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Eta-CMAQ modeling system's capability to provide PM2.5 and aerosol optical thickness forecast

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1. INTRODUCTION

In 2003, NOAA and the U.S. EPA signed a Memorandum of Agreement to work together to develop a National Air Quality Forecasting (AQF) 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 Northeastern U.S. (Davidson et al, 2004). The NWS / National Center for Environmental Prediction (NCEP) Eta model at 12 km was used (Rogers et al, 1996), to drive the EPA Community Multi-scale Air Quality (CMAQ) model (Byun et al, 1999) to produce up to 48 hour ozone predictions.

From the outset of the AQF System (AQFS) design, there has been considerable commitment to include predictions of fine particles with diameter less than 2.5 μm (PM2.5). High volume of particle-matter suspended in the atmosphere is hazardous to human health and impairs visibility. The scientific challenges accompanied with PM2.5 modeling and verification are manifold. It involves better understanding of complex aerosol microphysics and chemistry (e.g., particle size distributions), multi-phase constituent dynamics, and

heterogeneous chemical reactions. Preliminary works on PM2.5 modeling demonstrated the difficulty of getting the correct speciation and their partitioning (Morris et al, 2004). In general uncertainties in PM2.5 modeling arise from uncertainties in emissions from wild fires, sea salt and crust soil sources of particles.

In lieu of all these necessary pieces of revamping on PM2.5 modeling, the current work is a simple illustration of one of the potential methodologies NOAA/EPA is pursuing to provide numerical forecast guidance for two additional 2-D surface fields: PM2.5 concentration, and Aerosol Optical Thickness (AOT). The following sections describe some model assumptions of the CMAQ aerosol module, and the methodology to derive the PM2.5 and AOT fields. Finally a preliminary comparison will be conducted using imageries from the GOES satellite system (NOAA, 2004a) for a high ozone/PM2.5 episode occurred on July 22, 2004.

2. DERIVING PM2.5 AND AOT

CMAQ's aerosol module adopts a modal approach to represent the particles suspended in air (Binkowski and Roselle, 2003; Mebust et al, 2003). It uses the superposition of 3 log-normal sub-distributions to represent the size distribution of these particles. PM2.5 are represented by two of these sub-distributions called the Aitken (i), particles have diameters up to 0.1 μm , and the accumulation (j), particles have diameters between 0.1 and 2.5 μm , modes. The third modal sub-distribution represents particles of the coarse mode, particles have diameters between 2.5 to 10 μm . Table 1 shows the speciation of the particles in the i and j modes. The i mode particles usually represent particles freshly formed from nucleation or from direct emission, whereas the larger j mode particles represents aged particles. The chemical species treated in these modes are also tabulated in Table 1.

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Table 1. Speciation and variable name used in the CMAQ aerosol module

Species description	Name
Accumulation mode sulfate mass	ASO4J
Aitken mode sulfate mass	ASO4I
Accumulation mode ammonium mass	ANH4J
Aitken mode ammonium mass	ANH4I
Accumulation mode nitrate mass	ANO3J
Aitken mode nitrate mass	ANO3I
Accumulation mode anthropogenic secondary organic mass	AORGAJ
Aitken mode anthropogenic secondary organic mass	AORGAI
Accumulation mode primary organic mass	AORGAJ
Aitken mode primary organic mass	AORGPAI
Accumulation mode secondary biogenic organic mass	AORGBJ
Aitken mode secondary biogenic organic mass	AORGBI
Accumulation mode elemental carbon mass	ACEJ
Aitken mode elemental carbon mass	ACEI
Accumulation mode unspecified anthropogenic mass	A25J
Aitken mode unspecified anthropogenic mass	A25I
Accumulation mode water mass	AH2OJ
Aitken mode water mass	AH2OI

