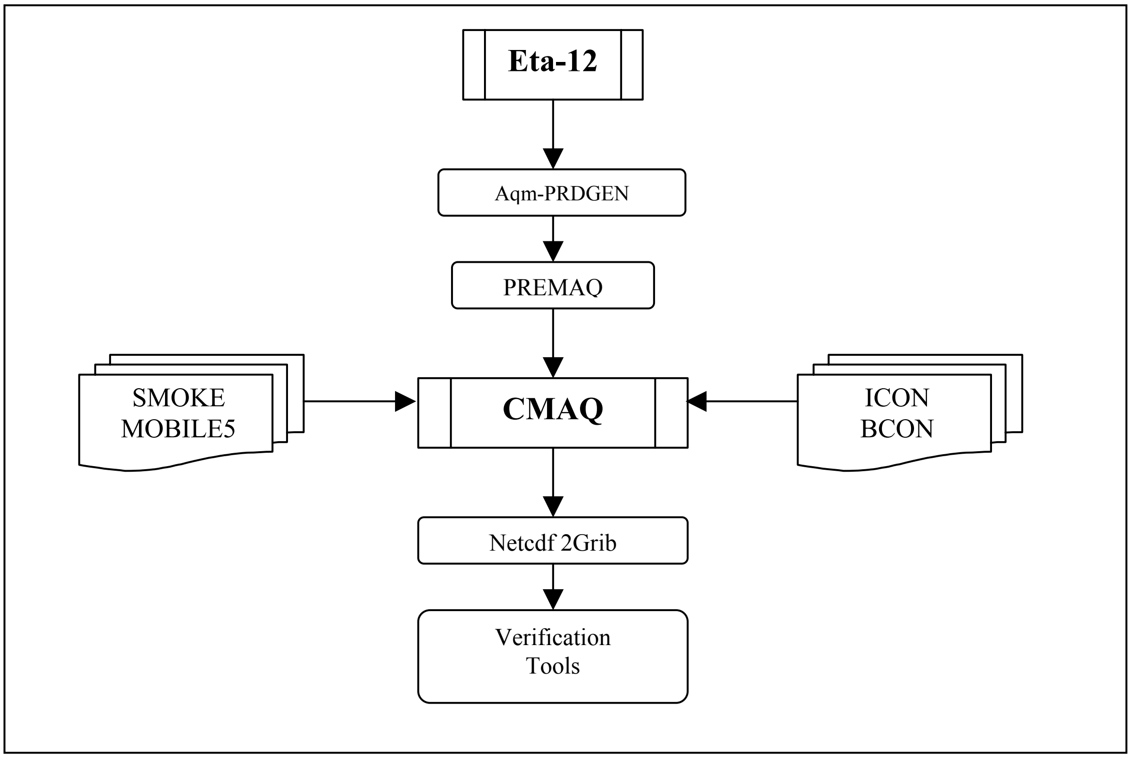

Figure 2. The Eta-12 and CMAQ coupled modeling system: From top to bottom: Aqm-PRDGEN is an extension of NCEP's PRDGEN; PREMAQ is EPA's CMAQ preprocessor; and the Netcdf to GRiB converter and Verification tools are explained in Sections 2 and 3 respectively.

