CMAQ Model Performance Evaluation for 2001: Updated March 2005

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I. Introduction

This report documents an evaluation of the Community Multiscale Air Quality Model (CMAQ) in comparison to ambient measurements[1]. The focus of this evaluation is PM2.5 species, visibility, and deposition. A comparison of model predictions to observations for PM2.5 precursor gases is also included in the analysis, to the extent that such data were available. The analysis was conducted in support of the Clean Air Interstate Rule (CAIR) which used CMAQ as the modeling tool to project PM2.5, visibility, and deposition for future case emissions scenarios. A description of CMAQ, references for this model, and details on the CMAQ model applications for CAIR can be found in the CAIR air quality modeling technical support document (AQMTSD) (EPA 2005a).

For this evaluation CMAQ was run for the year 2001 using a modeling domain covering the continental U.S. and adjacent portions of Mexico and Canada. Figure 1 shows a map of this domain. The 2001 model run was made using a horizontal grid resolution of 36 x 36 km. Year-specific meteorology, anthropogenic and biogenic emissions, and boundary conditions were used to drive the 2001 simulation. Additional information on the 2001 CMAQ model run and input data sets can be found in the AQMTSD and CAIR emissions inventory technical support document (EPA 2005b).

As noted above, this evaluation covers PM2.5 (specifically the component species: sulfate, nitrate, elemental carbon, organic carbon), visibility, and deposition (specifically: deposition of ammonium, nitrate, and sulfate). In addition, we have compared the CMAQ predictions to measurements of selected precursor gases including: ozone, sulfur dioxide, nitric acid, and nitrogen oxide. The analysis of precursor gases was limited by the extent of measurements available for these pollutants in 2001. As described below, we have examined model performance using a combination of traditional performance statistics and selected graphical techniques. The graphics include scatter plots of observed versus predicted concentrations, spatial plots, and time series plots.

Model performance for PM2.5 species, particularly sulfate and nitrate, is most important for the purposes of CAIR given that this rule prescribes emissions reductions of sulfur dioxide (SO2) and nitrogen oxides (NOx), which are fundamental to the formation of these two PM2.5 species. There are no universally accepted quantitative criteria for judging the adequacy or acceptability of model performance for PM2.5 species. However, in the absence of acceptance criteria, we have judged the performance of our 2001 CMAQ application by comparing our results to the range of performance obtained by other groups in the air quality modeling community who have conducted recent regional PM2.5 model applications.

The next section of this report (Section II) describes the analytical approach including (1)

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[1] This evaluation includes updates to the CMAQ Model Performance Evaluation Report of August 2004 (CAIR Docket OAR-2003-0053-1716).

a brief overview of the ambient monitoring data (i.e., observations) used in this analysis and the procedures for mapping observations to the corresponding CMAQ predictions and (2) a description of the statistical and graphical techniques. In Section III we present the performance results for PM2.5, visibility, and deposition. A comparison of our CMAQ performance for PM2.5 species to that of other regional model applications is also included in Section III. Finally, we provide the performance analysis for precursor gases in Section IV.

Figure 1. CMAQ Modeling Domain

II. Analytical Approach

A. Overview of Monitoring Data Used in this Analysis

This evaluation includes measurements from the following networks:
Clean **A**ir **S**tatus and **T**rends **Net**work (CASTNet);
Speciation **T**rend **N**etwork (STN);
Interagency **M**onitoring of **PRO**tected **V**isual **E**nvironments (IMPROVE);
Aerometric **I**nformation **R**etrieval **S**ystem (AIRS);
National **A**cid **D**eposition **P**rogram (NADP); and the
South **E**astern **A**erosol **R**esearch and **CH**aracterization monitoring network (SEARCH).

Appendix A provides maps showing the location of measurement sites used in this analysis. The pollutant measurements from each network which we analyzed are listed in Table 1.

Table 1. Measurements of Pollutant Concentrations Included in the Analysis, by Monitoring Network.

Ambient Monitoring Networks	**Particulate Species**							**Gaseous Precursor Species**				**Wet Deposition Species**		
	PM2.5 Mass	SO_4	NO_3	TNO_3*	EC	NH_4	OC	O_3	SO_2	HNO_3	NO	SO_4	NO_3	NH_4
IMPROVE	X	X	X		X	X	X							
CASTNet		X		X		X			X					
STN	X	X	X		X	X	X							
NADP												X	X	X
AIRS								X						
SEARCH		X	X	X	X	X	X	X	X	X	X			

* $TNO_3 = (NO_3 + HNO_3)$

The IMPROVE network is a cooperative visibility monitoring effort between EPA, federal land management agencies, and state air agencies (IMPROVE, 2001). Data are collected at Class I areas across the United States mostly at National Parks, National Wilderness Areas, and other protected pristine areas. There were approximately 134 IMPROVE rural/remote sites that had complete annual PM2.5 mass and/or PM2.5 species data for 2001. In 2001 there were

86 sites in the West[2] and 48 sites were in the East. IMPROVE data is collected once in every three days. Thus, for each site there is a total of 104 possible samples per year or 26 samples per season.

The STN network began operation in 1999 to provide nationally consistent speciated PM2.5 data for the assessment of trends at representative sites in urban areas. The STN data are collected 1 in every 3 days, whereas some supplemental site are collected 1 in every 6 days. For the 2001 analysis, CMAQ predictions were evaluated against 133 STN sites (105 sites in the East and 28 sites in the West).

The CASTNet dry deposition monitoring network consisted of a total of 79 sites in 2001. Of this there were 56 sites in the East and 23 in the West. CASTNet data are collected and reported as weekly average data (EPA, 2002). The data are collected in filter packs that sample the ambient air continuously during the week[3].

The NADP measurements were used in the evaluation of deposition (NADP 2002). In 2001 there were a total of 225 NADP sites (144 in the East and 81 in the West) which provided data in 2001. NADP data is collected and reported as weekly average data.

Ozone measurements from State/local monitoring sites in AIRS were used in the evaluation of 1-hour and 8-hour daily maximum ozone concentrations. We included ozone measurements from1156 sites 822 in the East and 334 in the West. The ozone data are measured and reported on an hourly basis.

The SEARCH network was established in 1998 and is a coordinated effort between the public and private sector to characterize the chemical and physical composition as well as the geographical distribution of PM2.5. SEARCH data are collected and reported on an hourly/daily basis. In our evaluation we included measurements from 6 SEARCH sites. These sites are:
Birmingham, Alabama (urban);
Centreville, Alabama (rural);
Gulfport Mississippi (urban);
Jefferson Street, Atlanta, Georgia (urban);
Oak Grove, Mississippi (rural); and
Yorkville, Georgia (rural).

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[2]The dividing line between the West and East was defined as the 100th meridian.

[3]The particulate nitrate concentration data collected by CASTNet are known to be problematic and subject to volatility due to the length of the sampling period. CASTNet also reports a total nitrate measurement, which is the combination of particulate nitrate and nitric acid. Since the total nitrate measurement is not affected by the partitioning between particulate nitrate and nitric acid, it is considered a more reliable measurement. Therefore, we chose to use the total nitrate data and not the particulate nitrate data in this evaluation.

B. Procedures for Mapping CMAQ Predictions to Observations

As indicated above, the observed data used in this analysis consisted of PM2.5 mass, sulfate PM, nitrate PM, elemental carbon, organic aerosols, crustal material (soils), ozone, sulfur dioxide, nitric acid and nitric oxide. The CMAQ model output species were postprocessed in order to achieve compatibility with the observation species. Below are the observations and corresponding CMAQ output species:

Observation	***CMAQ Output Species***
Sulfate PM:	PM_SULF = ASO4I + ASO4J
Nitrate PM:	PM_NITR = ANO3I + ANO3J
Total Nitrate:	TNO3 = ANO3I + ANO3J + (2140*HNO3*DENS)
Organic aerosols:	PM_ORG_TOT = AORGAI + AORGAJ + 1.167*AORGPAI + 1.167*AORGPAJ + AORGBI + AORGBJ
Elemental Carbon:	PM_EC = AECI + AECJ
Crustal Material (soils):	PM_OTH = A25I +A25J
PM2.5:	PM2.5 = ASO4I + ASO4J + ANH4I + ANH4J + ANO3I +ANO3J + AORGAI + AORGAJ + 1.167*AORGPAI + 1.167*AORGPAJ+ AORGBI + AORGBJ + AECI + AECJ + A25I + A25J
Coarse PM:	PM_COARS = ASOIL +ACORS + ASEAS
Ozone:	O3 = O3
Sulfur dioxide:	SO2 = SO2
Nitric acid:	HNO3 = HNO3
Nitric oxide:	NO = NO

where the CMAQ predictions are defined as follows:

PM_SULF is particulate sulfate,
ASO4J is accumulation mode sulfate mass,
ASO4I is aitken mode sulfate mass,
PM_NITR is particulate nitrate,
ANO3J is accumulation mode nitrate mass,
ANO3I is aitken mode aerosol nitrate mass,
ANH4J is accumulation mode ammonium mass,
ANH4I is aitken mode ammonium mass,
TNO3 is total nitrate, HNO3 is nitric acid,
DENS is air density,
PM_ORG_TOT is total organic aerosols,
AORGAJ is accumulation mode anthropogenic secondary organic mass,
AORGAI is aitken mode anthropogenic secondary organic mass,
AORGPAJ is accumulation mode primary organic mass,
AORGPAI is aitken mode primary organic mass,

AORGBJ is accumulation mode secondary biogenic organic mass,
AORGBI is aitken mode biogenic secondary biogenic organic mass,
PM_EC is primary elemental carbon, AECJ is accumlation mode elemental carbon mass,
AECI is aitken mode elemental carbon mass,
PM_OTH is primary fine particles (other unspeciated primary PM2.5),
A25J is accumulation mode unspecified anthropogenic mass,
A25I is aitken mode unspecified anthropogenic mass,
O3 is ozone,
SO2 is sulfur dioxide,
HNO3 is nitric acid, and
NO is nitric oxide.

PM2.5 is defined as the sum of the individual species. Note that a factor of 1.167 was applied to AORGPAI and AORGPAJ since the CMAQ model assumed the conversion factor between organic carbon to organic mass is 1.2 for primary organic aerosol emission, while we assumed a 1.4 factor for the IMPROVE and STN ambient data.

As stated above, the monitoring networks included in this evaluation provide measurements over various time intervals (i.e., hourly, daily, and weekly). In the calculation of model performance statistics and in the preparation of graphics we time-averaged the CMAQ predictions to correspond to the particular averaging time of the observations. For time periods with missing observations we excluded the CMAQ predictions from those time periods in our calculations.

C. Definition of Model Performance Statistics

Model performance statistics were calculated for PM2.5 and component species using data from the IMPROVE, CASTNet, and STN networks. Performance statistics were also calculated for the 1-hour and 8-hour ozone data in AIRS, SO2 from CASTNet, and the NADP ammonium, nitrate, and sulfate deposition data. Because of known or potential differences between networks in terms of measurement techniques and sampling protocols, we did not combine measurements from multiple networks in the calculation of statistics. Rather, we calculated statistics separately for each network. For each network and pollutant, statistics were calculated for all sites across the nation with separate breakouts for the East and West[4]. In terms of the time aggregation, we prepared statistics for the entire year using all observed-predicted pairs with separate statistics for each season using just those observed-predicted pairs in the season. Seasons are defined as follows: Winter includes the months of December, January, February; Spring includes the months of March, April, May; Summer includes the months of June, July, and August; and Fall includes the months of September, October, and November. Note that we did not calculate performance statistics for any of the SEARCH measurements because of the limited extent of samples.

[4] The dividing line between East and West is the 100^{th} meridian.

Below are the definitions of model performance statistics calculated as part of this evaluation.

Mean Observation: The time-average mean observed value (in µg/m^3)

$$OBS = \frac{1}{N} \sum_{i=1}^{N} Obs_{x,t}^{i}$$

Mean CMAQ Prediction: The time-average mean predicted value (in µg/m^3) paired in time and space with the observations.

$$PRED = \frac{1}{N} \sum_{i=1}^{N} Pred_{x,t}^{i}$$

Ratio of the Means: Ratio of the predicted over the observed values. A ratio of greater than 1 indicates on overprediction and a ratio of less than 1 indicates an underprediction.

$$RATIO = \frac{1}{N} \sum_{i=1}^{N} \frac{Pred_{x,t}^{i}}{Obs_{x,t}^{i}}$$

Mean Bias (µg/m^3): This performance statistic averages the difference (model - observed) over all pairs in which the observed values were greater than zero. A mean bias of zero indicates that the model over predictions and model under predictions exactly cancel each other out. Note that the model bias is defined such that positive values indicate that the model prediction exceeds the observation, whereas negative values indicate an underestimate of observations by the model. This model performance estimate is used to make statements about the absolute or unnormalized bias in the model simulation.

$$BIAS = \frac{1}{N} \sum_{i=1}^{N} (Pred_{x,t}^{i} - Obs_{x,t}^{i})$$

Normalized Mean Bias (percent): This statistic averages the difference (model - observed) over the sum of observed values. Normalized mean bias is a useful model performance indicator because it avoids over inflating the observed range of values.

$$NMB = \frac{\sum_{i=1}^{N} (Pred_{x,t}^{i} - Obs_{x,t}^{i})}{\sum_{i=1}^{N} (Obs_{x,t}^{i})} * 100$$

Mean Fractional Bias (percent): Normalized bias can become very large when a minimum threshold is not used. Fractional bias is used as a substitute. The fractional bias for cases with factors of 2 under- and over-prediction are -67 and + 67 percent, respectively (as opposed to -50 and +100 percent, when using normalized bias). Fractional bias is a useful indicator because it has the advantage of equally weighting positive and negative bias estimates. The single largest disadvantage is that the predicted concentration is found in both the numerator and denominator.

$$FBIAS = \frac{2}{N}\sum_{i=1}^{N}\frac{(Pred_{x,t}^{i} - Obs_{x,t}^{i})}{(Pred_{x,t}^{i} + Obs_{x,t}^{i})} * 100$$

Mean Error (μg/m³): This performance statistic averages the absolute value of the difference (model - observed) over all pairs in which the observed values are greater than zero. It is similar to mean bias except that the absolute value of the difference is used so that the error is always positive.

$$ERR = \frac{1}{N}\sum_{i=1}^{N}\left|Pred_{x,t}^{i} - Obs_{x,t}^{i}\right|$$

Normalized Mean Error (percent): This performance statistic is used to normalize the mean error relative to the observations. This statistic averages the difference (model - observed) over the sum of observed values. Normalized mean error is a useful model performance indicator because it avoids over inflating the observed range of values.

$$NME = \frac{\sum_{i=1}^{N}\left|Pred_{x,t}^{i} - Obs_{x,t}^{i}\right|}{\sum_{i=1}^{N}(Obs_{x,t}^{i})} * 100$$

Mean Fractional Error (percent): Normalized error can become very large when a minimum threshold is not used. Therefore fractional error is used as a substitute. It is similar to the fractional bias except the absolute value of the difference is used so that the error is always positive.

$$FERROR = \frac{2}{N}\sum_{i=1}^{N}\frac{\left|Pred_{x,t}^{i} - Obs_{x,t}^{i}\right|}{Pred_{x,t}^{i} + Obs_{x,t}^{i}} * 100$$

Correlation Coefficient (R^2): This performance statistic measures the degree to which two variables are linearly related. A correlation coefficient of 1 indicates a perfect linear relationship; whereas a correlation coefficient of 0 means that there is no linear relationship between the variables.

$$CORRCOEFF = \frac{\sum_{i=1}^{N} (Pred_i - \overline{Pred})(Obs_i - \overline{Obs})}{\sqrt{\sum_{i=1}^{N} (Pred_i - \overline{Pred})^2 \sum_{i=1}^{N} (Obs_i - \overline{Obs})^2}}$$

D. Procedures for Preparing Scatter Plots and Spatial and Time Series Graphics

In addition to the model performance statistics, we have included scatter plots, spatial maps and time series comparisons in the analysis to further reveal similarities and differences between model predictions and observations. Scatter plots were prepared for annual and seasonal average observed/predicted pairs. These plots were prepared for sulfate PM, nitrate PM, ammonium PM, organic carbon, elemental carbon, and ozone. Separate scatter plots were prepared for each network that measured these pollutants.

Spatial plots were prepared for observed and predicted sulfate PM, total nitrate (NO3 + HNO3), and ammonium PM for 2001 to provide a way to compare the spatial patterns in predictions versus observations. The spatial plots of observed data were prepared using measurements from the CASTNet STN monitoring networks. We combined the measurements from CASTNet and STN only because the measurement techniques of these two networks for sulfate PM and ammonium PM are reasonably similar, although there are some minor differences. Because no two networks measure nitrogen aerosols in a similar manner (due to problems in the partitioning of nitric acid and nitrate PM), we chose to use total nitrate reported by CASTNet for the spatial analysis of nitrate.

To overcome difference in sample collection between the CASTNet and STN in preparing spatial fields for sulfate PM and ammonium PM, we constructed 28 day averages (lunar months) using the data from each network, with the start date corresponding to the CASTNet sampling schedule. We also constructed lunar month averages for total nitrate using the CASTNet data. Sites were included if more than 75% of the data for the month were available. The monthly averages at each site were then interpolated to the CMAQ grid. After exploring the development of reliable spatial models for the monitoring data using a variety of gridding approaches (e.g. kriging, nearest neighbor, natural neighbor, polynomial regression, etc.), we chose the radial basis functions interpolation procedure for the sulfate PM, total nitrate, and ammonium PM fields (Hardy, 1990; Carlson and Foley, 1991). For the CMAQ predictions of sulfate PM, total nitrate and ammonium PM, we prepared monthly average concentrations that correspond to the monitoring periods.

We have also included a time series analysis to compare the temporal patterns in the

CMAQ predictions to those in the observations. Time series plots were created for nearly all sites and pollutants included in this evaluation. For this report we have selected a subset of plots for monitoring sites in the East in order to illustrate the various differences and similarities between predicted and observed temporal patterns. For STN, IMPROVE, and CASTNet we chose six sites in each network to present in this report. Collectively, these site provide a temporal comparison of predictions and observations in urban and rural portions of the Northeast, Southeast, and Midwest. The time series plots for PM2.5 species are in Appendix D and the plots for gaseous species are in Appendix E. Note that we have prepared plots for various averaging times for each network.

