VERIFICATION OF NOAA-EPA DEVELOPMENTAL AEROSOL FORECASTS

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1. INTRODUCTION

Since July 2006, the Meteorological Development Laboratory (MDL) has provided categorical verification metrics for aerosol forecasts. The Air Quality Forecasting (AQF) system links the National Centers for Environmental Prediction's (NCEP) North American Mesoscale (NAM) model with EPA's Community Multiscale Air Quality (CMAQ) modeling system to produce gridded 1-h ground-level aerosol predictions for the developmental (5x) conterminous U.S. (CONUS) domain (Binkowski and Roselle 2003). We used bilinear interpolation to calculate predicted daily maximum values at the locations of the observation sites. We compared these interpolated predicted values to the observed daily maximum to produce 2x2 contingency tables, with a threshold of 40 $\mu gm/m^3$. Our verification metrics included Percent Correct (FC), Threat Score (TS) or Critical Success Index (CSI), Probability of Detection (POD), and the False Alarm Rate (FAR). We populated two-by-two contingency tables as follows:

	Observed
Forecast	| a | b |
	| c | d |

where,
a = forecast, observed (yes/yes)
b = forecast, no observed (yes/no)
c = no forecast, observed (no/yes)
d = no forecast, no observed (no/no).

The corresponding scores were computed as follows:

$$PC = (a + d)/(a + b + c + d) \times 100 \quad (1)$$
$$TS = a/(a + b + c) \quad (2)$$
$$POD = a/(a + c) \quad (3)$$
$$FAR = b/(a + b) \quad (4).$$

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For a more detailed discussion about 2x2 contingency table analyses, see Wilks (1995).

We computed weekly statistics displayed in the form of bar charts, scatterplots, and graphs. Spatial maps showed daily maximum predicted aerosol values overlaid with the corresponding point observations.

In this paper we describe how the CMAQ model was configured to handle aerosol predictions. We evaluated the daily maximum of 1-h average predictions over the CONUS and over six sub-CONUS regions. We also provide verification results of the daily maximum of the 24-h running average over the CONUS.

2. AEROSOLS

CMAQ's aerosol module takes a modal approach to represent the particles suspended in air (Binkowski and Roselle, 2003 and Mebust et al., 2003). The module uses the superposition of 3 log-normal sub-distributions to represent the size distribution of these particles. Aerosols are represented by two of these sub-distributions called the Aitken (i) particles with diameters up to 0.1 µm, and the accumulation (j) particles with diameters between 0.1 and 2.5 µm. The third modal sub-distribution represents particles of the coarse mode, particles with diameters between 2.5 to 10 µm. Table 1 shows the types 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 represent aged particles.

The model approach treats the interaction between the fine modes and the coarse mode as follows. When the fine mode particles grow beyond 2.5 µm in diameter, they are merged into the coarse mode. But once the fine mode particles are merged into the coarse mode, they can not go back to the fine modes again. In the CMAQ model, there is no mechanism for fine particles to coagulate with coarse particles nor is there a mechanism for fine particles to be transferred to the coarse mode via condensational growth. These processes are thought to be of minor importance.

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	AORGPAJ
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

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. 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 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-mode and j-mode particles are wet removed in proportion to that of sulfate wet scavenging.

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

For the purpose of comparing modeled values to observed (2.5 μm) mass, predicted (2.5 μm) mass is derived by summing the masses of the species from Table 1. Here, (2.5 μm) is defined as particulate matter with diameter less than or equal to 2.5 μm. Particle bound water (i.e., AH2OI and AH2OJ) is excluded from this derivation of predicted (2.5 μm) mass.

3. AEROSOL VERIFICATION FOR CONUS

During 2007, MDL generated categorical verification metrics for the CONUS developmental (5x) domain. All daily maxima of 1-h average aerosol predictions or observations that were equal to or greater than the threshold during a predefined 24-h period were counted as exceedances. The 24-h window for counting exceedances was midnight to midnight, beginning at hour 22 for the 0600 UTC CMAQ forecast period. The EPA provided ozone observations for 661 sites within the CONUS domain. If an observation or interpolated model prediction for a station was missing, we excluded that station from our calculations.