The model treats the interaction between these fine modes and the coarse mode in a one-way merging manner into the coarse mode, when the fine modes particles grow beyond 2.5 μm in diameter. However, there is no implementation of coagulation between the fine modes and the coarse mode. A justification of such a simplification is discussed in Binkowski and Roselle (2003). The coarse mode modeling has not been emphasized due to the large uncertainty in the determination of its emissions. By the same token, the current CMAQ model does not include coarse mode particles in its visual range calculations. Therefore the AOT calculation in AQF does not account for the effect of coarse mode particles. The fine mode particles also participate in cloud micro-physics. The assumptions of the CMAQ aerosol module in relation to cloud activity are: (1) the i mode particles form the interstitial aerosols subjected

to in-cloud scavenging, (2) the j mode particles form cloud condensation nuclei which are subjected to redistribution within the cloud water, (3) all new sulfate mass produced by aqueous phase production is added to the j mode, (4) the shape of the j mode size distribution, quantified by the geometric standard deviation σ_g , stays constant throughout a cloud's lifetime, and (5) the i and j mode particles are wet removed in proportion to that of sulfate wet scavenging.

In the aerosol module, the equilibrium of the sulfate, nitrate, ammonium and water system is considered. This assumption is used due to the large uncertainty about the sea salt and soil particle data to validate a more vigorous methodology.

It is these interplays of the gaseous, heterogeneous, and aqueous phase chemistry that governs the growth of the i and j mode particles. The size and number distribution of these particles in turn govern the visibility calculation. A visibility calculation measures the furthest distance one can see and identify an object in the atmosphere. Conversely, since atmospheric particles reflect and absorb light, AOT is a measure of visibility impairment due to the existence of these particles. AOT, a dimensionless quantification of visibility impairment, is defined in the following equation.

$$AOT = \int_0^{ModelTop} B_{sp} dz$$

Where B_{sp} is the aerosol extinction coefficient in km^{-1} , z is altitude in km. CMAQ calculates B_{sp} through Q_{ext} , the extinction efficiency, a measure of light scattering efficiency which in turn is estimated using approximations to the Mie theory (Binkowski, 1999):

$$B_{sp} = \frac{3\pi}{2\lambda} \int_{-\infty}^{\infty} \frac{Q_{ext}}{\alpha} \frac{dV}{d \ln \alpha}$$

Where $\alpha = \pi D / \lambda$, D is the particle diameter, V is the volume of the particle, and λ is the wavelength of the incident light.

3. EXAMPLES OF PM2.5 AND AOT FIELDS

Figures 1b and 2b show the overlays of these two additional predicted 2-D fields which the AQFS is capable of producing as examples on July 21st and 22nd at 19 UTC. In these simulations CMAQ was spun-up for 3 and 4 days respectively starting on July 17th, 2004. The shaded fields, using the side color bar color code, depict the dimensionless AOT field. It was obtained by evaluating Equations (2) and (1) through the use of predicted instantaneous aerosol concentrations. The colored line contours depict PM_{2.5} concentrations in $\mu\text{g m}^{-3}$. They sum up all the aerosol masses tabulated in Table 1 at the first layer of the CMAQ model. During this particular period, some rather large Alaskan fires had been burning since late June 2004 (NOAA, 2004b), resulting in smoke particle plumes that were transported into the central and eastern U.S. These particle emissions are not accounted for in the model. EPA AIRNOW observations (EPA, 2004) showed that this 2-day pollution episode affected most noticeably the cities of NYC, Philadelphia, and Atlanta (Fig. 1a and 2a). On July 21st and 22nd, surface ozone concentrations were high along the NYC to Philadelphia Corridor and around Atlanta, GA, which were both at around 105 ppb for their daily 1 h averaged maximum.