- For IMPROVE and STN we have prepared time series for:
    + 24-hour measured values (referred to as "daily")
    + two-week averages (referred to as biweekly)

- For CASTNet we have prepare time series comprised of weekly values that correspond to the measurement periods

- For SEARCH we have prepared time series for:
    + daily values, weekly, and monthly averages for precursor gases
    + monthly averages for particulate species

Weekly, and/or bi-weekly and monthly average plots were created to smooth out the short-term variability in the daily samples in order to reveal temporal patterns associated with regional scale meteorological cycles.

Table 2. Measurements of Pollutant Concentrations Included in the Time-series Analysis, by Monitoring Network and Sites.

Ambient Monitoring Network Sites	**Particulate Species**						**Gaseous Species**			
	SO_4	NO_3	TNO_3^*	NH_4	EC	OC	SO_2	O_3	HNO_3	NO
CASTNet										
Sand Mountain, AL	X		X	X			X			
Georgia Station, GA	X		X	X			X			
Vincennes, IN	X		X	X			X			
Arendtsville, PA	X		X	X			X			
Shenandoah Ntl. Park, VA	X		X	X			X			
Perkinstown, WI	X		X	X			X			
IMPROVE										
Chassahowitzka, FL	X	X		X	X	X				

Mammoth Cave Ntl. Park, KY	X	X		X	X	X				
Mingo, MO	X	X		X	X	X				
Brigantine NWR, NJ	X	X		X	X	X				
Great Smoky Mountains Ntl. Park, TN	X	X		X	X	X				
Shenandoah Ntl. Park, VA	X	X		X	X	X				
STN										
Jefferson, AL	X	X		X	X	X				
Marion, IN	X	X		X	X	X				
Baltimore, MD	X	X		X	X	X				
Wayne, MI	X	X		X	X	X				
Wright, MO	X	X		X	X	X				
Bronx, NY	X	X		X	X	X				
SEARCH										
Birmingham, AL (urban)	X	X		X	X	X	X	X	X	X
Centreville, AL (rural)	X	X		X	X	X	X	X	X	X
Jefferson Street, Atlanta, GA (urban)	X	X		X	X	X	X	X	X	X
Yorkville, GA (rural)	X	X		X	X	X	X	X	X	X
Gulfport, MS (urban)	X	X		X	X	X	X	X	X	X
Oak Grove, MS (rural)	X	X		X	X	X	X	X	X	X

* $TNO_3 = (NO_3 + HNO_3)$

III. Performance Evaluation Results for PM2.5 Species, Deposition, and Visibility

In this section we provide the results of the model performance evaluation. The evaluation for PM2.5 is provided first and includes performance statistics[5] supplemented with observed-predicted scatter plots and spatial and time series comparisons for selected species.

[5] Selected PM2.5 performance statistics are included in the discussion of results. The values for all statistics can be found in Appendix A.

The PM2.5 performance statistics from our CMAQ evaluation are then compared to the results from other regional model applications. This is followed by the performance analysis for PM2.5 precursor gases. The evaluation for visibility and deposition is provided last.

A. CMAQ Performance Results for PM2.5 Species

The performance results are presented for each PM2.5 species then for total PM2.5 mass. As noted above, we have analyzed performance separately for each network with annual and seasonal statistics for the entire domain, the East, and the West. Scatter plots of annual and seasonal averages are included for the aggregation of sites, by network in the East.

1. Sulfate Concentrations

The overall model performance of sulfate PM is remarkably well compared against a suite of available monitoring data listed in Tables 3, 4, and 5. The seasonal plots and annual time series plots also show that the model was able to capture the seasonal and weekly/daily trends of sulfate PM. The model predictions of sulfate closely match observations particularly in the East and in the summer where and when the sulfate PM is most abundant. The model predicted comparable magnitudes of sulfate PM with high accuracy for both rural and urban sites in the East. The model slightly underpredicted the sulfate PM in the West over both rural and urban sites.

a. Sulfate PM Performance at IMPROVE sites

Table 3 lists the performance statistics for particulate sulfate at the IMPROVE sites. Domainwide, sulfate is overpredicted by 2%. Sulfate for the East is overpredicted by 9% and underpredicted 13% in the West. The annual sulfate performance (especially in the East) is better than most of the other PM2.5 species. The annual fractional error in the East is ~46% and the R^2 is 0.74**.**

Table 3. Annual sulfate PM performance at IMPROVE sites.

	No. of Obs.	Mean CMAQ Predictions (µg/m^3)	Mean Observations (µg/m^3)	Ratio of Means (pred/obs)	Bias (µg/m^3)	Fractional Bias (%)	Error (µg/m^3)	Fractional Error (%)	Correlation Coefficient
National	13447	1.72	1.68	1.02	0.04	0.94	0.67	45.67	0.74
East	4771	3.62	3.34	1.09	0.29	7.00	1.22	39.56	0.68
West	8676	0.67	0.77	0.87	-0.10	-2.39	0.36	49.02	0.28

Figures 2 and 3 show the annual and seasonal mean sulfate at IMPROVE sites versus CMAQ predictions, respectively. The scatter plots and linear regressions indicate that the predictions are highly correlated with the observations (annual: R^2 = 0.96; summer: R^2 = 0.94; fall: R^2 = 0.96; spring: R^2 = 0.94; and winter: R^2 = 0.80).

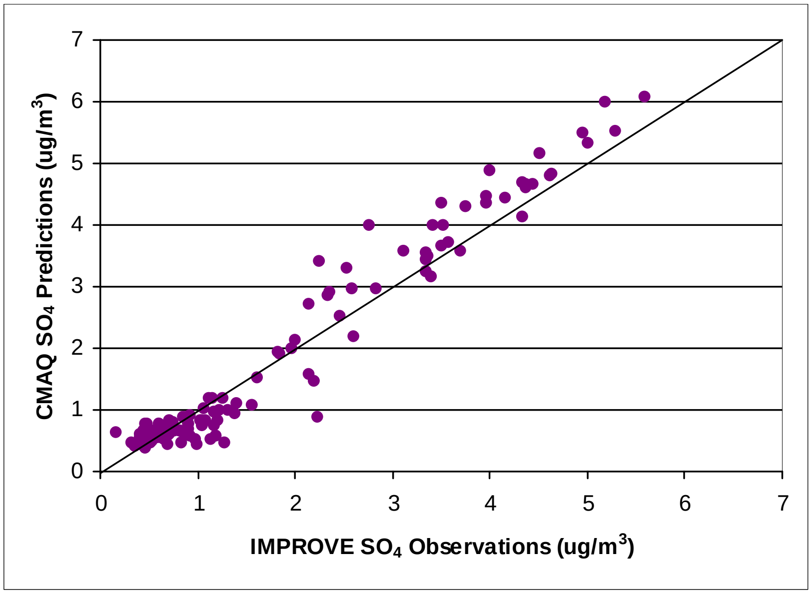


Figure 2. Annual mean sulfate PM: IMPROVE observations versus CMAQ predictions.

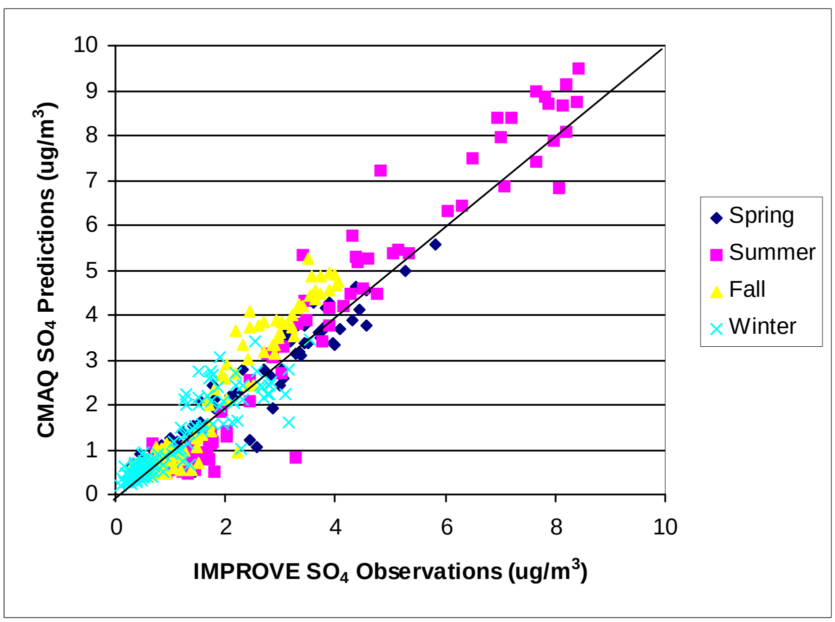


Figure 3. Seasonal mean sulfate PM: observations at IMPROVE sites versus CMAQ predictions.

b. Sulfate PM Performance at STN sites

Table 4 lists the performance statistics for particulate sulfate at the STN sites. Nationally, CMAQ overpredicted sulfate by only 6% compared for the STN network sites. The annual mean sulfate for the East is overpredicted by 11% and underpredicted by 36% in the West. The annual sulfate performance is encouraging (similar to IMPROVE SO4 performance) and better than most of the other PM2.5 species. The annual fractional error in the East is ~46% and the R^2 is 0.61**.**

Table 4. Annual sulfate PM performance at STN sites.

	No. of Obs.	Mean CMAQ Predictions (µg/m³)	Mean Observations (µg/m³)	Ratio of Means (pred/obs)	Bias (µg/m³)	Fractional Bias (%)	Error (µg/m³)	Fractional Error (%)	Correlation Coefficient
National	6970	3.62	3.40	1.06	0.22	-0.54	1.47	46.15	0.61
East	5414	4.37	3.93	1.11	0.44	8.43	1.67	44.53	0.59
West	1556	1.00	1.56	0.64	-0.55	-31.74	0.78	51.78	0.16

Figures 4 and 5 show the annual and seasonal average sulfate at STN sites versus CMAQ predictions, respectively. The scatter plots and linear regressions indicate that the predictions are highly correlated with observations (annual: R^2 = 0.83; summer: R^2 = 0.82; fall: R^2 = 0.67; spring: R^2 = 0.54; and winter: R^2 = 0.56).

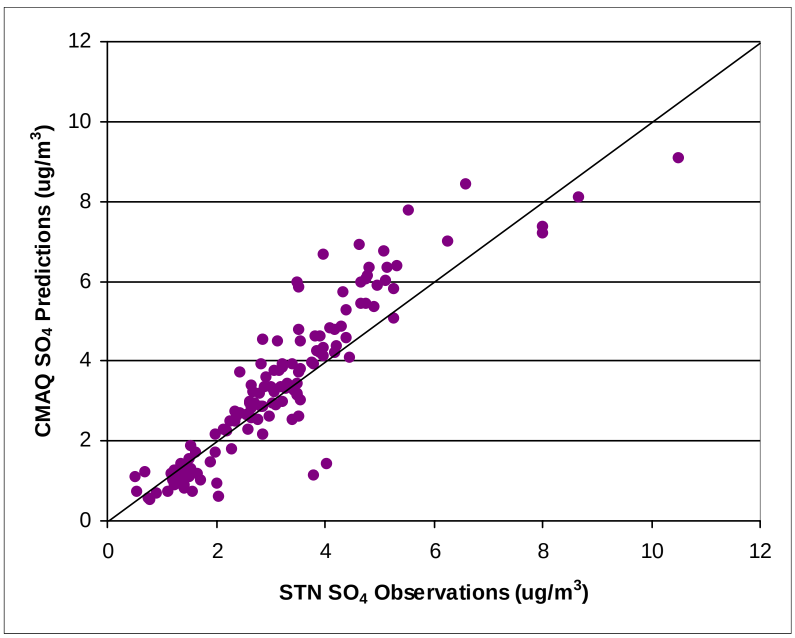


Figure 4. Annual mean sulfate: STN observations versus CMAQ predictions.

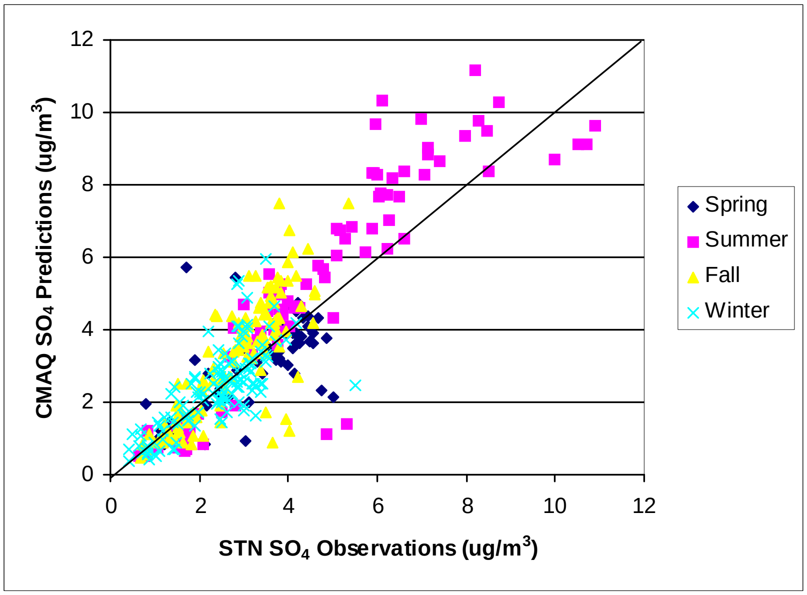


Figure 5. Seasonal mean sulfate: STN observations versus CMAQ predictions.

c. Sulfate PM Performance at CASTNet Sites

Table 5 lists the performance statistics for particulate sulfate at the CASTNet sites. Nationally, CMAQ underpredicted sulfate by only 4% compared to the CASTNet network sites. The annual mean sulfate performance for the East is quite good, neither over- nor underpredicting. Likewise, the annual sulfate performance is encouraging (similar to IMPROVE and STN SO4 performance). The annual fractional error in the East is ~24% and the R^2 is 0.81.

Table 5. Annual sulfate PM performance at CASTNet sites.

	No. of Obs.	Mean CMAQ Predictions ($\mu g/m^3$)	Mean Observations ($\mu g/m^3$)	Ratio of Means (pred/obs)	Bias ($\mu g/m^3$)	Fractional Bias (%)	Error ($\mu g/m^3$)	Fractional Error (%)	Correlation Coefficient
National	3736	3.09	3.21	0.96	-0.12	-11.61	0.77	31.43	0.85
East	2639	4.10	4.11	1.00	-0.01	-2.09	0.89	23.77	0.81
West	1097	0.66	1.04	0.64	-0.38	-34.51	0.46	49.84	0.34

Figures 6 and 7 shows the seasonal mean CASTNet observations versus CMAQ predictions for total sulfate. The scatter plot and linear regression of sulfate show very good agreement, with strong correlations among all seasons (annual: R^2 = 0.97; summer: R^2 = 0.95; fall: R^2 = 0.95; spring: R^2 = 0.95; winter: R^2 = 0.89). The performance of sulfate at the CASTNet sites looks better than at the IMPROVE sites.

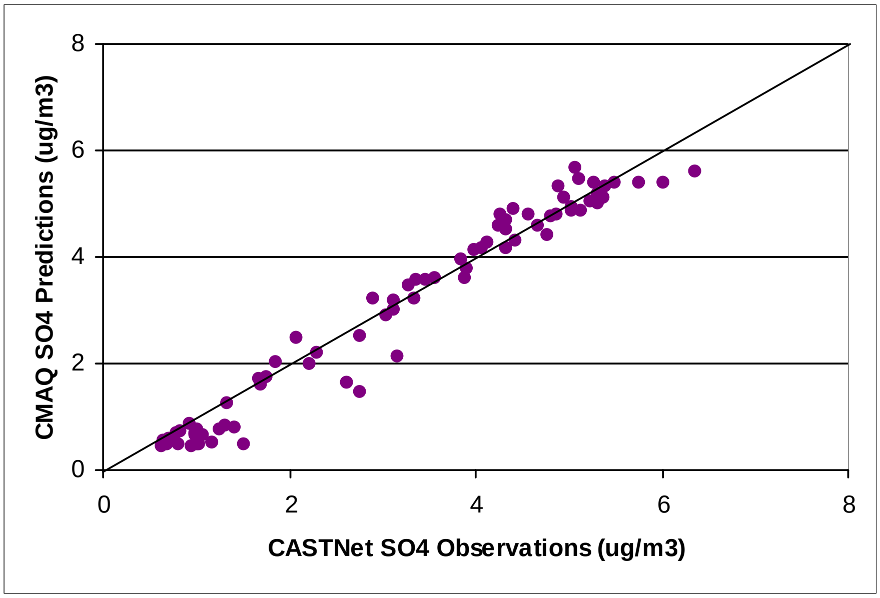


Figure 6. Annual mean sulfate PM: CASTNet observations versus CMAQ predictions.

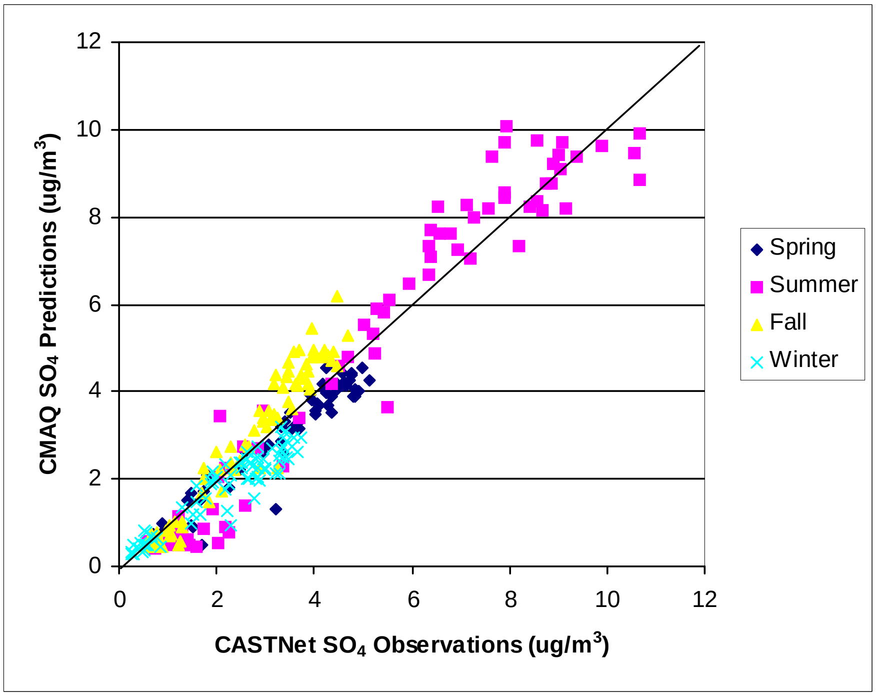


Figure 7. Seasonal mean sulfate PM: CASTNet observations versus CMAQ predictions.

d. Sulfate PM Spatial Pattern Analysis

Figures 8-13 show the spatial patterns of observed and predicted sulfate concentrations for three summer periods when sulfate concentrations are high (i.e., May 22 - June 18, 2001; June 19 - July 16, 2001; July 17 - August 13, 2001). Comparing the observed and predicted fields indicates that predictions closely replicate the observed patterns of sulfate PM. The predicted magnitude and gradients correspond well with the observations in the East.