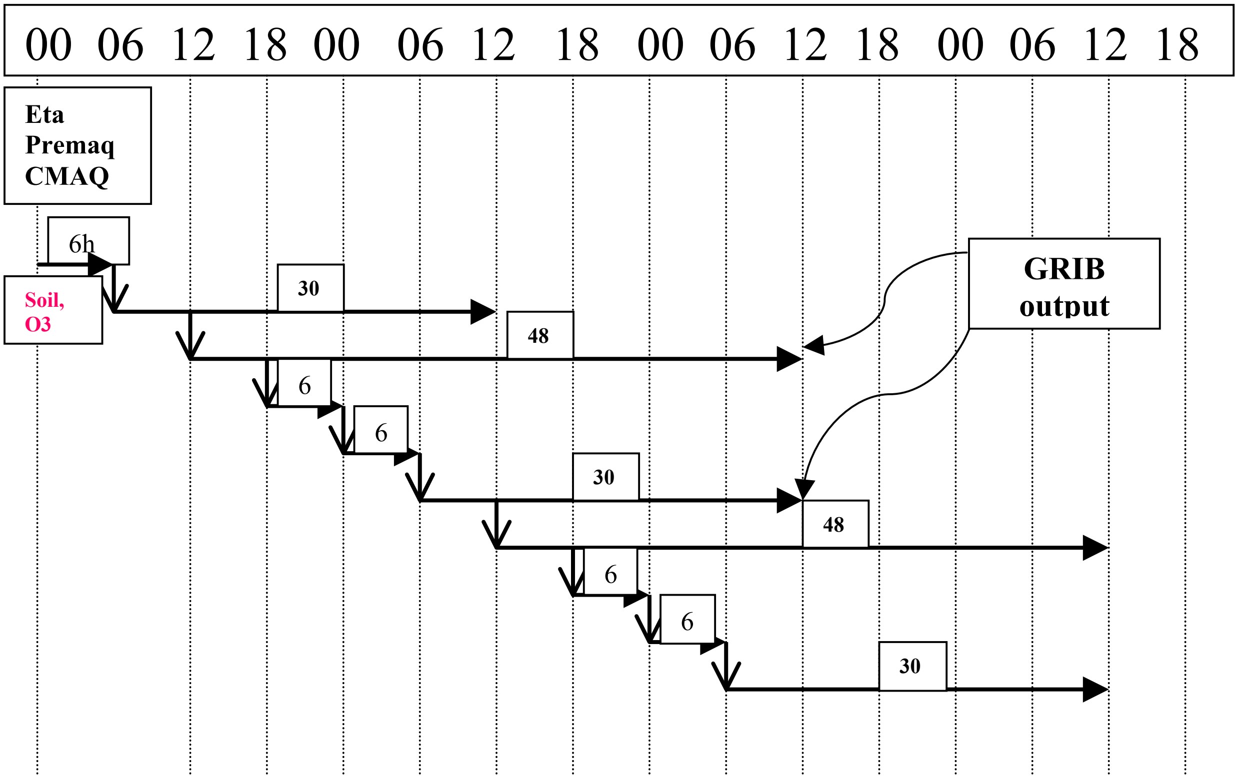

Figure 3. CMAQ four times/day 6-hour cycling and forecast schematic. At 0600 and 1200 UTC, CMAQ is run to produce 30 and 48 h predictions, respectively.

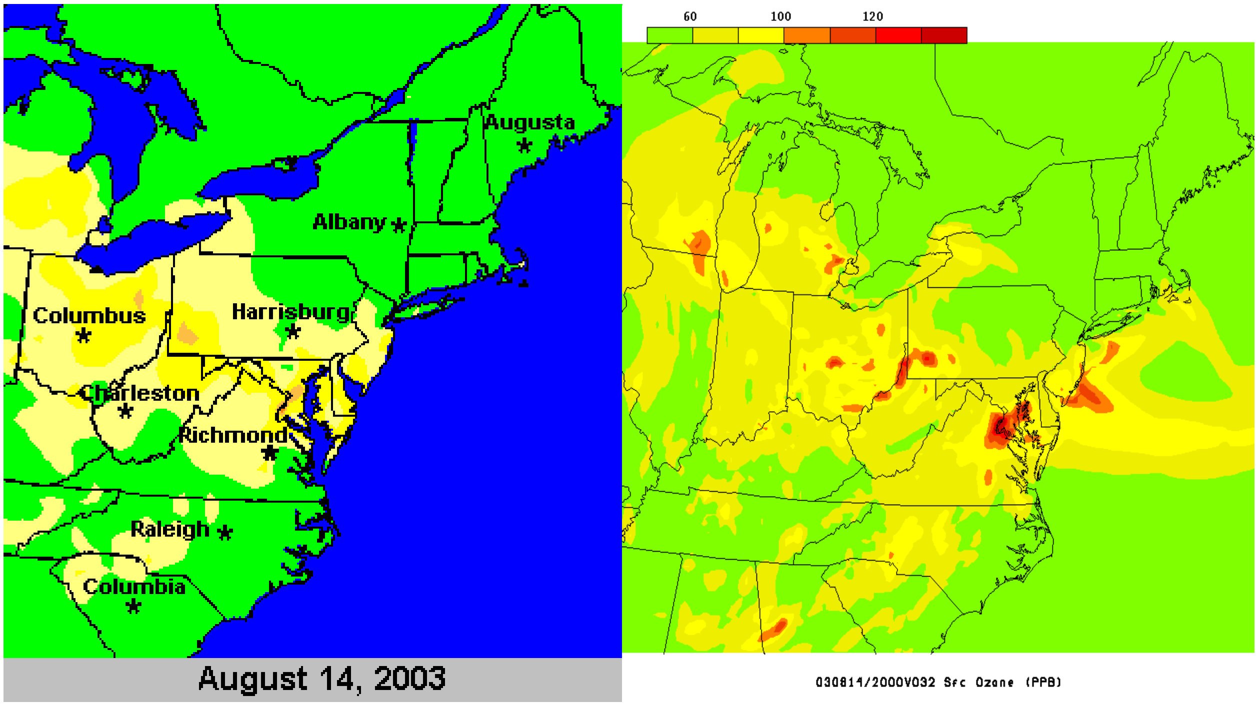

Figure 4. a) AIRNOW observed peak 1 hr surface ozone concentrations and b) Corrected CMAQ 32 hr 1 hour average predictions (ppb) for August 30, 2003 at 20:00 UTC. Color key: green (0-59 ppb), lgt yellow(60-79), yellow (80-99), orange (100-110), red (111-124).