Fig. 1 shows a comparison of the percent correct of the daily maximum of 1-h average predictions (in blue) and the daily number of observed exceedances (in red), for May 29–August 30, 2007. There were several drops below 80%. Comparing the two plots in Fig. 1, we can see that decreases in the percent correct were associated with elevated aerosol episodes. There were six days in the sample period where 100 or more observed exceedances occurred, namely, June 1, June 18, June 26, July 4, August 3, and August 16. On these days, the percent correct dropped below 80%. During elevated aerosol episodes, there is greater potential for false alarms and missed exceedance predictions.

Fig. 2 is a map of aerosol predictions and observations, for the daily maximum of the 1-h average for August 3, 2007. The predicted exceedances are shown in dark blue and the observed exceedances as red points. Table 2 shows monthly scores derived from contingency tables for March–August, 2007. The total number of cases for May was below 10,000 because observations were missing for May 20–28, 2007.

4. REGIONAL AEROSOL VERIFICATION

Fig. 3 shows a map of the CONUS broken into six regions (Mathur, 2006). This map was previously used for regional analyses of CMAQ ozone predictions. We evaluated the CMAQ aerosol forecasts for these six regions. We compared monthly verification results for the Pacific Coast (PC), Rocky Mountains (RM), Lower Midwest (LM), Upper Midwest (UM), South East (SE), and Northeast (NE). Fig. 4 shows the monthly TS for the six regions for March–August, 2007. The Pacific Coast (PC) had the highest TS in June but it dropped in August because of a high FAR. Table 3 shows the regional contingency table for June, 2007. The CMAQ model seemed to handle the aerosol activity in the PC region better than in the other regions. Fig. 5 shows a scatterplot for the PC region for June, 2007. Vertical and horizontal pink lines at 40 $\mu gm/m^3$ split the scatterplot into four quadrants. Under-forecasts of exceedance predictions are shown in the upper left quadrant. Over-forecasts are shown in the lower right quadrant. Except for a cluster of under-forecasts for predictions < 15 $\mu gm/m^3$, the model showed some degree of skill. There were a few more over-forecasts of predictions > 40 $\mu gm/m^3$, than under-forecasts.

Fig. 6 shows the monthly regional bias for the 1-h average aerosol predictions for August, 2007. The x-axis shows the forecast projection by hour. The vertical lines at projections 22/46 show midnight, UTC. The PC region shows the highest bias. All regions over-predict a diurnal drop in aerosol concentrations. Fig. 7shows the monthly regional Mean Absolute Error (MAE) for August, 2007. The PC region shows the highest diurnal variation in MAE, while the UM region shows the lowest. Fig. 8 shows the monthly regional mean observations for August, 2007. The PC region shows the lowest mean of all of the regions. The SE and UM regions show a morning spike near projection 7 (0900 UTC).

5. DAILY MAXIMUM OF 24-H RUNNING AVERAGE

MDL used one hour average model predictions to produce spatial maps of the daily maximum of the 24-h running average. We evaluated these model predictions by generating 24-h running averages from the 1-h average observations provided by the EPA. We produced 2x2 contingency tables using a threshold of 40 $\mu gm/m^3$.

Fig. 9 shows a comparison of the percent correct of the daily maximum of the 24-h running average predictions (in blue) and the daily number of observed exceedances (in red), for June 2-August 30, 2007. Notice that there are fewer observed exceedances in Fig. 9 than Fig. 1. Fig. 9 shows similar behavior to Fig. 1, decreases in the percent correct were associated with elevated aerosol episodes. We can see that except for August 5 (percent correct = 89.4), the percent correct of the daily maximum of the 24-h running average predictions stayed above 90% for the entire period. The daily maximum of the 24-h running average predictions had better percent correct scores than the daily maximum of the 1-h average because the 24-h running average predictions contained much fewer observed threshold exceedances than the 1-h average predictions. MDL also produced spatial maps of the daily maximum of the 24-h running average. Fig. 10 is a map of aerosol predictions and observations, for the daily maximum of the 24-h running average for August 3, 2007. As with the 1-h maps, predicted exceedances are shown in dark blue and the observed exceedances as red points.

6. CONCLUSIONS

The CMAQ model was configured to produce gridded 1-h ground-level aerosol predictions for the 5x CONUS domain. MDL computed verification metrics of the daily maximum of the 1-h aerosol predictions over the CONUS as well as for six regions. MDL derived the daily maximum of the 24-h running average predictions from 1-h aerosol predictions over the CONUS domain. We evaluated these predictions by deriving 24-h running averages from the 1-h average observations provided by the EPA. State and local authorities are interested in the 1-h average aerosol predictions and the 24-h running average predictions. Daily maps of the 1-h average and 24-h running average were provided to aid the modelers in their development. The maps showed where missed exceedance predictions were located. This information was useful for investigating systematic under prediction or over prediction issues in selected geographic areas.