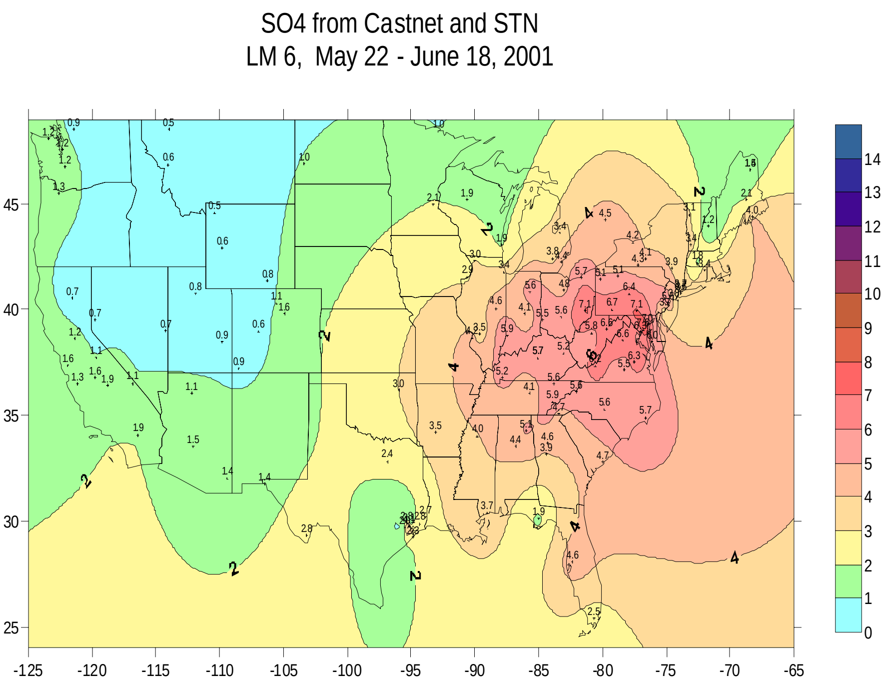


Figure 8. Sulfate PM: average of the period May 22 - June 18, 2001 CASTNet and STN observations.

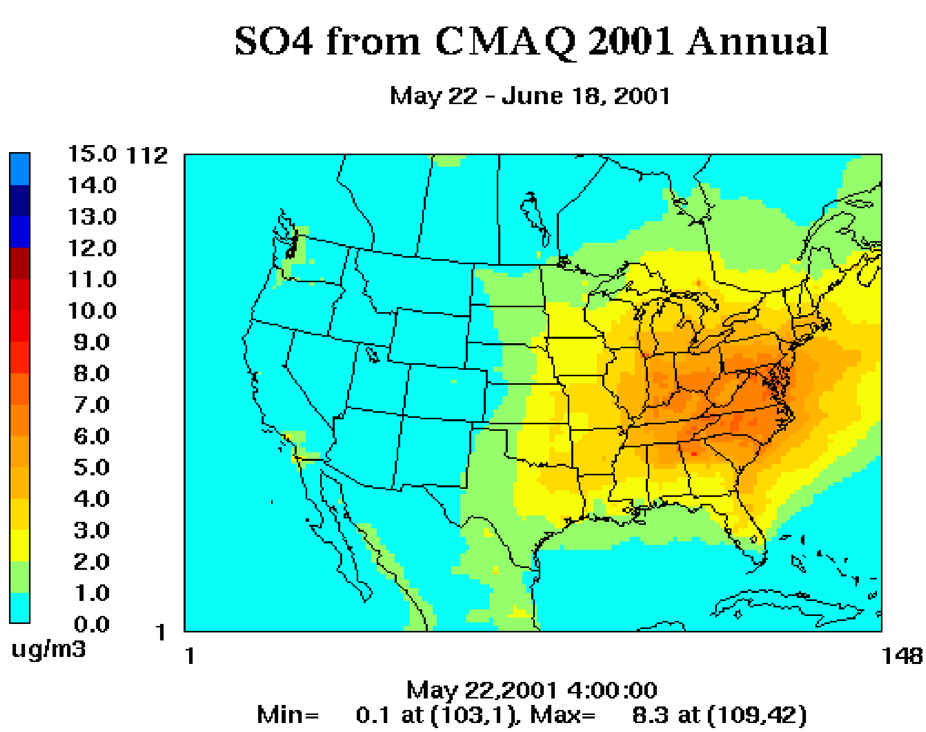


Figure 9. Sulfate PM: average of the period May 22 - June 18, 2001 CMAQ predictions.

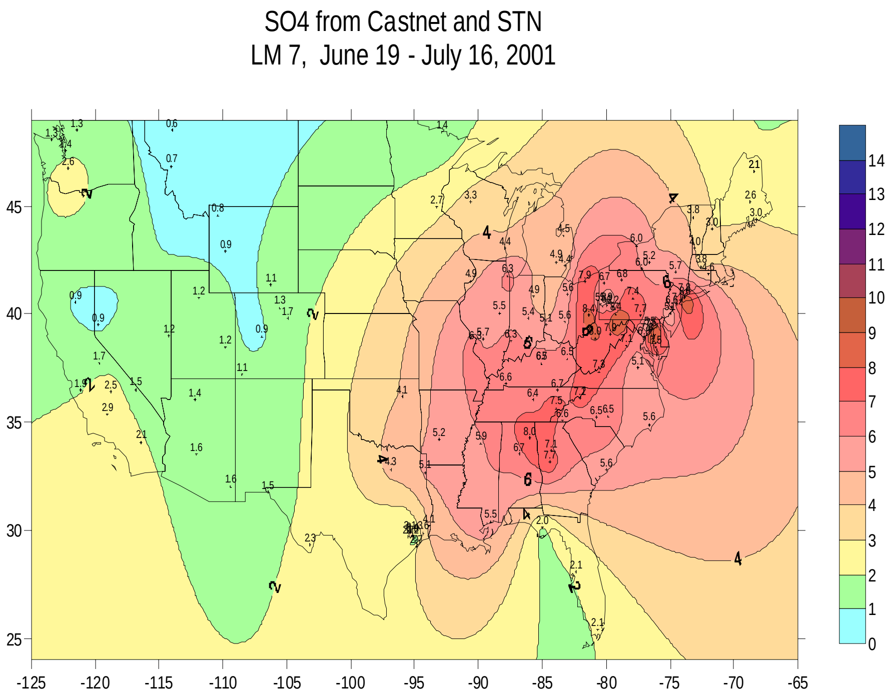


Figure 10. Sulfate PM: average of the period June 19 - July 16, 2001 CASTNet and STN observations.

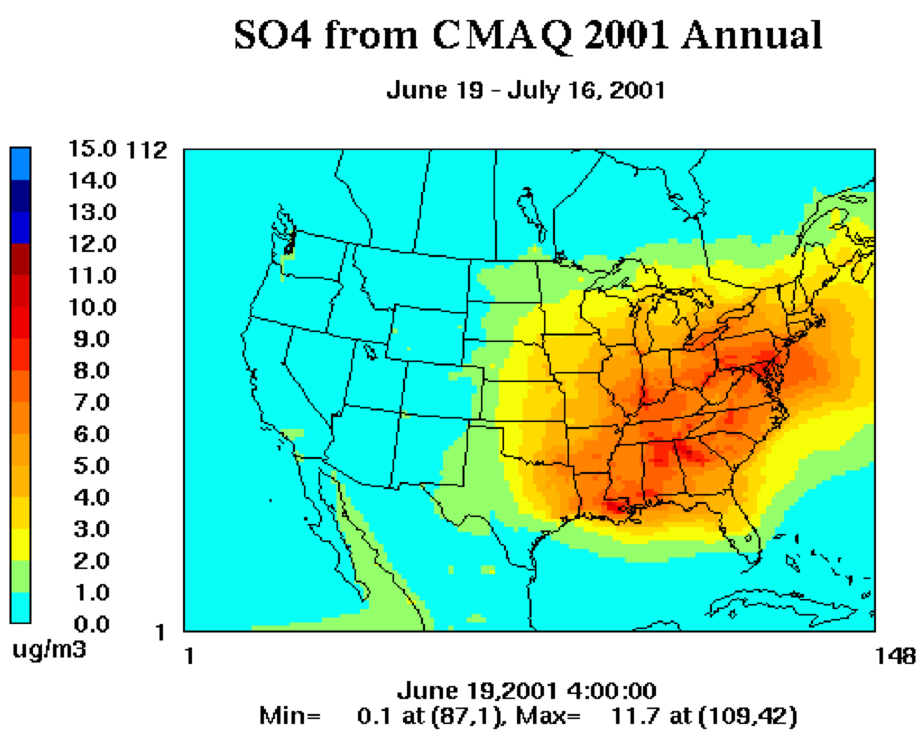


Figure 11. Sulfate PM: average of the period June 19 - July 16, 2001 CMAQ predictions.

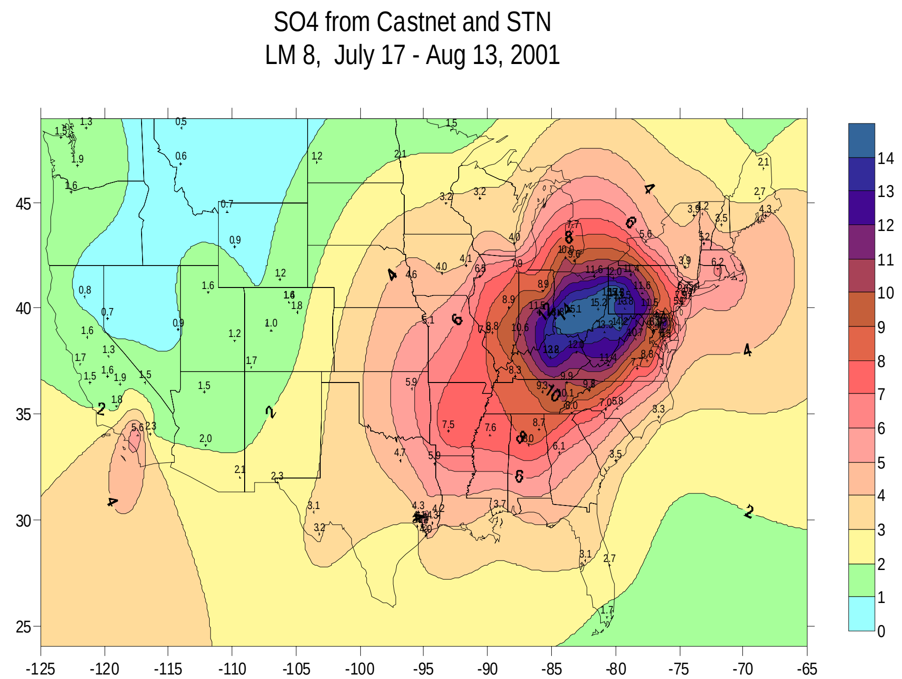


Figure 12. Sulfate PM: average of the period July 17 - August 13, 2001 CASTNet and STN observations.

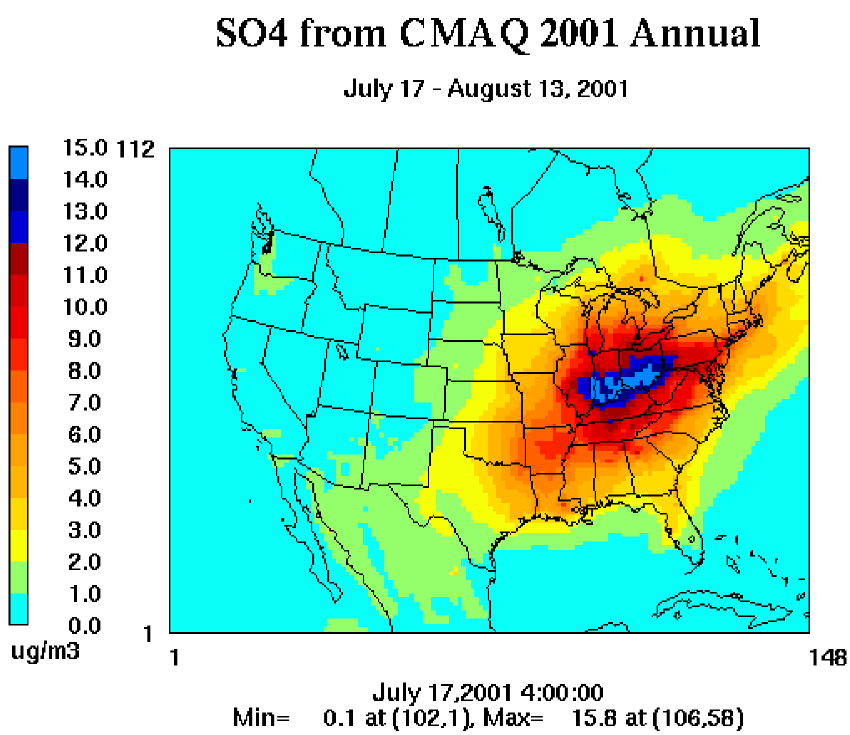


Figure 13. Sulfate PM: average of the period July 17 - August 13, 2001 CMAQ predictions.

e. Sulfate PM Time Series Analysis

Overall, the temporal trends in sulfate PM predicted by CMAQ correspond closely with the observations at both urban and rural locations in the East throughout much of the year. The results for the weekly and bi-weekly averages indicate that the modeling system (i.e., CMAQ and the meteorological and emissions inputs) replicates well the regional scale meteorological and chemical processes affecting sulfate formation and transport in the East.

2. Nitrate Concentrations

The overall model performance of nitrate PM and total nitrate is reasonably well compared against the available monitoring data. The seasonal plots and annual time series plots also show that the model was able to capture the seasonal and weekly variations of total nitrate and nitrate PM. However, the nitrate PM was overpredicted in the East, especially in the winter when nitrate PM is most abundant, and was underpredicted in the West, especially over urban sites.

a. Nitrate PM Performance at IMPROVE Sites

Table 6 lists the performance statistics for nitrate PM at the IMPROVE sites. Nitrate is overpredicted by 27% domainwide. Nitrate is generally overpredicted in the East (58%) and underpredicted in the West (2%).

Table 6. Annual nitrate PM performance at IMPROVE sites.

	No. of Obs	Mean CMAQ Predictions (μg/m^3)	Mean Observations (μg/m^3)	Ratio of Means (pred/obs)	Bias (μg/m^3)	Fractional Bias (%)	Error (μg/m^3)	Fractional Error (%)	Correlation Coefficient
National	13398	0.61	0.48	1.27	0.13	-39.71	0.49	112.04	0.35
East	4755	1.04	0.66	1.58	0.38	-31.90	0.74	107.04	0.44
West	8643	0.37	0.38	0.98	-0.01	-44.01	0.36	114.79	0.23

Figures 14 and 15, which provide the scatter plots of the annual mean (R^2= 0.63) and seasonal mean (summer: R^2= 0.49; fall: R^2= 0.43; spring: R^2= 0.77; winter: R^2= 0.50) nitrate PM for IMPROVE observations versus CMAQ predictions.

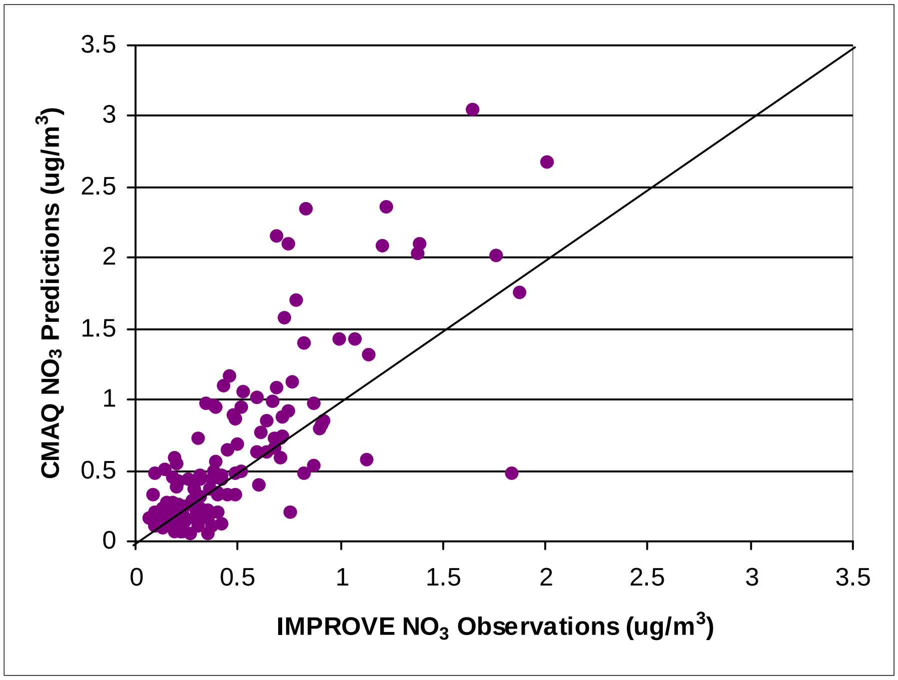


Figure 14. Annual mean nitrate PM: IMPROVE observations versus CMAQ predictions.

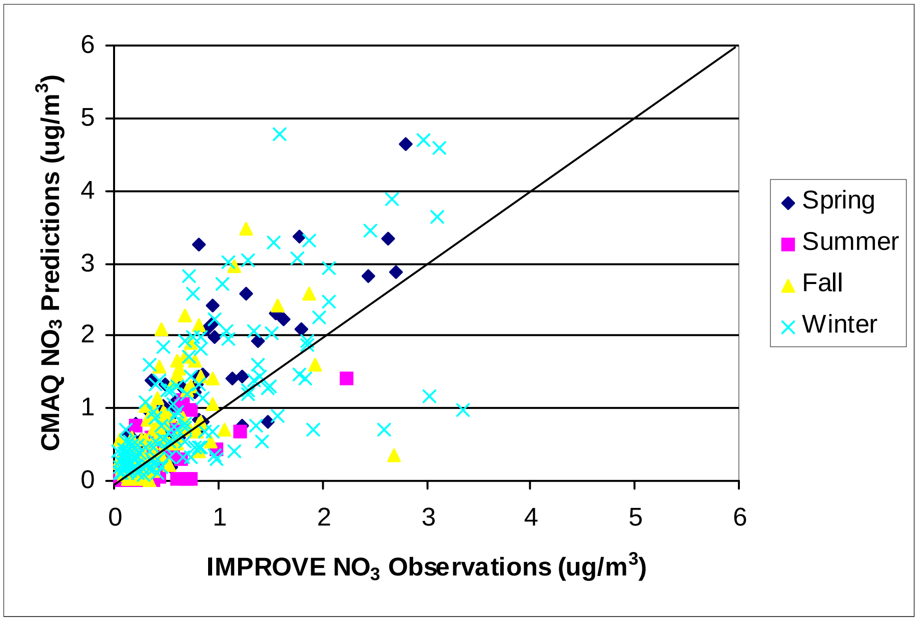


Figure 15. Seasonal mean nitrate PM: IMPROVE observations versus CMAQ predictions.