In terms of observed PM_{2.5}, Figures 1a and 2a show data from the AIRNOW PM_{2.5} network (EPA, 2004). The data provided by AIRNOW are daily averages from 4 UTC the current day to 4 UTC the next day. For the July 21st results, there was spatial agreement between the PM_{2.5} fields (Fig. 1a and b). The peaks on either sides of Lake Erie and around Philadelphia, PA, were captured by the AQFS simulation. AIRNOW indicated a concentration level of 30-40 $\mu\text{g m}^{-3}$, while AQFS consistently under-predicted concentrations at around 20-25 $\mu\text{g m}^{-3}$. Similar performance can also be seen in the July 22nd results. The peak PM_{2.5} concentration band along the NYC – Philadelphia Corridor were reproduced, as were the peaks around central, NC and Atlanta, GA. AIRNOW observed PM_{2.5} concentrations of 30-40 $\mu\text{g m}^{-3}$ for these peaks, while AQFS was able to locate these local peaks, yet their predicted magnitudes were consistently deficient by 10-15 $\mu\text{g m}^{-3}$ compared to observed values. The bias can partially be attributed to the neglect of the wild fire emissions to the west of the AQFS domain. Improvement of the aerosol concentration boundary conditions will be

considered to address these situations and other situations, such as volcanic eruptions in the upcoming implementation of AQFS at NOAA.

To evaluate the model predicted AOT we used observations from the GOES Imager because of its diurnal coverage. Satellite sensors such as MODIS (IDEA, 2004), which also observe AOT from polar-orbiting satellites only once a day, do not offer much information to track changes in aerosol composition during the day.

The cloudiness around the Great Lakes shown in Figures 1c and 2c was a result of two warm fronts: one spanning on the south skirt of the lakes, and the other spanning north of the lakes lying North of the U.S.-Canadian border. Temperatures in Eastern U.S. were slightly higher than seasonal norms with daily maximum temperatures in the 30-32°C range for all three locations for the days in question.

The predicted AOT values did not match well with those observed by GOES. Despite the fact that the model captured the peaks over Lake Erie and a high AOT value band between offshore MA to offshore NC, the magnitudes predicted were around 0.3-0.5 compared to the observed 0.7-0.9. The model did not capture the high values in the southern states. On July 22nd, the cloudiness in the Mid-Atlantic region and in the areas north of it voided the opportunity for comparison, as shown in Figure 2c. The model captured the peaks between Raleigh, NC, and Atlanta, GA. The model predicted the values of AOT for these locations to be around 0.5 while the satellite data indicated that observed values lay between 0.7 and 1.0. The under prediction of AOT values can be partially explained by the incomplete representation of aerosol sources from forest fires. In addition to this, other uncertainties might exist in the model physics and chemistry.

4. VERIFICATION METHODOLOGY

Quantitative evaluation procedures, similar to those used for surface ozone forecast, for CMAQ predicted AOT will be developed in the future. For the ozone forecast, which became operational at NWS lately, the NOAA Forecast Verification System (FVS) has been used to provide model verification (Tsidulko et al, 2004). This system can be used as a model for PM_{2.5} and AOT forecast verifications. The EPA AIRNOW site provides continuous PM_{2.5} measurements. In addition to the AIRNOW data,

automated near real time comparison between the AQFS AOT forecasts and the satellite observed AOT measurements will be useful to evaluate the atmospheric particle forecast system.

5. SUMMARY

The NOAA/EPA AQFS had been used to make a rough estimate of surface level PM_{2.5} and AOT for a pollution episode occurred in July, 2004. The results have been qualitatively compared against AIRNOW's PM_{2.5} observations and AOT imageries obtained from the GOES Imager. Verification tools aimed at utilizing NOAA's FVS systems are under development.