7. ACKNOWLEDGMENTS

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8. REFERENCES

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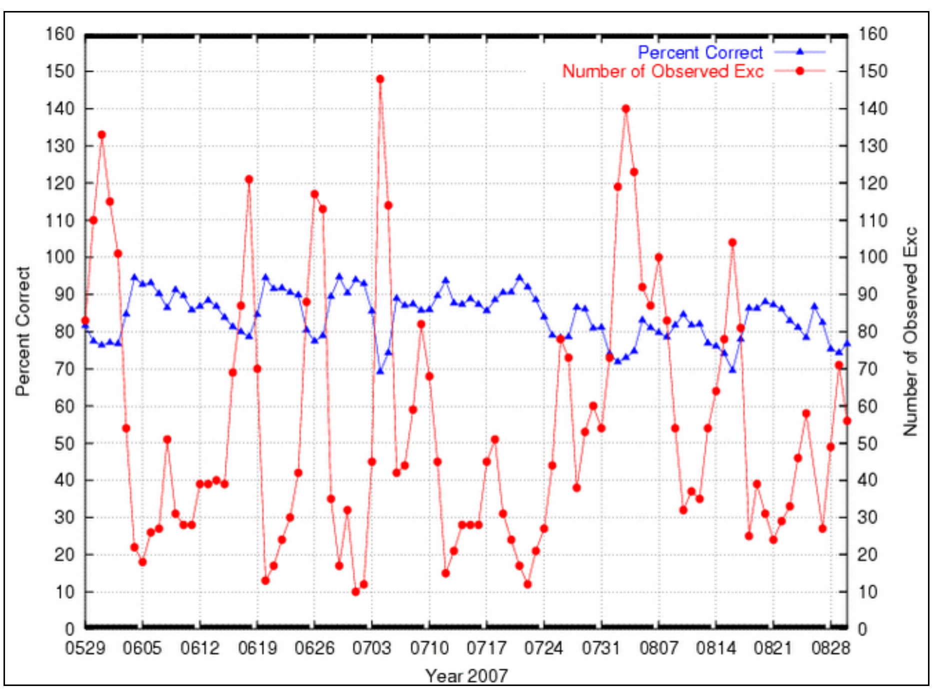

Figure 1. Percent correct vs. number of observed exceedances, daily maximum of 1-h average aerosol predictions, May 29–Aug 30, 2007.

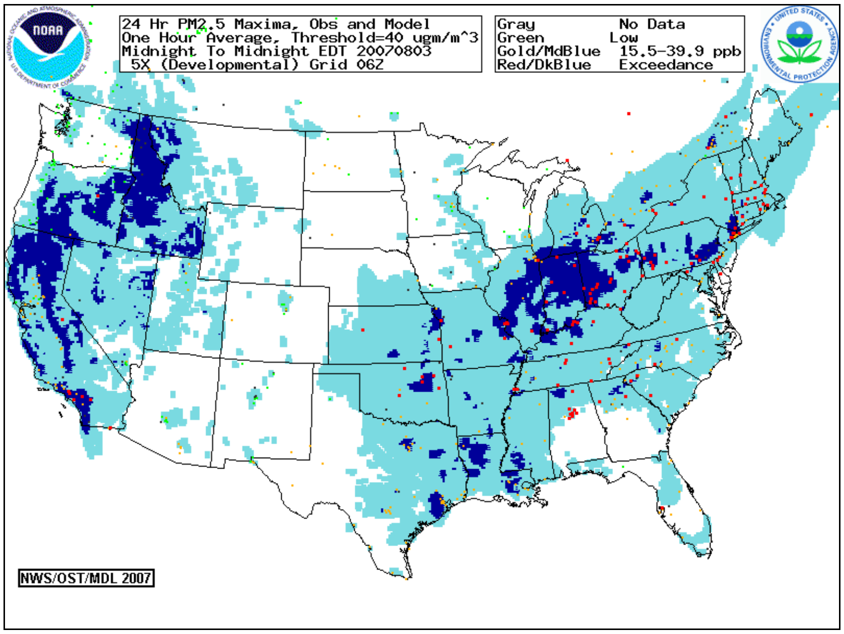

Figure 2. Daily maximum 1-h aerosol predictions and observations, Aug 3, 2007.