It is important to consider these results in the context that the observed nitrate PM concentrations at the IMPROVE sites are very low. The mean nationwide observations are only 0.48 µg/m^3. It is often difficult for models to replicate very low concentrations of secondarily formed pollutants. Nitrate is generally a small percentage of the measured PM2.5 at almost all of the IMPROVE sites. Nonetheless, it has been recognized that the current generation of PM air quality models generally overpredict particulate nitrate. Numerous improvements have been made to the CMAQ modeling system and nitrate performance has continued to improve, Additional ongoing efforts are expected to further improve nitrate predictions over time.

b. Nitrate PM Performance at STN Sites

Table 7 lists the performance statistics for nitrate PM at the STN sites. Nitrate is underpredicted by 5% domainwide. Nitrate is generally overpredicted in the East (28%) and underpredicted in the West (66%).

Table 7. Annual nitrate PM performance at STN sites.

	No. of Obs.	Mean CMAQ Predictions (µg/m^3)	Mean Observations (µg/m^3)	Ratio of Means (pred/obs)	Bias (µg/m^3)	Fractional Bias (%)	Error (µg/m^3)	Fractional Error (%)	Correlation Coefficient
National	6130	1.69	1.77	0.95	-0.08	-31.19	1.41	93.02	0.18
East	4662	1.94	1.52	1.28	0.42	-11.90	1.23	86.03	0.38
West	1468	0.86	2.55	0.34	-1.68	-92.44	1.99	115.22	0.21

Figures 16 and 17, which show the scatter plots of the annual (R^2= 0.12) and seasonal mean (summer: R^2= 0.16; fall: R^2= 0.08; spring: R^2= 0.63; winter: R^2= 0.13) nitrate PM for STN observations verus CMAQ predictions.

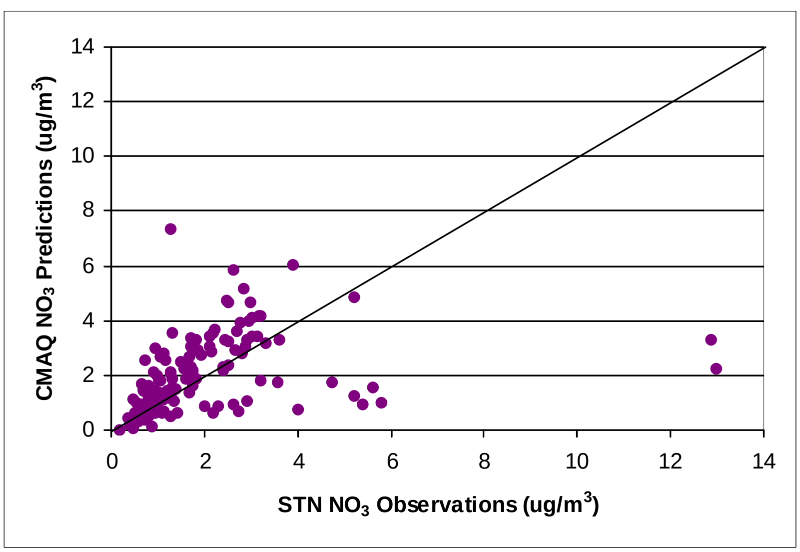


Figure 16. Annual mean nitrate PM: STN observations versus CMAQ predictions.

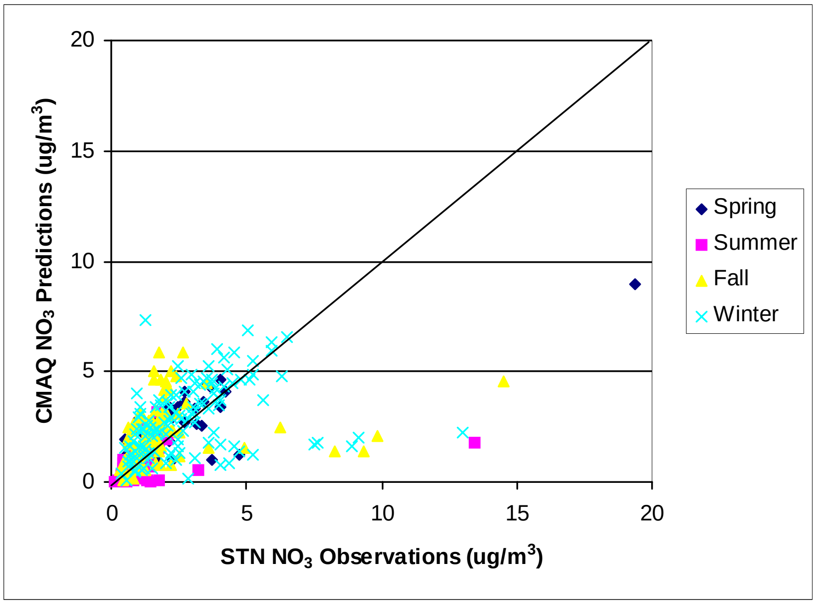


Figure 17. Seasonal mean nitrate PM: STN observations versus CMAQ predictions.

c. Total Nitrate Performance at CASTNet Sites

Table 8 lists the performance statistics for total nitrate (NO3 + HNO3) at the CASTNet sites. Total Nitrate is overpredicted by 26% domainwide. Total nitrate is generally overpredicted in the East (36%) and underpredicted in the West (34%). In the East, fractional bias is ~16% with a fractional error of ~81%.

Table 8. Annual total nitrate performance at CASTNet sites.

	No. of Obs.	Mean CMAQ Predictions (μg/m^3)	Mean Observations (μg/m^3)	Ratio of Means (pred/obs)	Bias (μg/m^3)	Fractional Bias (%)	Error (μg/m^3)	Fractional Error (%)	Correlation Coefficient
National	3735	1.25	0.99	1.26	0.26	-6.40	0.75	88.11	0.53
East	2638	1.64	1.20	1.36	0.43	15.84	0.90	81.14	0.53
West	1097	0.32	0.48	0.66	-0.16	-59.89	0.39	104.87	0.09

Figures 18 and 19 show the annual and seasonal mean CASTNet observations versus CMAQ predictions for total nitrate. The scatter plots and linear regressions of total nitrate showed modest agreement, with weaker correlations within each season (annual: R^2 = 0.53; summer: R^2 = 0.02; fall: R^2 = 0.43; spring: R^2 = 0.48; winter: R^2 = 0.60). Nationwide, the overprediction bias is 25%. This is not surprising given the overprediction bias of modeled particulate nitrate. The overprediction of total nitrate indicates that nitric acid concentrations may be overpredicted. This may be one of the reasons for the general overprediction of particulate nitrate. Model developers are continuing to examine the nitric acid production and destruction pathways. There are continuing improvements being made to the daytime and nighttime nitric acid formation reactions. Dry deposition of nitric acid is also being studied as a possible cause of overprediction.

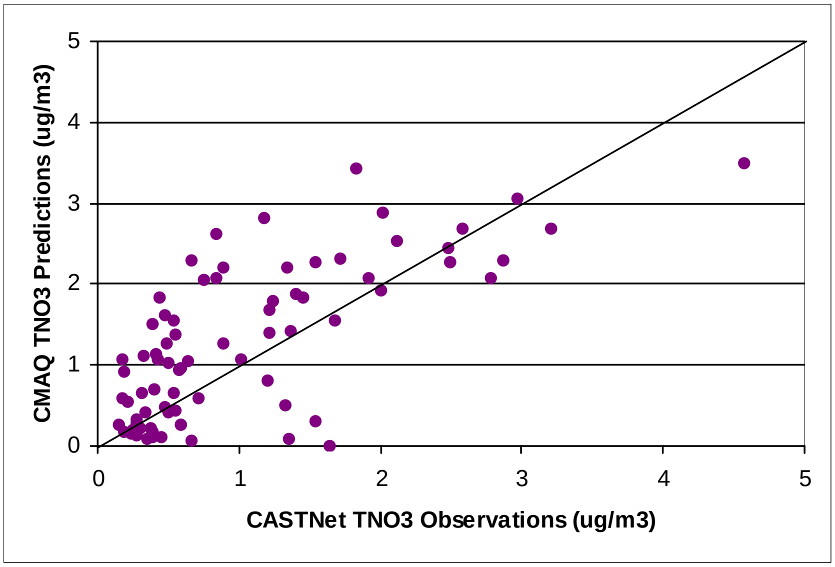


Figure 18. Annual mean total nitrate: CASTNet observations versus CMAQ predictions

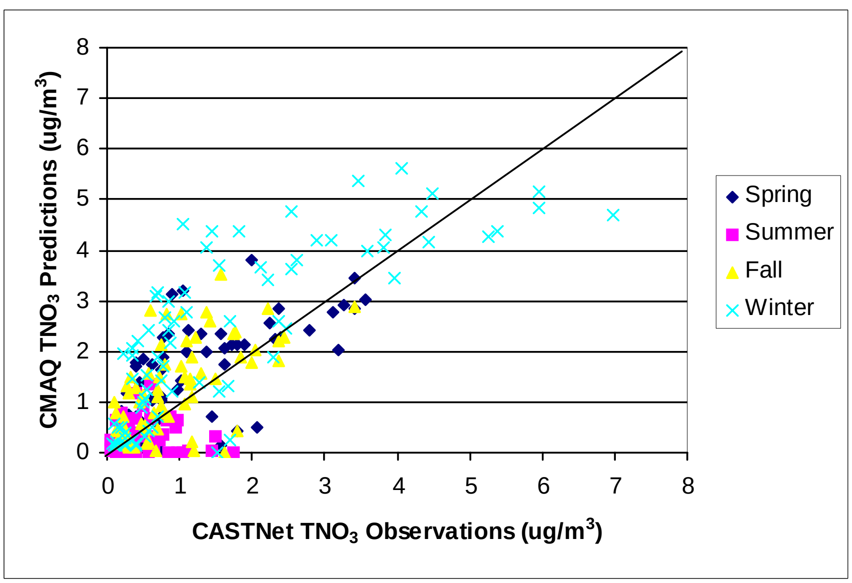


Figure 19. Seasonal mean total nitrate: CASTNet observations versus CMAQ predictions.

d. Nitrate Spatial Pattern Analysis

Observed and predicted spatial fields for total nitrate are shown in Figures 20 - 23 for two winter periods (i.e., January 2-29, 2001; January 30 - February 26, 2001. The location and magnitude of the highest predicted concentrations and spatial gradients generally correspond to that of the observations, although the model tends to over predict the concentrations as is also evident from the performance statistics. At least part of the differences between predictions and observations are believed to be associated with ammonia emissions input to the model which may be too high in some parts of the region.

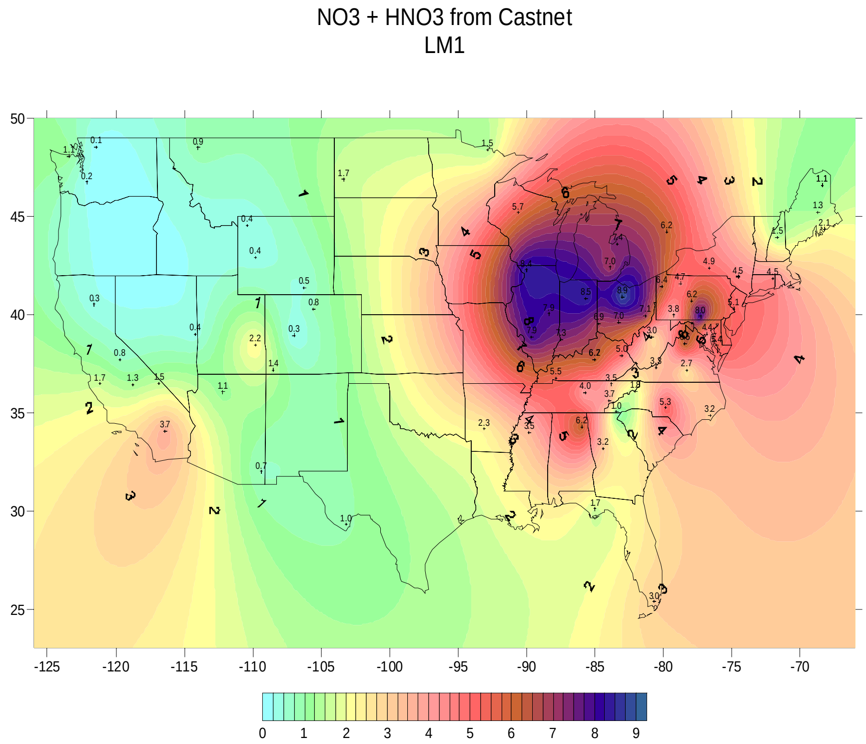


Figure 20. Total nitrate: average of the period January 2- 29, 2001 CASTNet observations.

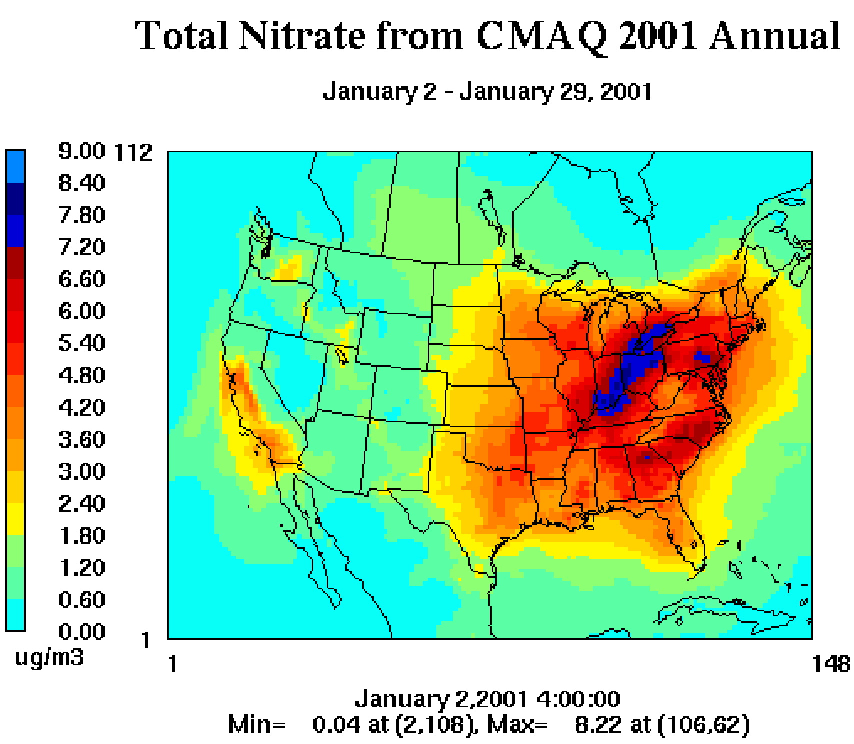


Figure 21. Total nitrate: average of the period January 2- 29, 2001 CMAQ predictions.

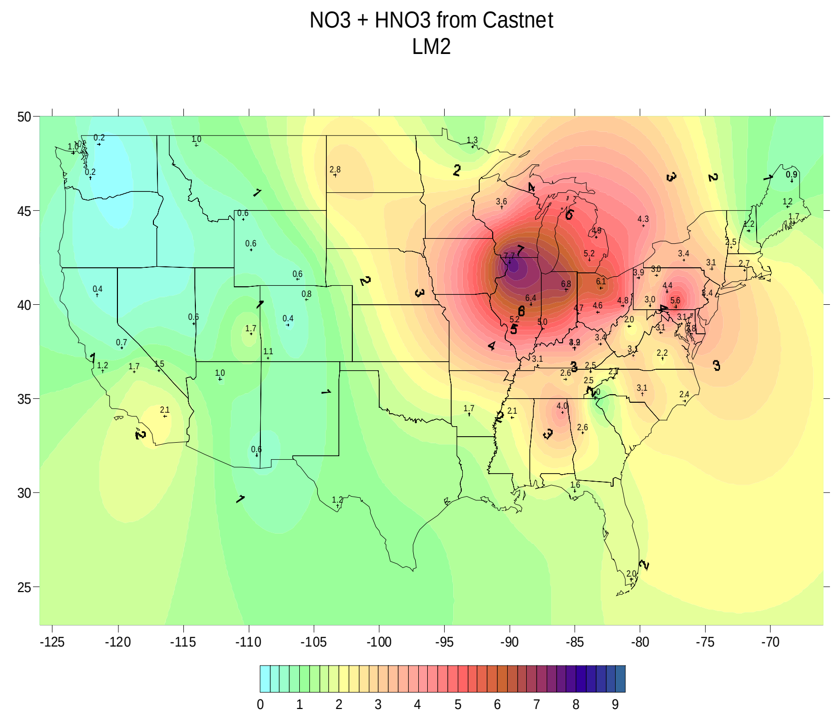


Figure 22. Total nitrate: average of the period January 30 - February 26, 2001 CASTNet observations .