6. ACKNOWLEDGEMENT AND DISCLAIMER

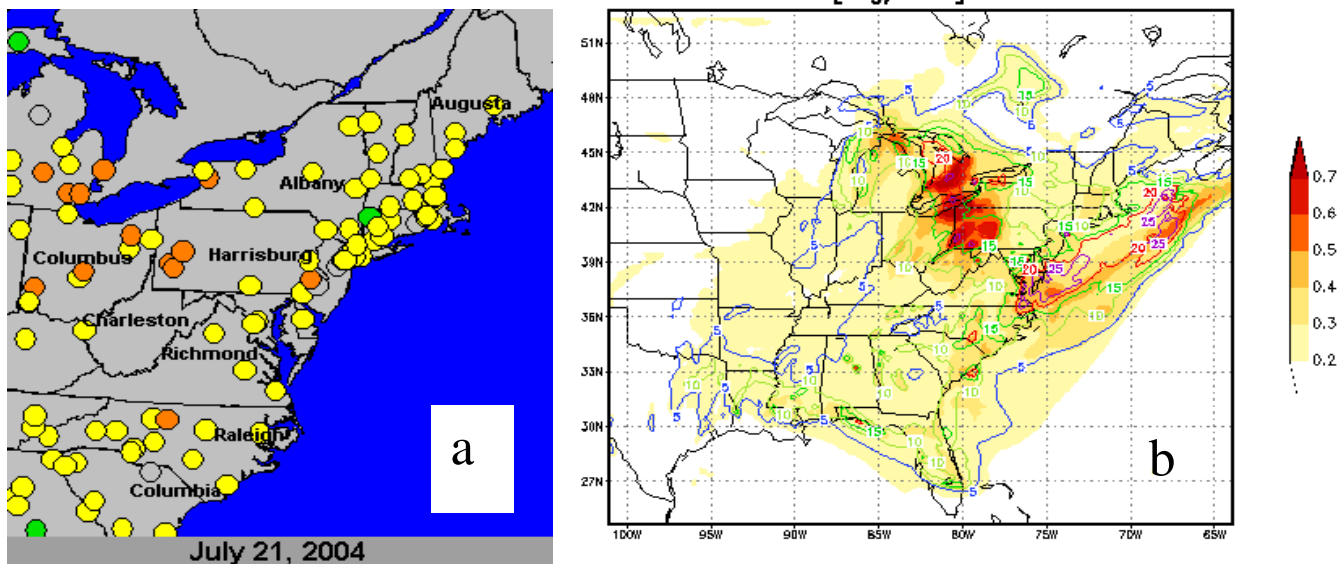
The views expressed are those of the authors and do not necessarily represent those of NOAA or the EPA. The EPA AIRNOW program staff provided the observations necessary for quantitative model evaluation.

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AOT and PM2.5 contours [mg/m³] 07H VALID 19Z 21 JUL2004