Table 2. Contingency table results for CONUS, 2007, daily maximum of 1-h average aerosol predictions.

SCORE	March	April	May	June	July	August
a	247	79	147	347	309	524
b	542	358	431	761	1019	1686
c	862	469	701	1081	1098	1318
d	12430	13006	8575	12285	12547	11264
PC	0.900	0.941	0.885	0.873	0.859	0.797
TS	0.150	0.087	0.115	0.159	0.127	0.149
POD	0.223	0.144	0.173	0.243	0.220	0.284
FAR	0.687	0.819	0.746	0.687	0.767	0.763

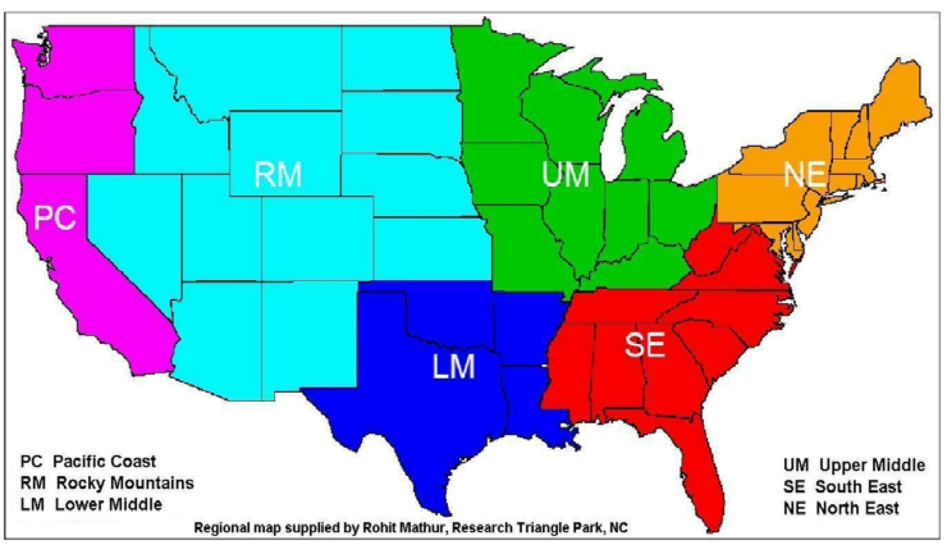

Figure 3. Map of the U.S. showing six regions, Pacific Coast (PC), Rocky Mountains (RM), Lower Midwest (LM), Upper Midwest (UM), South East (SE), and Northeast (NE).

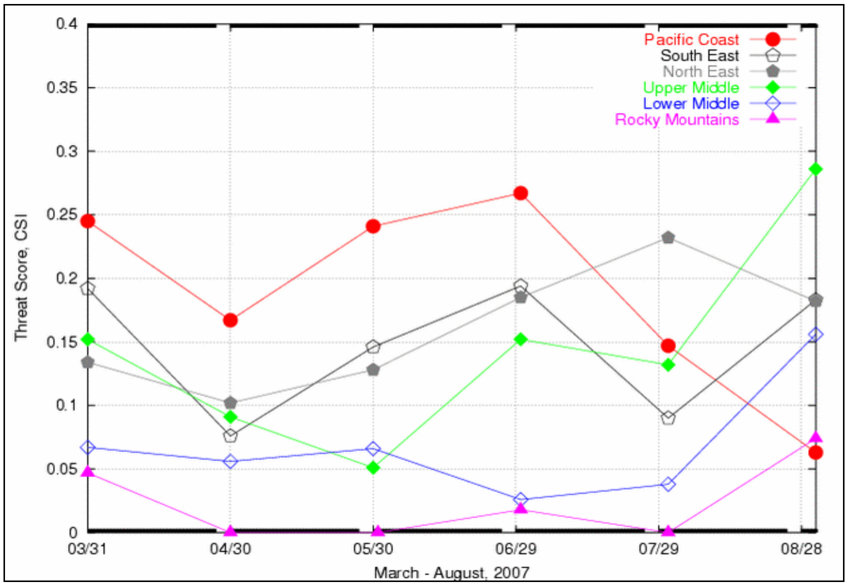

Figure 4. , Monthly average, threat score for the six regions, Mar–Aug, 2007.