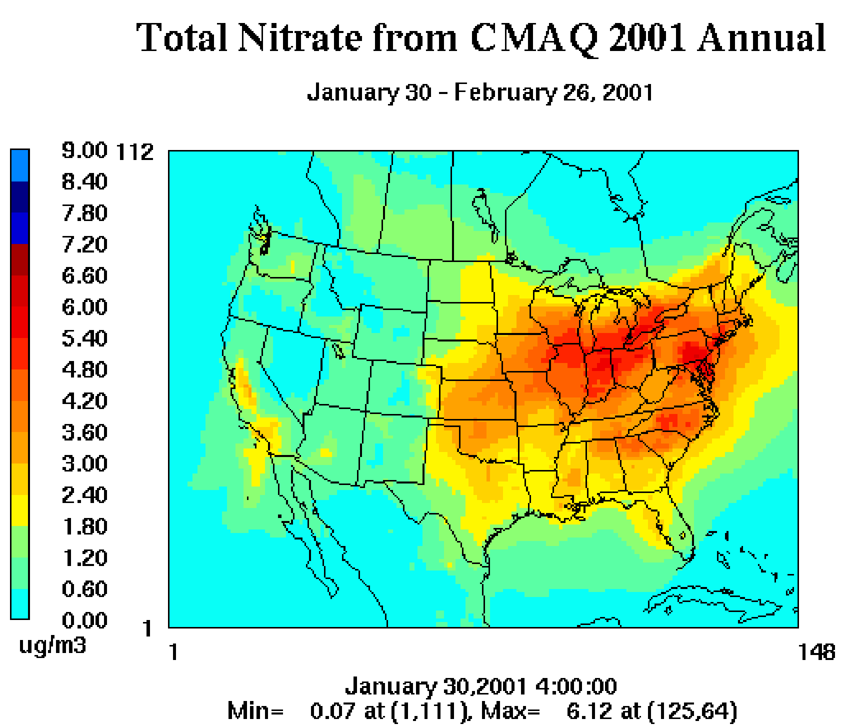


Figure 23. Total nitrate: average of the period January 30 - February 26, 2001 CMAQ predictions.

e. Nitrate Time Series Analysis

In general, CMAQ performed reasonably well for nitrate PM and total nitrate among the four networks, IMPROVE, STN, CASTNet, and SEARCH (Appendix D, Figures D- 7 thru 12).

The time-series analysis shows that the model was able to capture the monthly and weekly trends in nitrate PM and total nitrate at most sites, but the concentrations tend to be overpredicted in the cool seasons of the year, especially at some of the rural sites. However, the nitrate predictions closely tracked the observations at some sites, especially those in the Midwest. Also, there is a tendency for performance to be better in the period October through December compared to the period January through March. These differences suggest that the temporal factors used to distribute annual ammonia emissions to each month may have overestimated emissions during the first quarter of the year in some parts of the region. Excessive ammonia would not only contribute to the overprediction of nitrate PM because of the conversion of excessive HNO3 to nitrate PM, but also would result in an imbalance that leads to the overprediction of total nitrate. This would occur since nitrate PM has significantly lower dry deposition velocity than HNO3, and thus partitioning toward nitrate PM would result in lower removal rate of total nitrate due to lower dry deposition rate.

3. Ammonium Concentrations

The overall model performance of ammonium PM is fairly good compared against available monitoring data from CASTNet and STN. The seasonal plots and annual time series plots also show that the model was able to capture the seasonal and weekly/daily trends of ammonium PM. The model slightly overpredicted ammonium PM over both rural and urban sites in the East where the ammonium PM is most abundant. The model slightly underpredicted the ammonium PM over both rural and urban sites in the West.

a. Ammonium PM Performance at IMPROVE Sites

Table 9 lists the performance statistics for ammonium PM at the IMPROVE sites. Note that because the sample size is relatively small the results may not be meaningful. Ammonium PM is overpredicted by 25% domainwide. In the East, ammonium PM is generally overpredicted by 38%, and underpredicted in the West by 18%.

Table 9. Annual ammonium PM performance at IMPROVE sites.

	No. of Obs	Mean CMAQ Predictions (μg/m³)	Mean Observations (μg/m³)	Ratio of Means (pred/obs)	Bias (μg/m³)	Fractional Bias (%)	Error (μg/m³)	Fractional Error (%)	Correlation Coefficient
National	330	1.72	1.38	1.25	0.35	26.19	0.69	47.10	0.36
East	326	1.74	1.38	1.26	0.36	26.93	0.69	46.19	0.36
West	4	0.46	0.82	0.57	-0.36	-34.51	0.92	121.54	0.22

Figures 24 and 25, which provide the scatter plots of the annual mean (R^2= 0.10) and seasonal mean (summer: R^2= 0.12; fall: R^2= 0.88; spring: R^2= 0.96; winter: R^2= 0.02) ammonium PM for IMPROVE observations versus CMAQ predictions. Overall, correlations showed modest agreement considering the limited amount of data collected, with better performance in Spring and Fall.

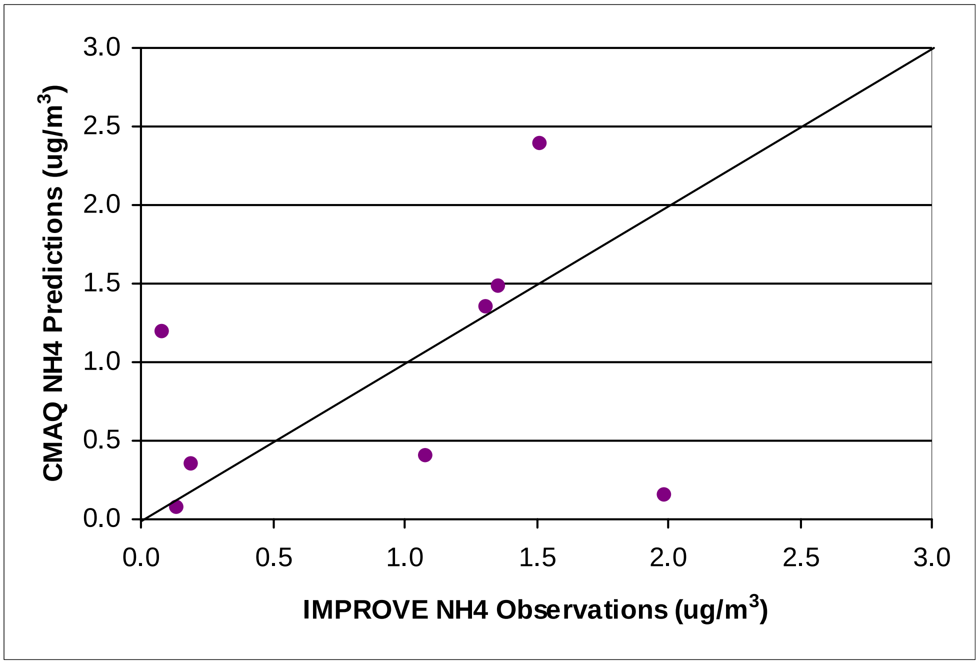


Figure 24. Annual mean ammonium PM: IMPROVE observations versus CMAQ predictions.

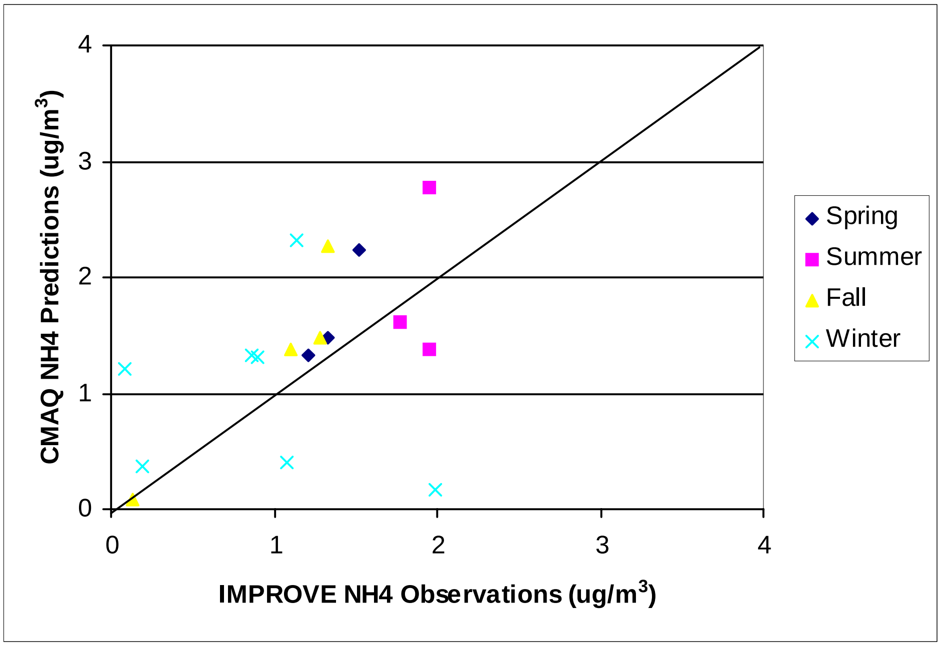


Figure 25. Seasonal mean ammonium PM: IMPROVE observations versus CMAQ predictions.

b. Ammonium PM Performance at STN Sites

Table 10 lists the performance statistics for ammonium PM at the STN sites. Ammonium PM is overpredicted by 25% domainwide. Ammonium PM is generally overpredicted in the East (36%) and underpredicted in the West (6%).

Table 10. Annual ammonium PM performance at STN sites.

	No. of Obs.	Mean CMAQ Predictions (µg/m^3)	Mean Observations (µg/m^3)	Ratio of Means (pred/obs)	Bias (µg/m^3)	Fractional Bias (%)	Error (µg/m^3)	Fractional Error (%)	Correlation Coefficient
National	6970	1.58	1.26	1.25	0.32	35.50	0.84	68.24	0.34
East	5414	1.87	1.36	1.37	0.51	44.10	0.89	67.16	0.43
West	1556	0.61	0.94	0.65	-0.33	5.57	0.66	72.01	0.20

Figures 26 and 27, which show modest agreement among the scatter plots of the annual (R^2= 0.29) and seasonal mean (summer: R^2= 0.54; fall: R^2= 0.13; spring: R^2= 0.52; winter: R^2= 0.31) nitrate PM for STN observations verus CMAQ predictions.

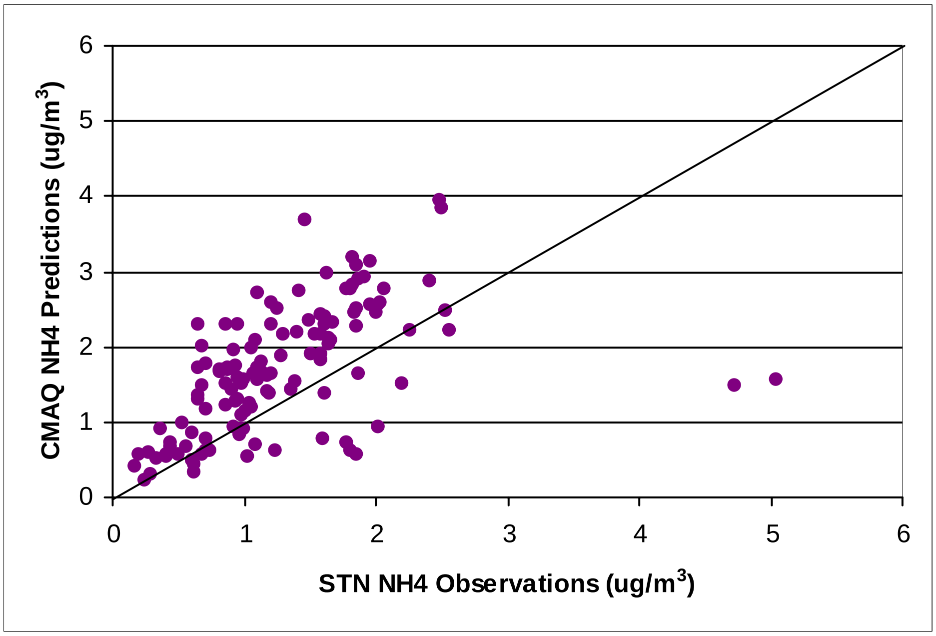


Figure 26. Annual mean ammonium PM: STN observations versus CMAQ predictions.

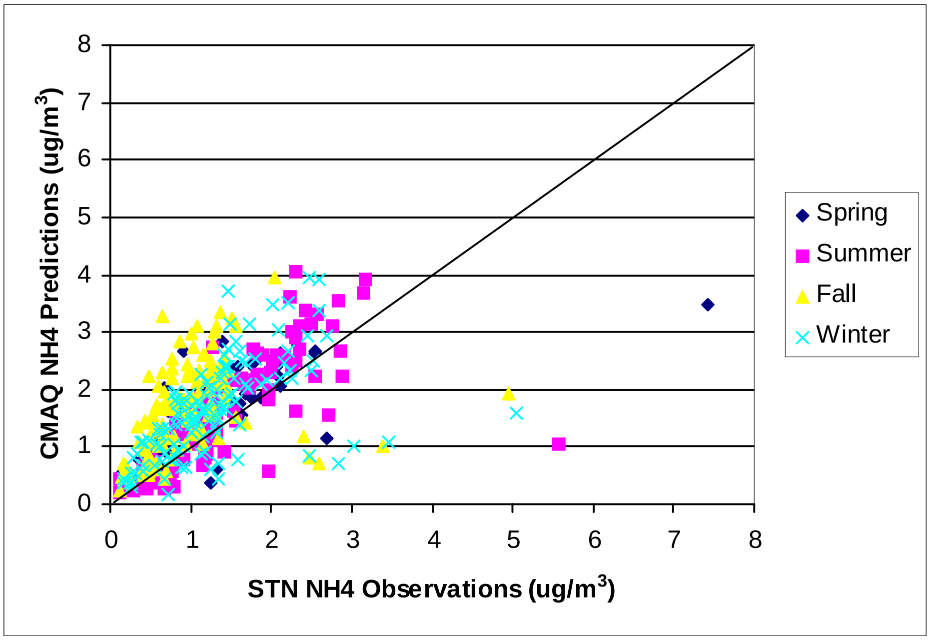


Figure 27. Seasonal mean ammonium PM: STN observations versus CMAQ predictions.

c. Ammonium PM Performance at CASTNet Sites

Table 11 lists the performance statistics for ammonium PM at the CASTNet sites. Nationally, ammonium PM is overpredicted by only 7% domainwide. Generally, the model performs well for ammonium PM, overpredicting in the East by only 9% and underpredicting in the West by 17%. In the East, fractional bias is ~14% with a fractional error of ~33%.

Table 11. Annual ammonium PM performance at CASTNet sites.

	No. of Obs.	Mean CMAQ Predictions (μg/m^3)	Mean Observations (μg/m^3)	Ratio of Means (pred/obs)	Bias (μg/m^3)	Fractional Bias (%)	Error (μg/m^3)	Fractional Error (%)	Correlation Coefficient
National	3736	1.24	1.16	1.07	0.08	5.85	0.39	37.97	0.67
East	2639	1.63	1.49	1.09	0.14	13.91	0.48	32.94	0.54
West	1097	0.32	0.38	0.83	-0.06	-13.54	0.18	50.06	0.12

Figures 28 and 29 shows the seasonal mean CASTNet observations versus CMAQ predictions for ammonium PM. The scatter plots and linear regressions of annual and seasonal ammonium PM showed good agreement, (annual: R^2 = 0.89; summer: R^2 = 0.85; fall: R^2 = 0.85; spring: R^2 = 0.87; winter: R^2 = 0.82).

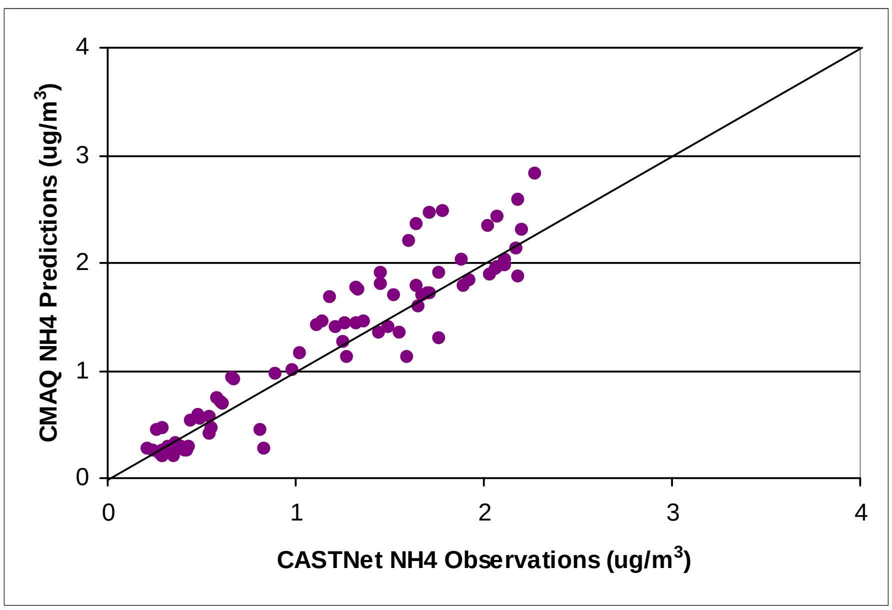


Figure 28. Annual mean ammonium PM: CASTNet observations versus CMAQ predictions.

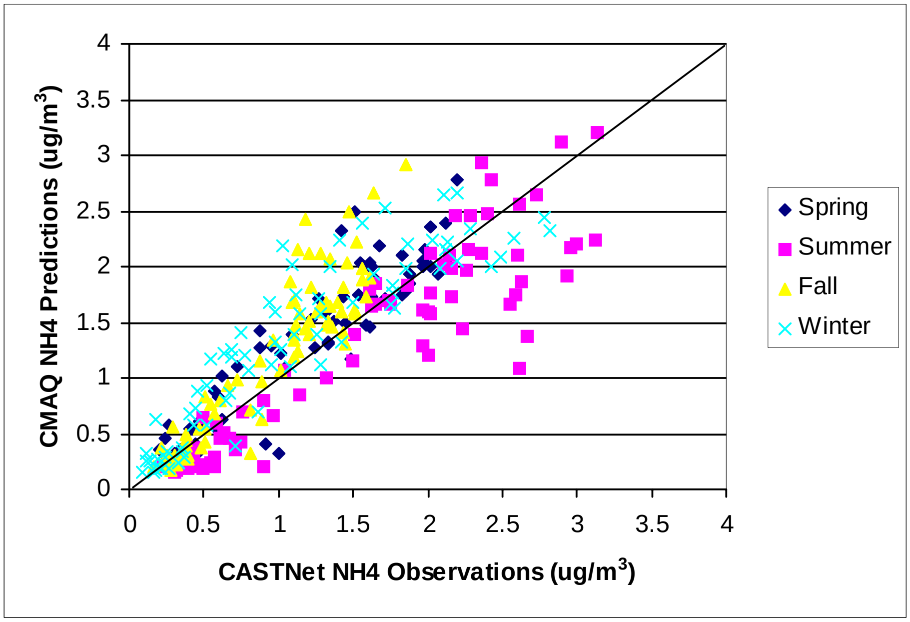


Figure 29. Seasonal mean ammonium PM: CASTNet observations versus CMAQ predictions.

d. Ammonium PM Spatial Pattern Analysis

Figures 30-33 show the two summer periods analyzed for ammonium PM (i.e., June 19 - July 16, 2001; July 17 - August 13, 2001) when ammonium PM is at its peak. In general, the spatial patterns of ammonium PM predicted by CMAQ are very similar to those spatial patterns extracted from the observations, in both location and magnitude, especially in the East. Note that in the Central and Western US, observations are limited compared to the East, hence, comparisons in those areas should be viewed with caution.