GASP Aerosol Optical Depth 19:45UTC 7/21/04

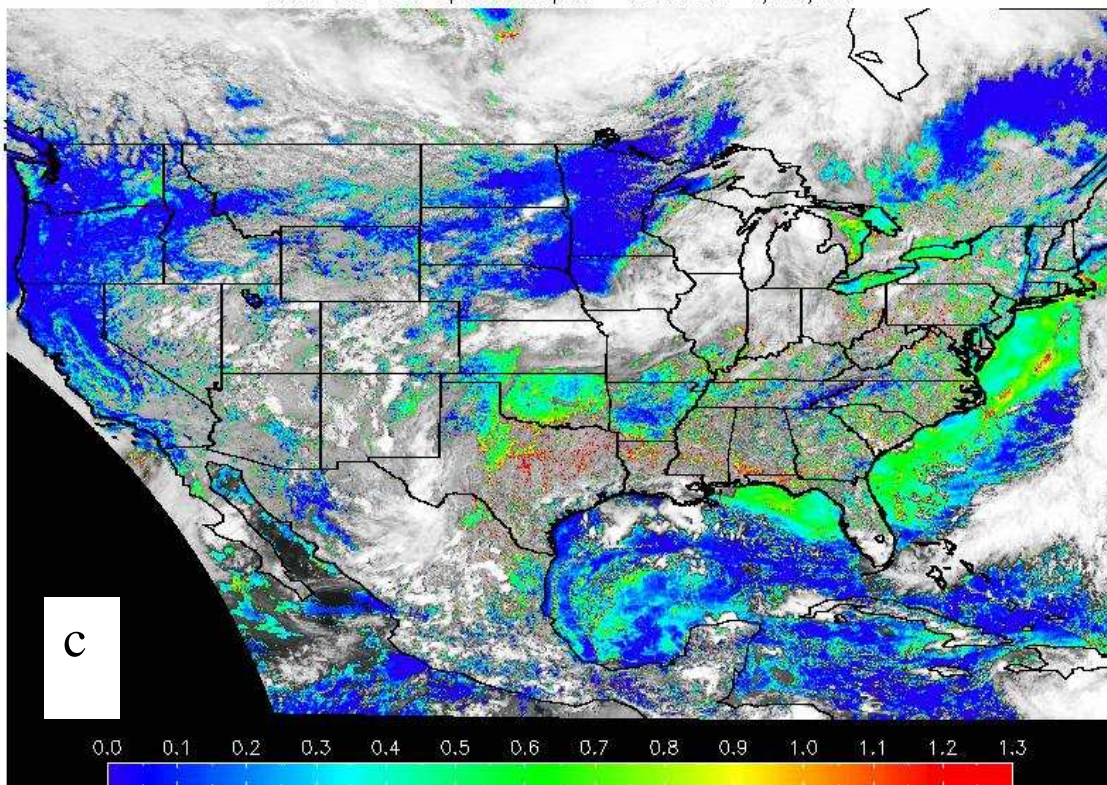
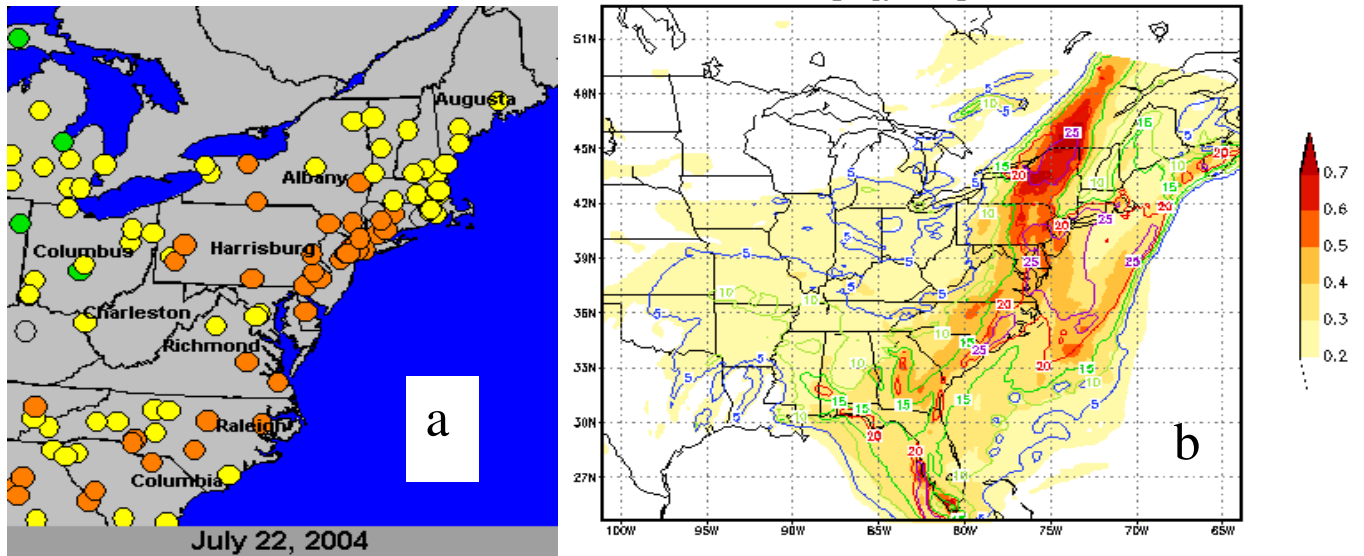