Table 3. Regional contingency table results, June, 2007, daily maximum of 1-h average predictions.

SCORE	CONUS	LM	NE	PC	RM	SE	UM
a	347	4	89	52	3	95	75
b	761	104	105	68	98	194	90
c	1081	44	286	75	68	201	329
d	12285	1407	1361	2300	1390	1644	2181
PC	0.873	0.905	0.788	0.943	0.894	0.815	0.843
TS	0.159	0.026	0.185	0.267	0.018	0.194	0.152
POD	0.243	0.083	0.237	0.409	0.042	0.321	0.186
FAR	0.687	0.963	0.541	0.567	0.970	0.671	0.545

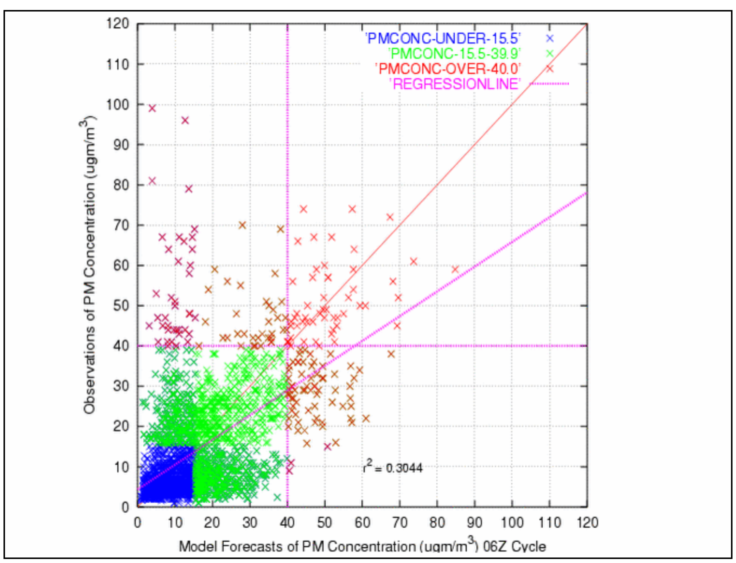

Figure 5. Scatterplot for Pacific Coast (PC) region, June, 2007, daily maximum of 1-h average predictions.

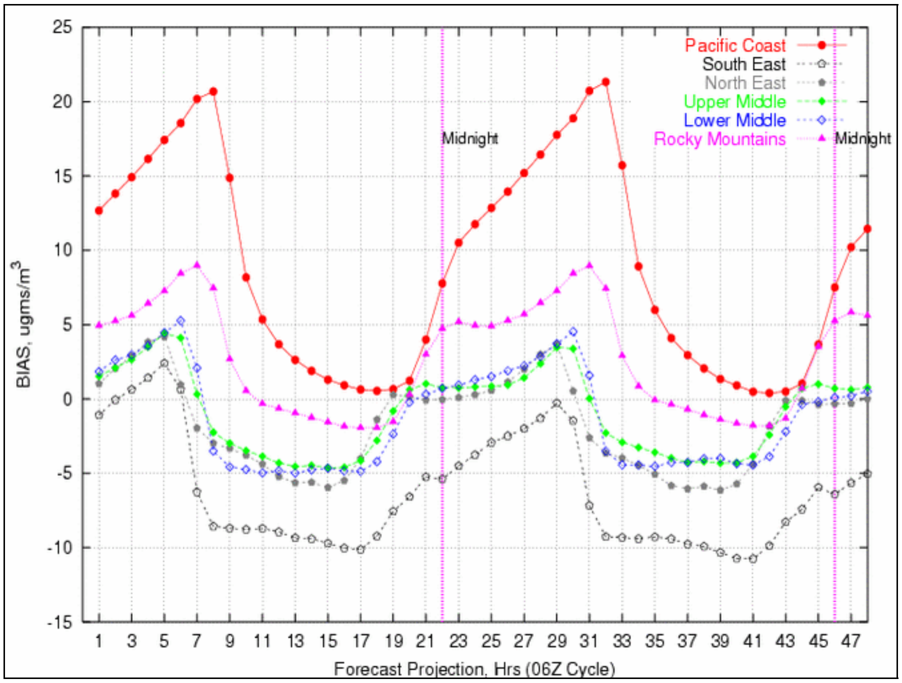

Figure 6. Monthly regional bias, by projection, 1-h average aerosol predictions, August, 2007.