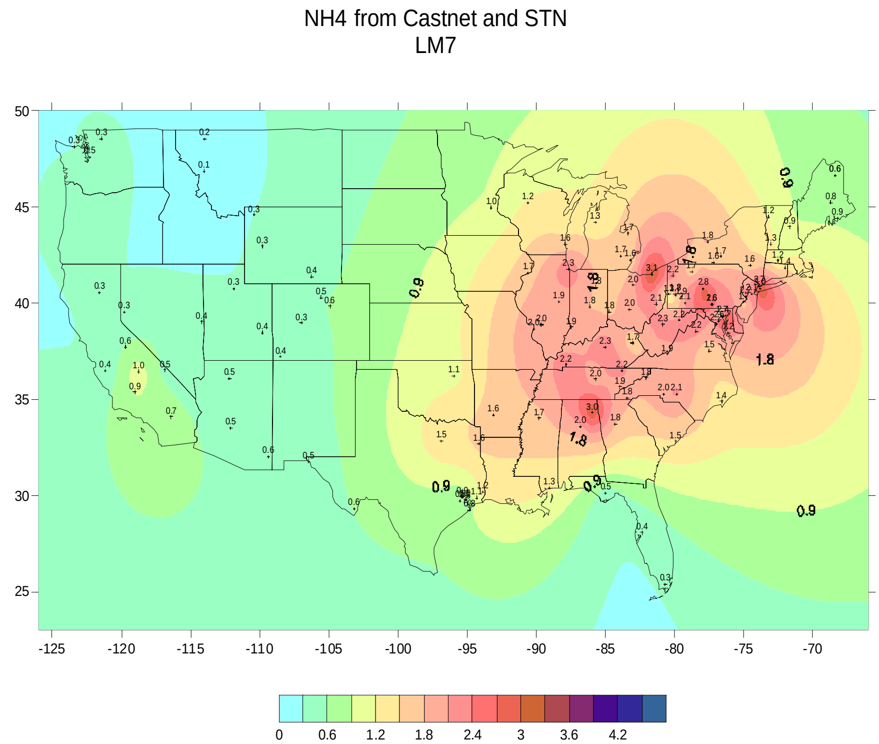


Figure 30. Ammonium PM: average of the period June 19 - July 16, 2001 CASTNet and STN observations.

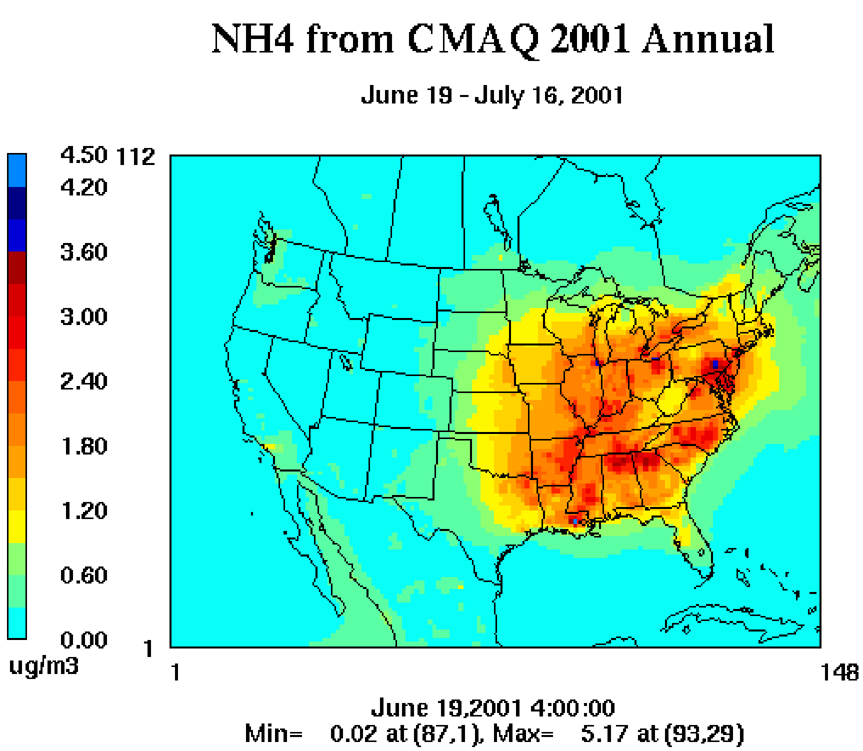


Figure 31. Ammonium PM: average of the period June 19 - July 16, 2001 CMAQ predictions.

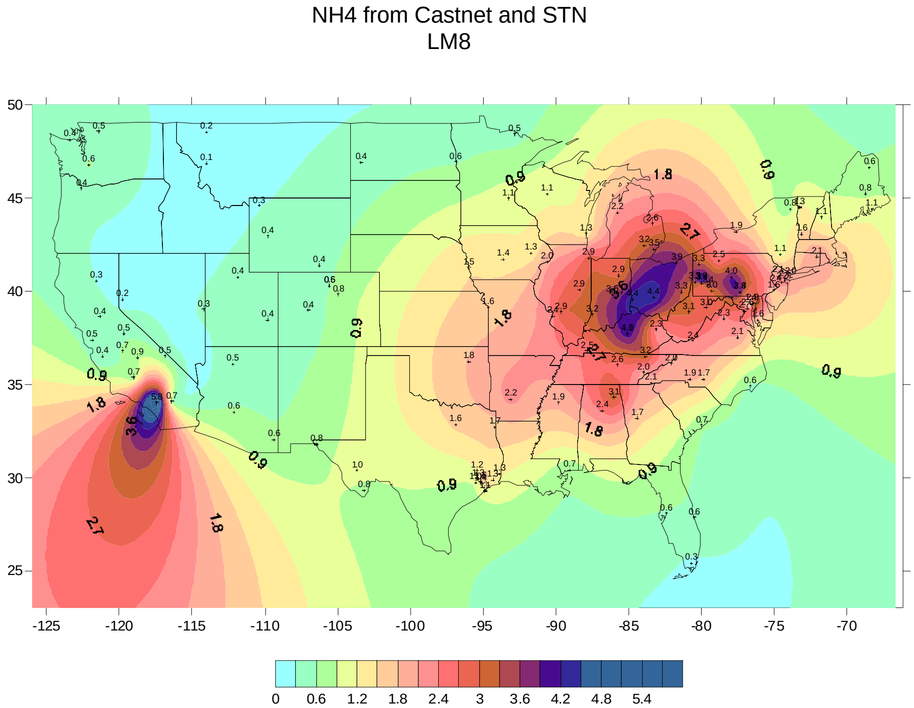


Figure 32. Ammonium PM: average of the period July 17 - August 13, 2001 CASTNet and STN observations.

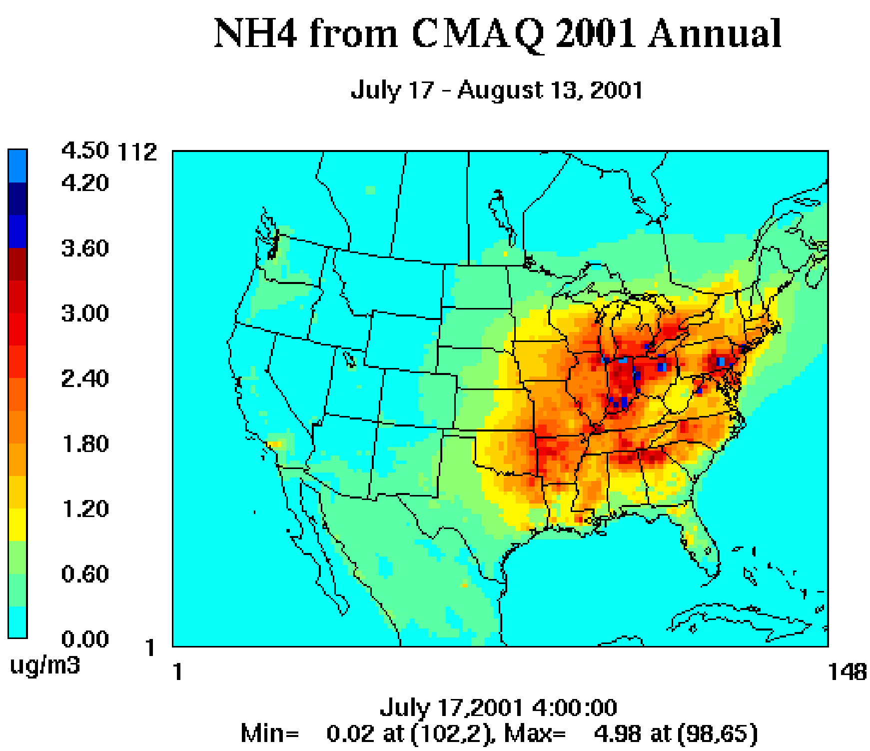


Figure 33. Ammonium PM: average of the period July 17 - August 13, 2001 CMAQ predictions.

e. Ammonium PM Time-series Performance

CMAQ performed reasonably well for ammonium PM when compared to STN CASTNet, and SEARCH monitoring networks (Appendix D, Figures D- 13-16). Since the level of ammonium PM is highly correlated to the abundance of sulfate PM in the East, the performance of ammonium PM is anticipated to be consistent with that of sulfate PM. Indeed, similar to the time-series analysis of sulfate PM, CMAQ was able to capture the magnitude, trends and variations of ammonium PM reasonably well on a monthly, weekly and daily basis in the East. These ammonium PM time-series comparisons showed fairly good performance at both rural and urban sites, but the model seemed to slightly overpredict ammonium PM for most of the year. In regard to seasonal performance, the model performed slightly better for ammonium PM during the spring and summer months especially at the rural sites.

4. Elemental Carbon Concentrations

The overall model performance of elemental carbon is reasonably well without significant bias compared against the available monitoring data. The seasonal and annual plots show that the model predicted fairly well over rural sites (IMPROVE) both in the East and the West, but overpredicted in the East and underpredicted in the West over urban sites (STN), indicating that the elemental carbon may be more a local concern. The seasonal performance evaluation also shows that the model seemed to predict the elemental carbon better in the warmer months than in the colder months.

a. Elemental Carbon Performance at IMPROVE Sites

Table 12 lists the performance statistics for elemental carbon at the IMPROVE sites. Elemental carbon concentrations at IMPROVE sites are relatively low, but performance is generally good. There is a domainwide underprediction of only 2% with a western overprediction of 9%.

Table 12. Annual elemental carbon performance at IMPROVE sites.

	No. of Obs.	Mean CMAQ Predictions (μg/m^3)	Mean Observations (μg/m^3)	Ratio of Means (pred/obs)	Bias (μg/m^3)	Fractional Bias (%)	Error (μg/m^3)	Fractional Error (%)	Correlation Coefficient
National	13441	0.23	0.24	0.98	-0.01	-16.26	0.15	60.77	0.22
East	4759	0.31	0.35	0.87	-0.04	-22.57	0.16	50.74	0.28
West	8682	0.19	0.17	1.09	0.02	-12.81	0.13	66.25	0.14

Figures 34 and 35 show scatter plots of annual and seasonal mean elemental carbon for IMPROVE observations versus CMAQ predictions, respectively. The annual scatter plot and linear regression shows some scatter, however good agreement with a R^2 of 0.42. Overall, spring and fall linear regressions had relatively good agreement (spring: R^2 = 0.47; fall: R^2 = 0.49), whereas winter and summer had the weakest correlations (winter: R^2 = 0.38; and spring: R^2 = 0.19).

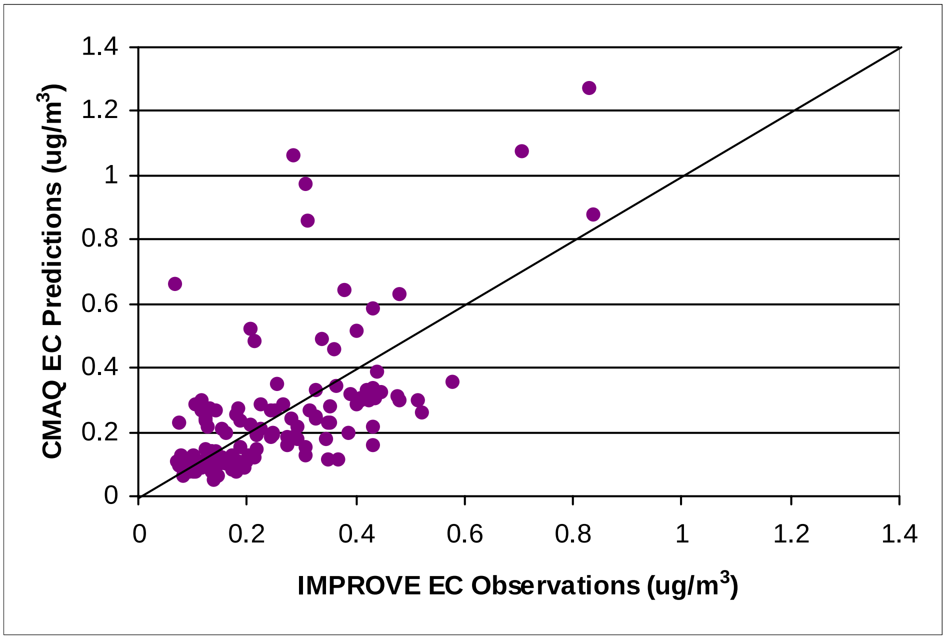


Figure 34. Annual mean elemental carbon: IMPROVE observations versus CMAQ predictions.

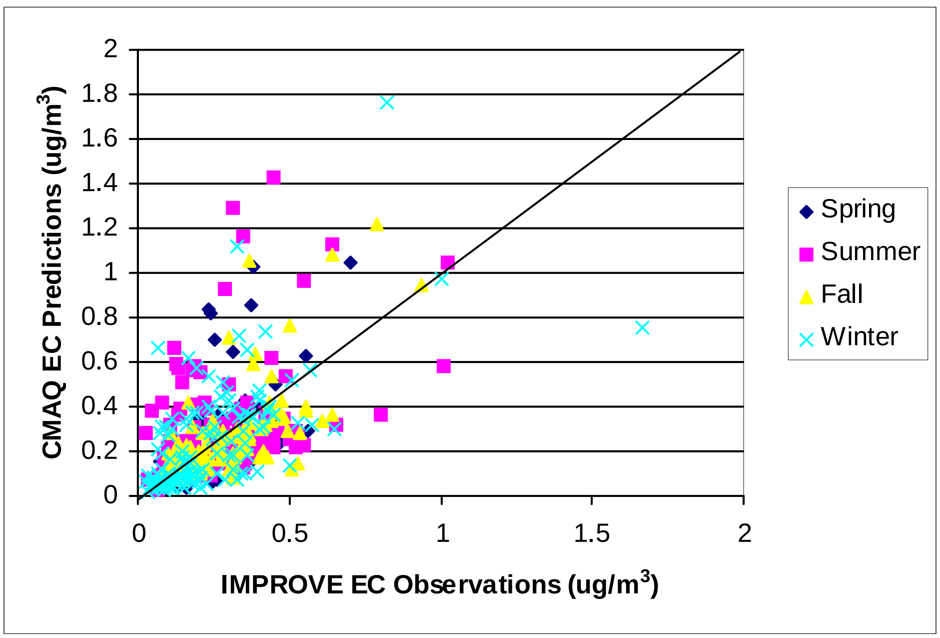


Figure 35. Seasonal mean elemental carbon: IMPROVE observations versus CMAQ predictions.

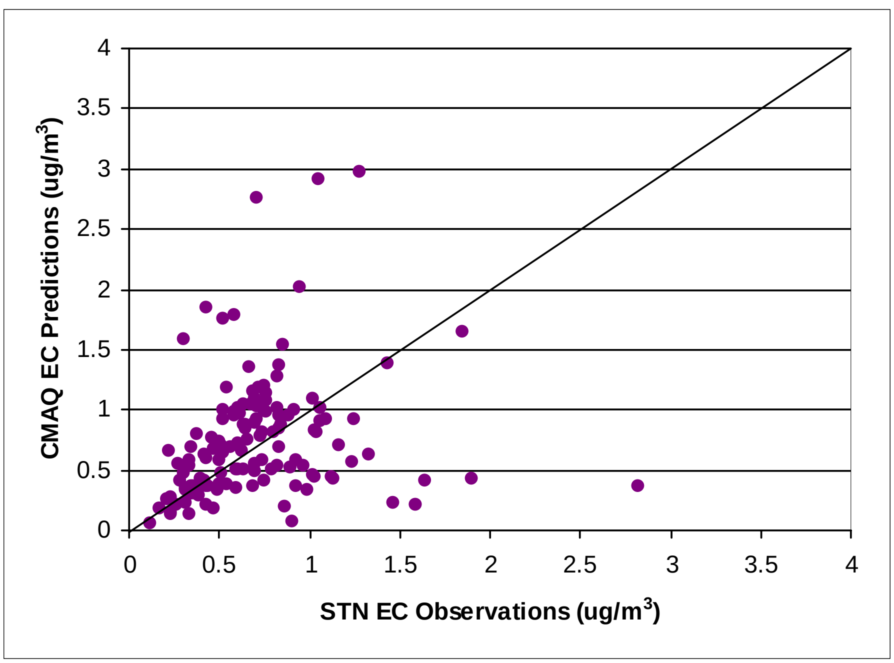
b. Elemental Carbon Performance at STN Sites

Table 13 lists the performance statistics for elemental carbon at the STN sites. Observed elemental carbon concentrations are extremely low, which CMAQ predicts domainwide an overprediction of 30%; 53% overprediction in the East and 23% underprediction in the West.

Table 13. Annual elemental carbon performance at STN sites.

	No. of Obs.	Mean CMAQ Predictions (μg/m³)	Mean Observations (μg/m³)	Ratio of Means (pred/obs)	Bias (μg/m³)	Fractional Bias (%)	Error (μg/m³)	Fractional Error (%)	Correlation Coefficient
National	7108	0.85	0.65	1.30	0.20	20.24	0.52	64.22	0.09
East	5483	0.91	0.59	1.53	0.31	32.06	0.51	63.35	0.15
West	1625	0.65	0.85	0.77	-0.20	-19.63	0.52	67.16	0.08

Figures 36 and 37 show scatter plots of annual and seasonal mean elemental carbon for STN observations versus CMAQ predictions, respectively. The annual scatter plot and linear regression displayed scatter with a poor R^2 of 0.03. Summer and spring seasons had the best regressions: summer: $R^2 = 0.21$; spring: $R^2 = 0.18$), whereas winter and fall had the weakest correlations (winter: $R^2 = 0.01$; and fall: $R^2 = 0.09$).