Figure 1: Predicted and observed surface level AOT and PM2.5 values valid at around 19 UTC July 21, 2004: (a) Observed daily average PM2.5 by the AIRNOW network where green, yellow and orange data points represent concentration between 10 and 20; between 20 and 30; and between 30 and 40 $\mu\text{g m}^{-3}$ respectively, (b) AQFS predicted AOT, color shaded in accordance with the side color bar; and PM2.5, colored contour lines with labels, and (c) GOES imagery on AOT with cloud.

AOT and PM2.5 contours [mg/m³] 07H VALID 19Z 22 JUL2004



GASP Aerosol Optical Depth 19:45UTC 7/22/04

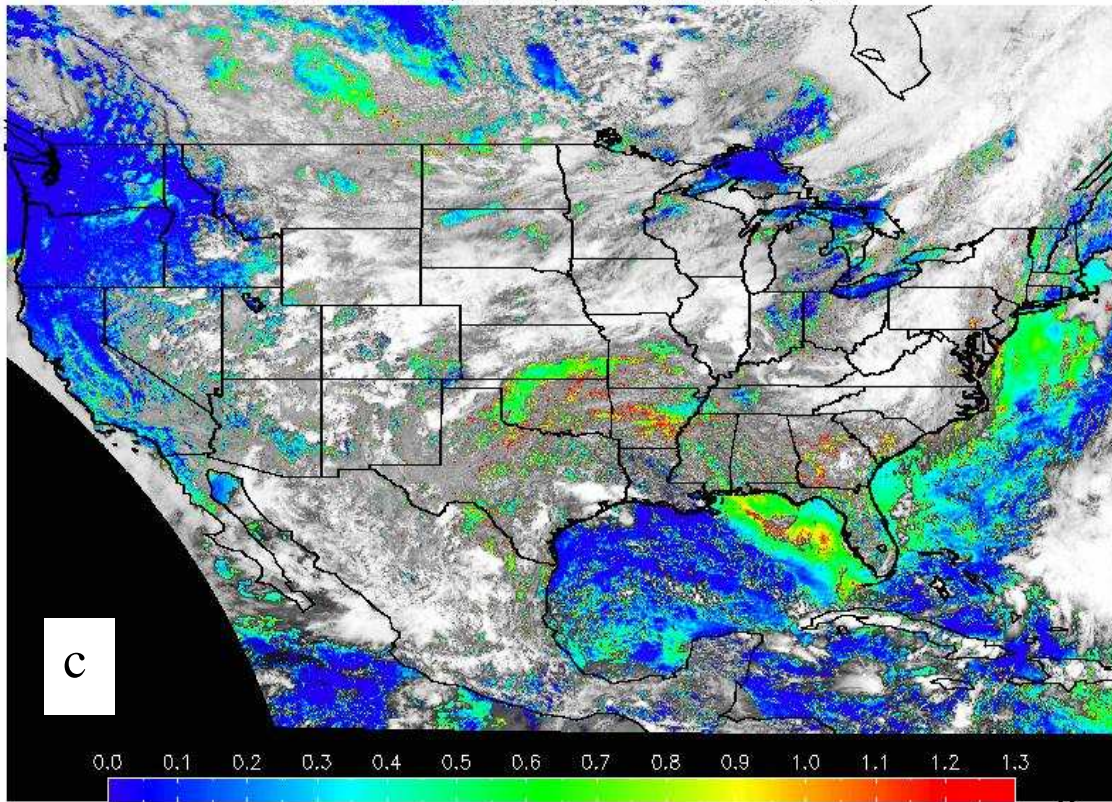


Figure 2: Same as Figure 1 but for July 22, 2004.