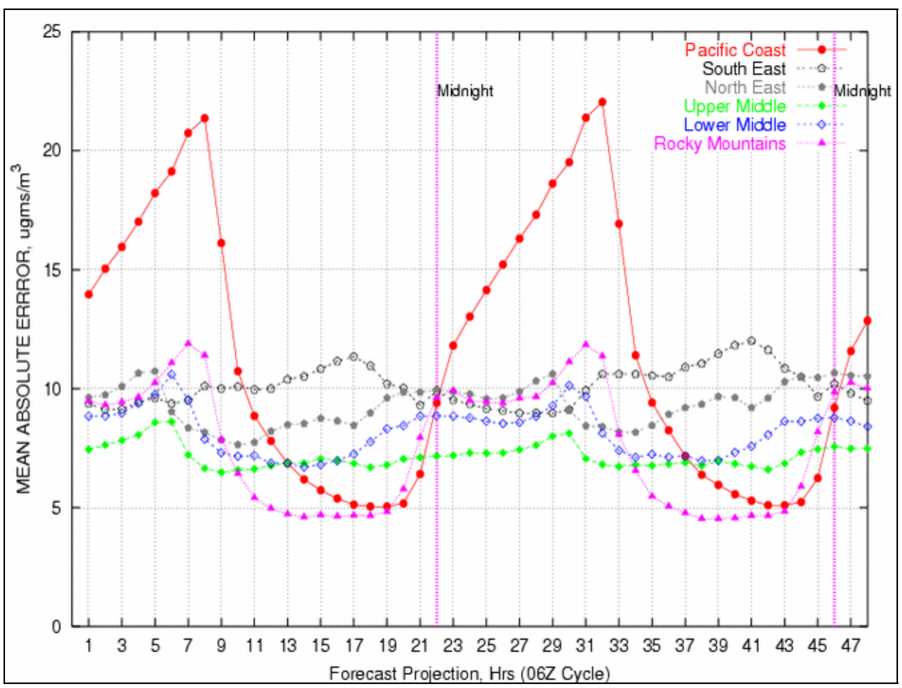

Figure 7. Monthly regional MAE, by projection, 1-h average aerosol predictions, August, 2007.

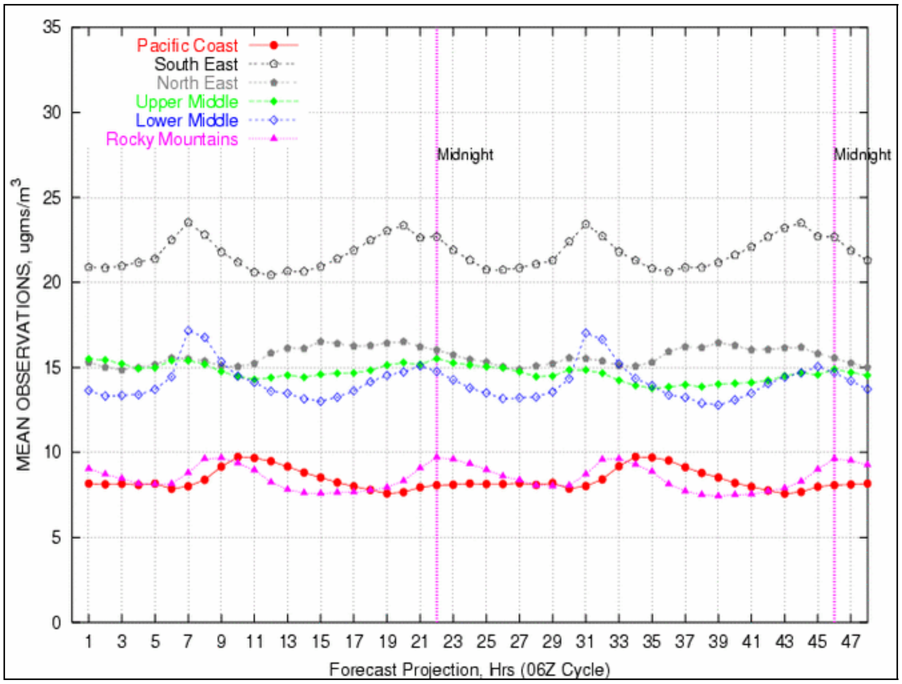

Figure 8. Monthly regional mean observations, 1-h average aerosol predictions, August, 2007.