Fgure 36. Annual mean elemental carbon: STN observations versus CMAQ predictions.

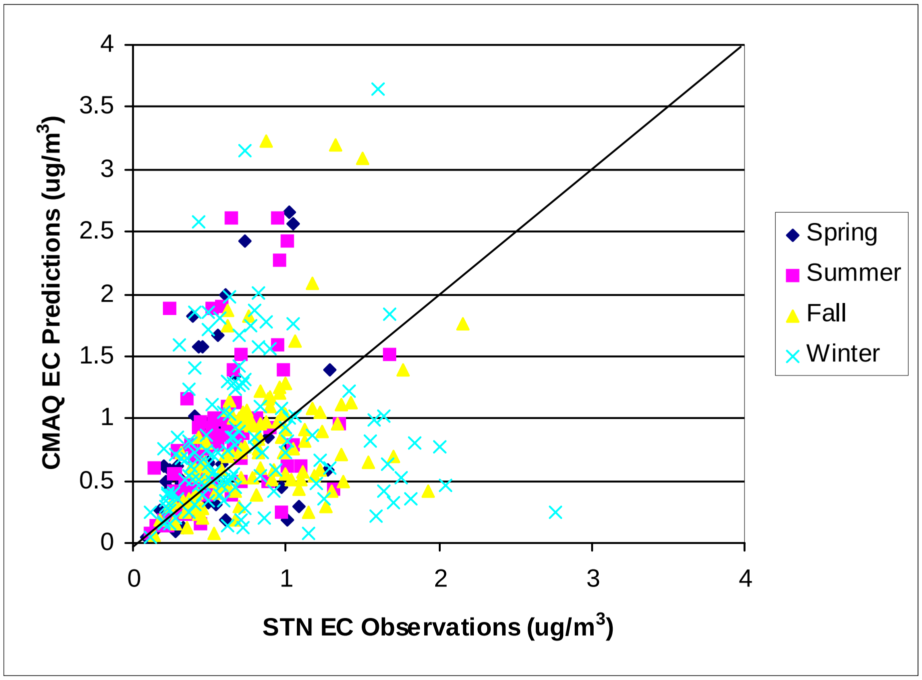


Figure 37. Seasonal mean elemental carbon: STN observations versus CMAQ predictions.

c. Elemental Carbon Time-series Performance

CMAQ performed reasonably well for elemental carbon (EC) when compared to STN, IMPROVE, and SEARCH monitoring networks (Appendix D, Figures D- 17-21). CMAQ was able to capture the magnitude, trends. and variations of EC reasonably well on a monthly, weekly and daily basis in the East. These EC time-series comparisons showed fairly good performance at both rural and urban sites, but the model seemed to slightly underpredict EC (specifically at the six SEARCH sites) for most of the year. In regard to seasonal performance, the model performed slightly better for EC during the spring and summer months especially at the rural sites.

5. Organic Carbon Performance

The overall model performance of organic carbon (OC) is in line with the monitoring data without significant bias. However, the model performance for OC is mixed, and correlations between the model and monitoring data are much lower than that for sulfate and nitrate. The model underpredicted organic carbon (OC) throughout the year over both rural (IMPROVE) and urban (STN) sites in the East, but overpredicted for both sites in the West. The uncertainties associated with the science and modeling of OC (e.g., anthropogenic and biogenic OC) along with primary OC emissions and measurement techniques (e.g., OC vs. EC) contribute to the relatively poor model performance of OC compared to that of sulfate and nitrate.

a. Organic Carbon Performance at IMPROVE Sites

Table 14 lists the performance statistics for organic carbon at the IMPROVE sites.

Organic carbon performance is generally good with a nationwide overprediction of 11%. Although there is a 75% overprediction in the West, the performance in the East is relatively good with an underprediction of 7%. But the correlation coefficients are low in the East and West.

Table 14. Annual organic carbon performance at IMPROVE sites.

	No. of Obs.	Mean CMAQ Predictions (µg/m³)	Mean Observations (µg/m³)	Ratio of Means (pred/obs)	Bias (µg/m³)	Fractional Bias (%)	Error (µg/m³)	Fractional Error (%)	Correlation Coefficient
National	13427	1.50	1.11	1.35	0.39	29.62	0.92	67.68	0.11
East	4764	1.45	1.56	0.93	-0.10	-9.73	0.77	51.78	0.23
West	8663	1.52	0.87	1.75	0.65	51.26	1.00	76.37	0.09

Annual and seasonal scatter plots (Figures 38 and 39) of mean organic carbon for IMPROVE observations versus CMAQ predictions show a fairly large differences in predictions compared to the observations. The correlations are weak with a low annual $R^2 = 0.11$. Seasonal correlations are summer: $R^2 = 0.01$; fall: $R^2 = 0.12$; spring: $R^2 = 0.22$; and winter: $R^2 = 0.28$.

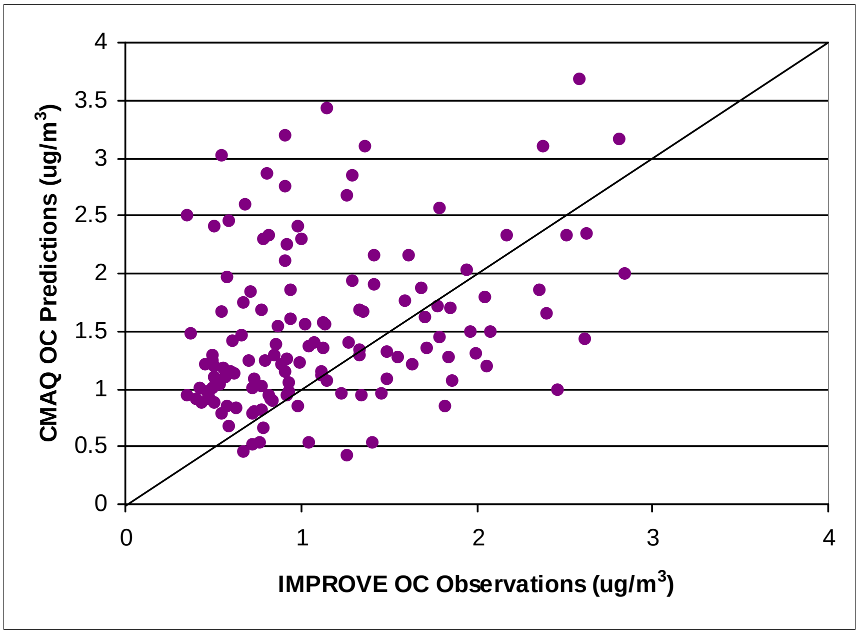


Figure 38. Annual mean organic carbon: IMPROVE observations versus CMAQ predictions.

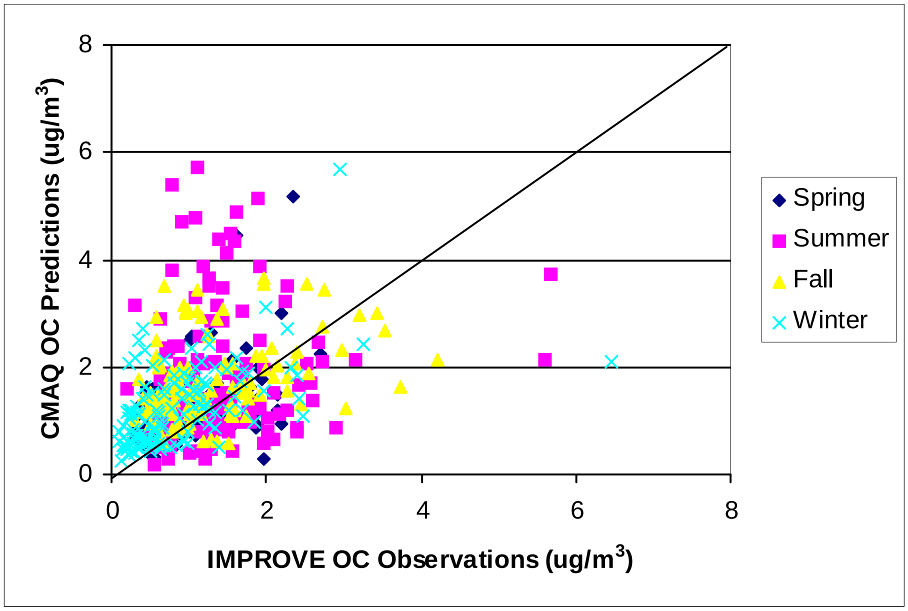


Figure 39. Seasonal mean organic carbon: IMPROVE observations versus CMAQ predictions.

b. Organic Carbon Performance at STN Sites

The performance statistics for organic carbon at the STN sites are listed in Table 15. Organic carbon performance has a nationwide underprediction of 25%. Organic carbon is underpredicted by 41% in the West, however performance was relatively good in the East with an underprediction of 18%. Correlation coefficients are low domainwide and in the East and West.

Table 15. Annual organic carbon performance at STN sites.

	No. of Obs.	Mean CMAQ Predictions (µg/m³)	Mean Observations (µg/m³)	Ratio of Means (pred/obs)	Bias (µg/m³)	Fractional Bias (%)	Error (µg/m³)	Fractional Error (%)	Correlation Coefficient
National	6947	2.40	3.20	0.75	-0.86	-9.58	1.75	73.13	0.11
East	5339	2.39	2.93	0.82	-0.60	-3.21	1.55	75.11	0.13
West	1608	2.44	4.12	0.59	-1.72	-31.05	2.42	66.44	0.11

Annual and seasonal scatter plots (Figures 40 and 41) of mean organic aerosol for STN observations versus CMAQ predictions show a fair amount of scatter, with a low annual correlation of $R^2 = 0.02$ and seasonal correlations in summer: $R^2 = 0.23$; fall: $R^2 = 0.03$; spring: $R^2 = 0.22$; and winter: $R^2 = 0.01$.

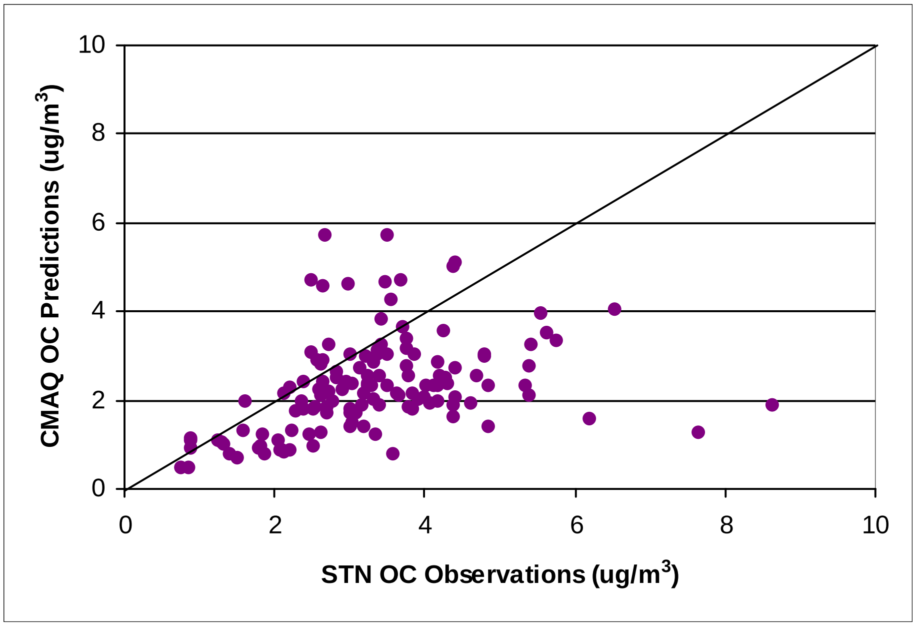


Figure 40. Annual mean organic carbon: STN observations versus CMAQ predictions.

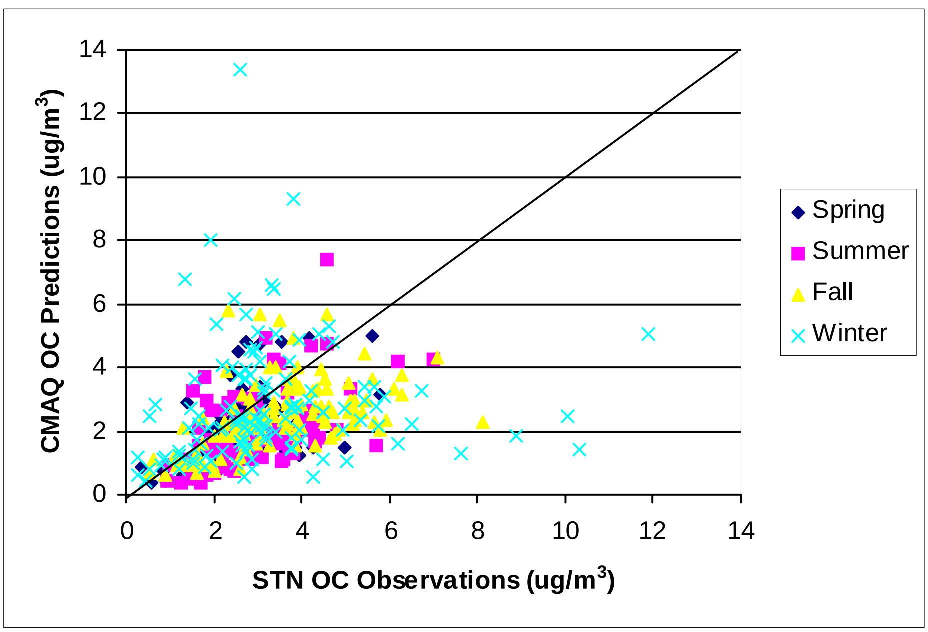


Figure 41. Seasonal mean organic carbon: STN observations versus CMAQ predictions.

c. Organic Carbon Time series Analysis

In general, CMAQ appeared to underestimate organic carbon (OC) at both rural and urban sites throughout the year when compared to IMPROVE, STN, and SEARCH monitoring networks (Appendix D, Figures D- 22-26) in the East. However, the model seems to perform better in the colder months in the East and at several STN sites (e.g. Marion, Indiana, and Bronx, New York) the model actually overestimate OC in the colder months. Since the major component of organic aerosols in the colder months should be primary organic aerosols (POA) and in the warmer months should be secondary organic aerosols (SOA), the underprediction in the warmer month could be attributed to the underprediction of photochemically produced SOA. Overall, the temporal trends and variations were not captured as good as sulfate PM and nitrate PM. This is not expected since there are well known uncertainties associated with the science and modeling of organic aerosols. Organic aerosols consist of several forms: POA, anthropogenic SOA, and biogenic SOA. Thus, the emissions of POA and photochemical formation of anthropogenic and biogenic SOA need to be well characterized in the model in order to adequately simulate the organic aerosols, and both of these still present major challenges in the modeling of organic aerosols. Moreover, the uncertainties associated with the measurement techniques of carbonaceous aerosols (e.g., OC/EC split, OC blank correction, etc.) also present an issue for model evaluation against ambient data.

6. PM2.5 Concentrations

a. PM2.5 Performance at IMPROVE Sites

Table 16 lists the performance statistics for PM2.5 at the IMPROVE sites versus CMAQ predictions. For the full domain, PM2.5 is overpredicted by only 9%. The ratio of the means is 1.09 with a bias of 0.54 μg/m^3. It can be seen that this overprediction is similar in both the East and West. The West is overpredicted by 10% while the East is overpredicted by 9%. The fractional bias is ~8% in the East, while the fractional error is 43%. The fractional bias and error in the West is ~14% and 57% respectively. The observed PM2.5 concentrations in the East are relatively high compared to the West. CMAQ displays an ability to differentiate between generally high and low PM2.5 areas seen in the East and West.

Table 16. Annual PM2.5 performance at IMPROVE sites.

	No. of Obs.	Mean CMAQ Predictions (μg/m^3)	Mean Observations (μg/m^3)	Ratio of Means (pred/obs)	Bias (μg/m^3)	Fractional Bias (%)	Error (μg/m^3)	Fractional Error (%)	Correlation Coefficient
National	13217	6.32	5.77	1.09	0.54	11.94	2.89	51.93	0.47
East	4724	9.86	9.04	1.09	0.82	8.32	3.80	43.27	0.48
West	8493	4.36	3.96	1.10	0.38	13.94	2.39	56.70	0.17

Figures 42 and 43 show the annual and seasonal mean PM2.5 IMPROVE observations versus CMAQ predictions, respectively. The annual and seasonal scatter plots show fairly good agreement, with annual R^2 = 0.72; summer R^2 = 0.65; fall R^2 = 0.64; spring R^2 = 0.72; and winter

R^2 = 0.60).

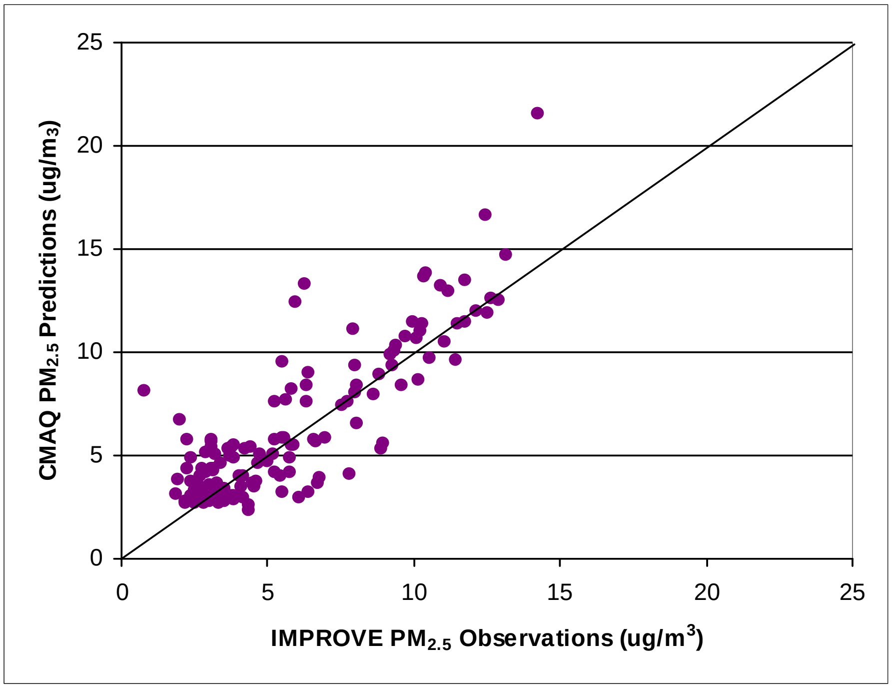


Figure 42. Annual mean PM2.5: IMPROVE observations versus CMAQ predictions.