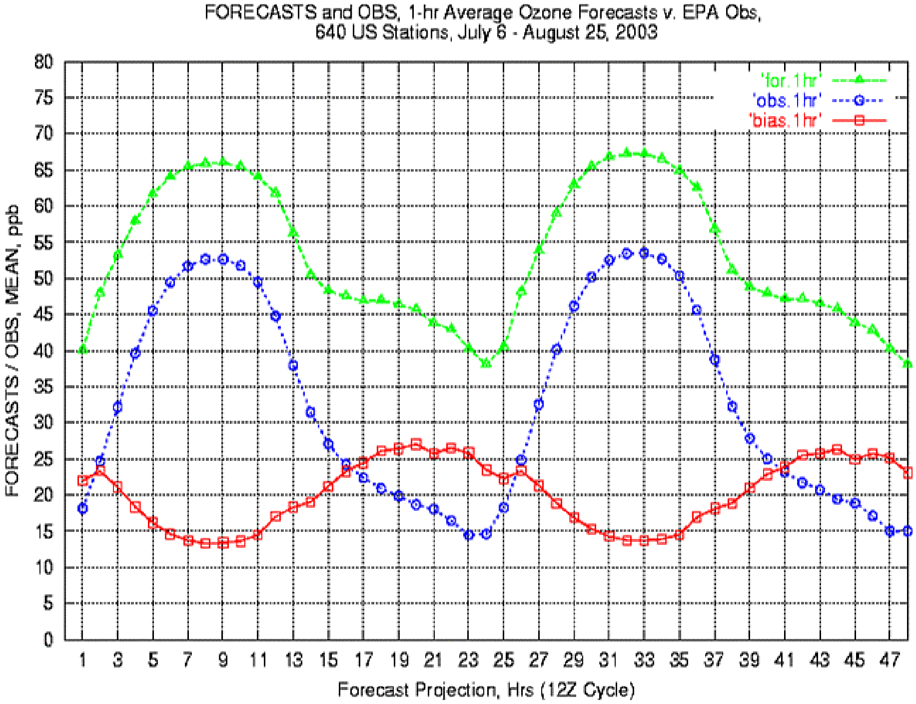

Figure 5. Mean predicted CMAQ ozone concentration (ppb, green line), AIRNOW observed (blue line, excluding Canadian Stations) and bias error (red line) by forecast hour for all available 12 UTC cycle CMAQ predictions from July 7 through August 25, 2003.

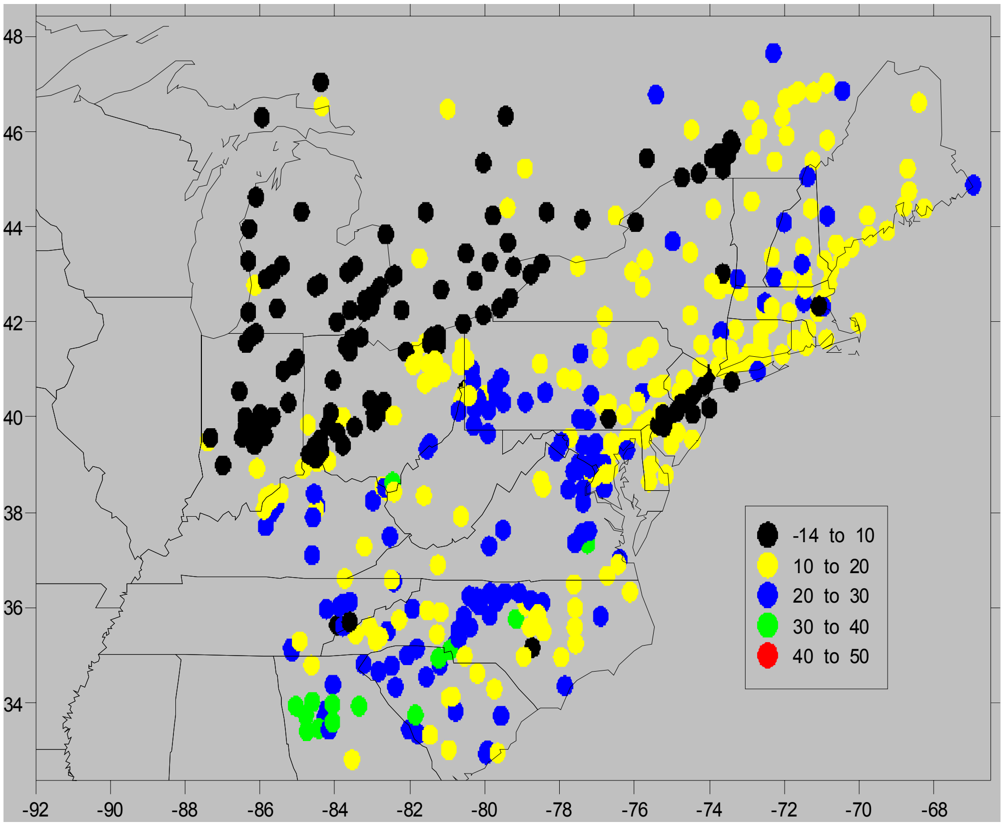

Figure 6. Mean bias of CMAQ 12 UTC cycle maximum 1-hour surface ozone predictions (ppb) vs. AIRNOW observations. CMAQ forecasts compared for all runs from July 7-August 31, 2003.