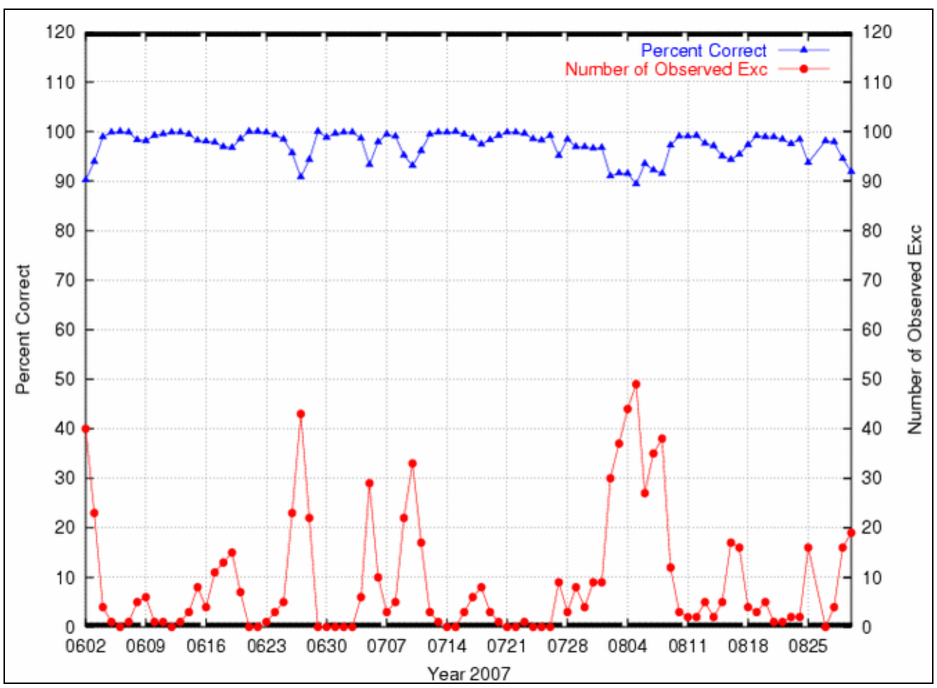

Figure 9. Percent correct vs. observed exceedances, daily maximum of 24-h running average aerosol predictions, Jun 2–Aug 30, 2007.

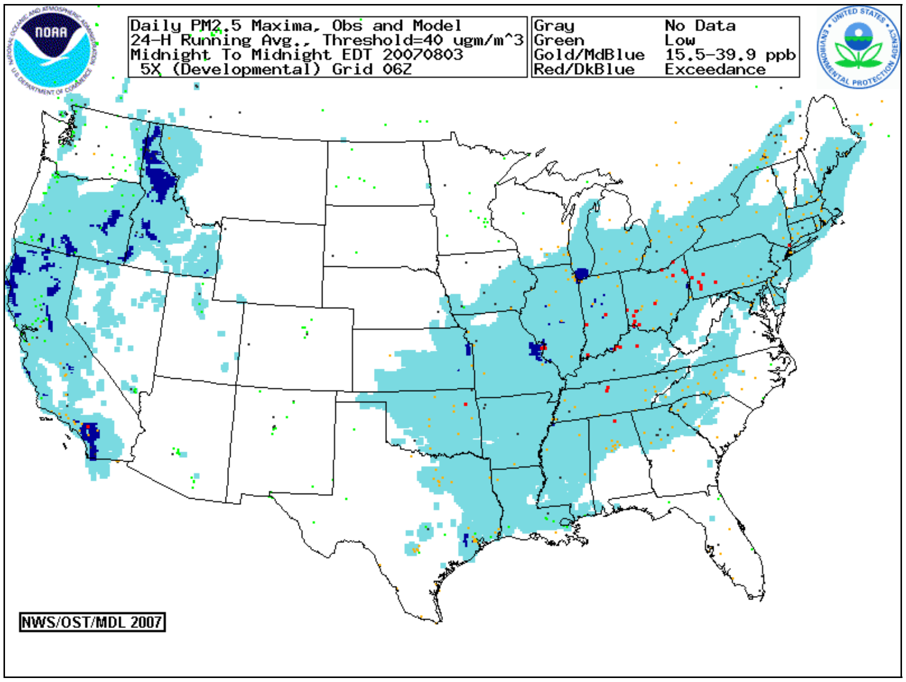

Figure 10. Daily maximum of 24-h running average aerosol predictions and observations, August 3, 2007.