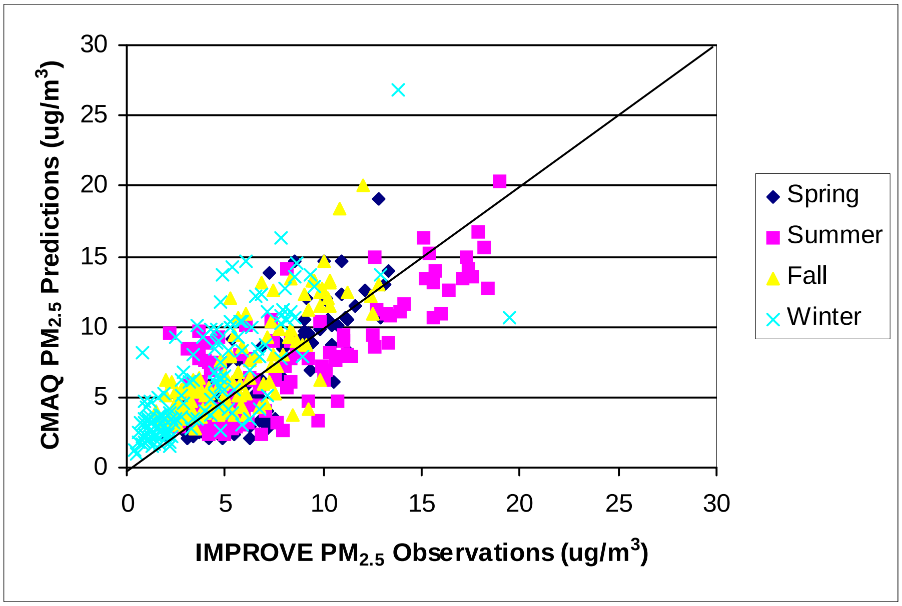


Figure 43. Seasonal mean PM2.5: IMPROVE observations versus CMAQ predictions.

b. PM2.5 Performance at STN sites

Table 17 lists the performance annual statistics for PM2.5 at the STN sites. Nationally, CMAQ underpredicted PM2.5 by 16%. The ratio of the means is 0.84 with a bias of -2.10 μg/m³. It can be seen that this underprediction is greater in the West (49%), whereas the East underpredicts by only 7%. The fractional bias is approximately 21% in the East, while the fractional error is 49%. The fractional bias and error is higher in the West with ~51% and 64% respectively.

Table 17. Annual mean PM2.5 performance at STN sites.

	No. of Obs.	Mean CMAQ Predictions (μg/m³)	Mean Observations (μg/m³)	Ratio of Means (pred/obs)	Bias (μg/m³)	Fractional Bias (%)	Error (μg/m³)	Fractional Error (%)	Correlation Coefficient
National	6419	10.79	12.89	0.84	-2.10	-21.11	5.48	48.54	0.29
East	4944	12.13	13.07	0.93	-0.94	-12.08	5.03	43.90	0.41
West	1475	6.29	12.30	0.51	-6.02	-51.33	6.96	64.09	0.19

Figures 44 and 45 show the annual and seasonal average PM2.5 2001 STN observations versus CMAQ predictions respectively. The annual and seasonal scatterplots showed some scatter, with correlations: annual R^2 = 0.28; summer R^2 = 0.58; fall R^2 = 0.19; spring R^2 = 0.40; and winter R^2 = 0.09.

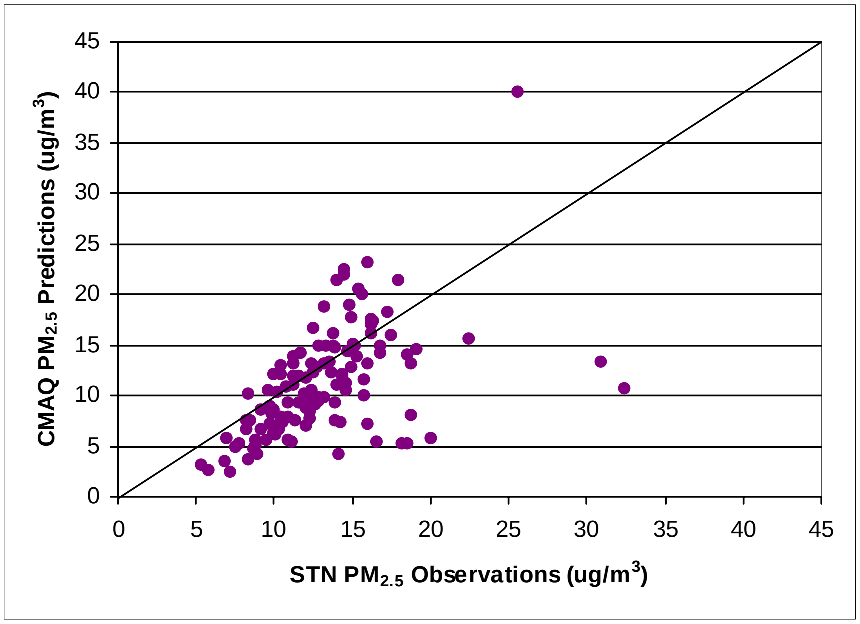


Figure 44. Annual mean PM2.5: STN observations versus CMAQ predictions.

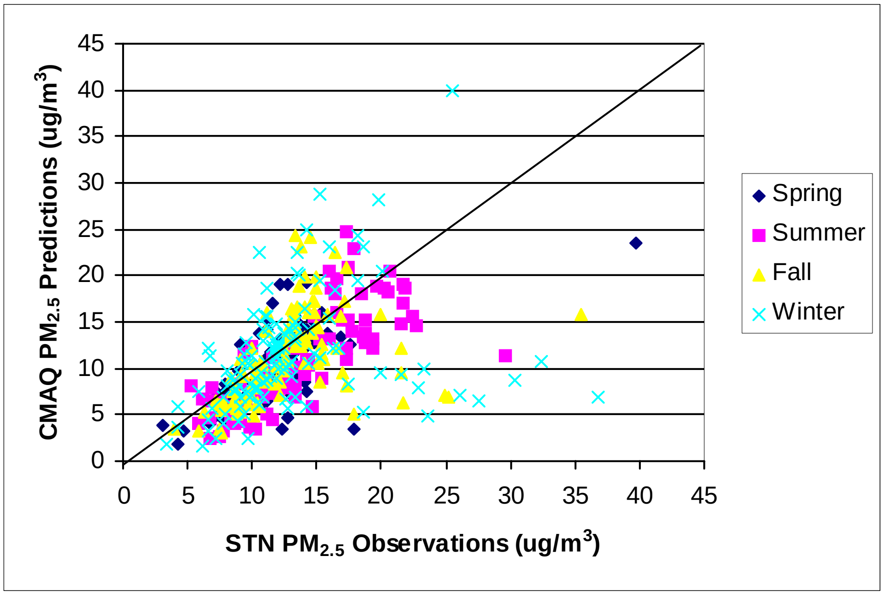


Figure 45. Seasonal mean PM2.5: STN observations versus CMAQ predictions.

B. Comparison of Model Performance Evaluations (conducted by other modeling groups)

Currently, there are no universally accepted or EPA- recommended quantitative criteria for judging the acceptability of PM2.5 model performance. In the absence of such model performance acceptance criteria, we have compared CMAQ 2001 performance results to the range of results obtained by other groups in the air quality modeling community who conducted other recent regional PM2.5 model applications.[6] Summaries of model performance for these other studies can be found in Appendix C. In addition, specific model performance ranges and criteria have been identified by other modeling applications which some contend should be achievable for sulfate and PM2.5, given the current state-of-science for aerosol modeling and measurement uncertainty. The specific values cited by these are ±30 percent to ±50 percent for fractional bias, 50 percent to 75 percent for fractional error, and 50 percent for normalized error.

Below is a summary of performance results from other, non-EPA modeling studies, for summer sulfate and winter nitrate. As noted previously, nitrate and sulfate are the two species most relevant for CAIR. Overall, the general range of fractional bias (FB) and fractional error (FE) statistics for the better performing model applications are as follows:

- summer sulfate is in the range of -10 percent to +30 percent for FB and 35 percent to 50 percent for FE; and
- winter nitrate is in the range of +50 percent to +70 percent for FB and 85 percent to 105 percent for FE.

[6] These other modeling studies represent a wide breath of modeling analyses which cover various models, model configurations, domains, years and/or episodes, chemical mechanisms, and aerosol modules.

The corresponding performance statistics for CAIR 2001 CMAQ application as well as the 1996 REMSAD application used for the CAIR proposal modeling are provided in Table 18. The results indicate that the performance for CMAQ in 2001 is within the range or better than that found by other groups in recent applications. The performance also meets the benchmark goals suggested by several modeling groups. In addition, the CMAQ performance is considerably improved over that of the REMSAD 1996 performance for summer sulfate and winter nitrate, which were near the bounds or outside the range of other recent applications. The CMAQ model performance results give us confidence that our applications of CMAQ using the new modeling platform provide a scientifically credible approach for assessing PM2.5 concentrations for the purposes of CAIR.

Table 18. Selected Performance Evaluation Statistics from the CMAQ 2001 Simulation and the REMSAD 1996 Simulation.

Eastern U.S.		CMAQ 2001		REMSAD 1996	
		FB (%)	FE (%)	FB (%)	FE (%)
Sulfate (Summer)	STN	14	44	-	-
	IMPROVE	10	42	-20	51
	CASTNet	3	22	-21	59
Nitrate (Winter)	STN	15	73	-	-
	IMPROVE	21	92	67	103

C. Wet Deposition Performance

1. Wet Sulfate Deposition Performance at NADP Sites

Table 19 lists the performance annual statistics for wet sulfate deposition at the NADP sites. Nationally, CMAQ overpredicted sulfate wet deposition by 15%. It can be seen that this overprediction is contributed to the East (25%), whereas the West underpredicts by 36%. The fractional bias is approximately 9% in the East, while the fractional error is 58%. The fractional bias and error is higher in the West with approximately -34% and 76% respectively.

Table 19. Annual mean sulfate wet deposition performance at NADP sites.

	No. of Obs.	Mean CMAQ Predictions (kg/ha)	Mean Observations (kg/ha)	Ratio of Means (pred/obs)	Bias (kg/ha)	Fractional Bias (%)	Error (kg/ha)	Fractional Error (%)	Correlation Coefficient
National	7619	1.68	1.46	1.15	0.22	-4.40	1.02	63.09	0.17
East	5299	2.21	1.77	1.25	0.44	8.61	1.24	57.51	0.12
West	2320	0.47	0.74	0.64	-0.26	-34.13	0.53	75.85	0.03

Figures 46 and 47 show the annual and seasonal total NADP observations versus CMAQ predictions for sulfate wet deposition. The annual scatter plot and linear regression show some scatter (underprediction bias sulfate wet deposition), but good agreement, with good correlation: $R^2 = 0.71$. The seasonal scatter plot showed some scatter, with correlations: summer $R^2 = 0.46$; fall $R^2 = 0.53$; spring $R^2 = 0.37$; and winter $R^2 = 0.63$.

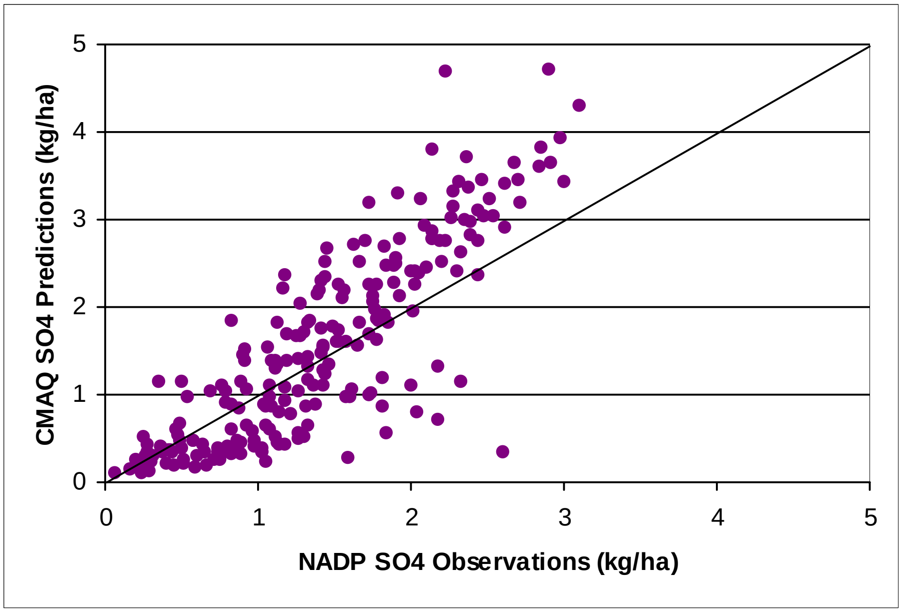


Figure 46. Annual total sulfate wet deposition: NADP observations versus CMAQ predictions.

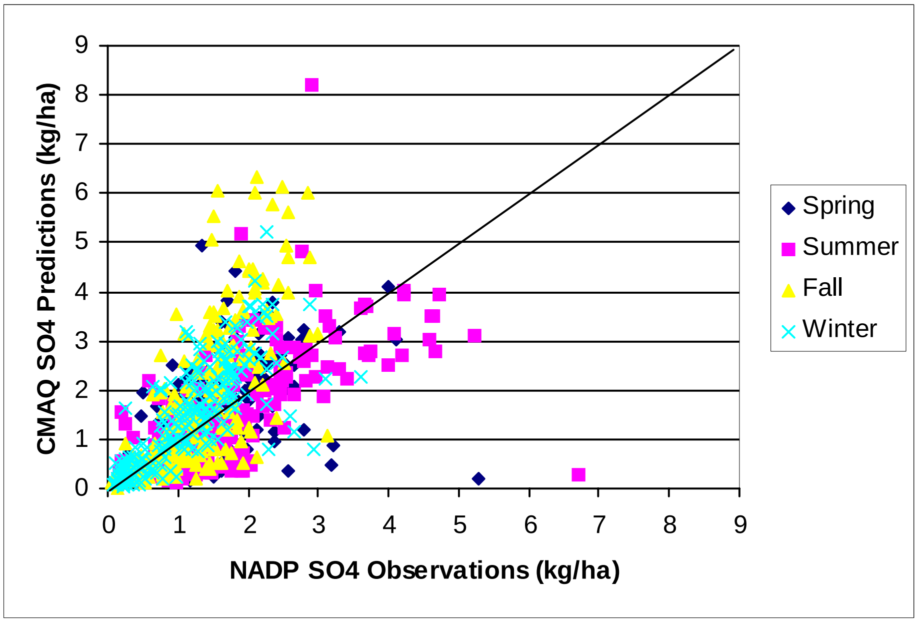


Figure 47. Seasonal total sulfate wet deposition: NADP observations versus CMAQ predictions**.**

2. Wet Nitrate Deposition Performance at NADP Sites

Table 20 lists the performance annual statistics for wet nitrate deposition at the NADP sites. CMAQ underpredicted nitrate wet deposition by 14% domainwide. In the East, performance for wet nitrate deposition is remarkably well, with only an underprediction of 1%. Whereas, in the West, CMAQ underpredicted by 56%. The fractional bias is approximately-21% in the East, while the fractional error is 69%. In the West, the fractional bias and error is higher, approximately -61% and 87% respectively.

Table 20. Annual mean wet nitrate deposition performance at NADP sites.

	No. of Obs.	Mean CMAQ Predictions (kg/ha)	Mean Observations (kg/ha)	Ratio of Means (pred/obs)	Bias (kg/ha)	Fractional Bias (%)	Error (kg/ha)	Fractional Error (%)	Correlation Coefficient
National	7619	1.31	1.52	0.86	-0.21	-33.47	1.13	74.92	0.11
East	5299	1.66	1.68	0.99	-0.02	-21.23	1.25	69.43	0.12
West	2320	0.51	1.16	0.44	-0.65	-61.41	0.85	87.47	0.05

Figures 48 and 49 show the annual total NADP observations versus CMAQ predictions for nitrate wet deposition. The annual scatter plot and linear regressions show an underprediction bias for nitrate with a correlation, R^2 = 0.35. The seasonal scatter plot showed scatter, with correlations: summer R^2 = 0.07; fall R^2 = 0.31; spring R^2 = 0.20; and winter R^2 = 0.40.

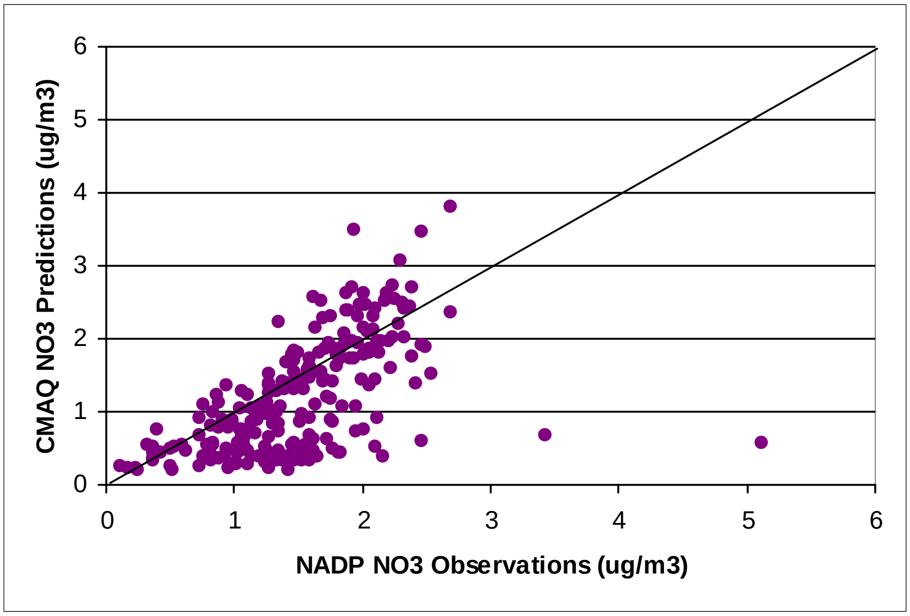


Figure 48. Annual total nitrate wet deposition: NADP observations versus CMAQ predictions**.**

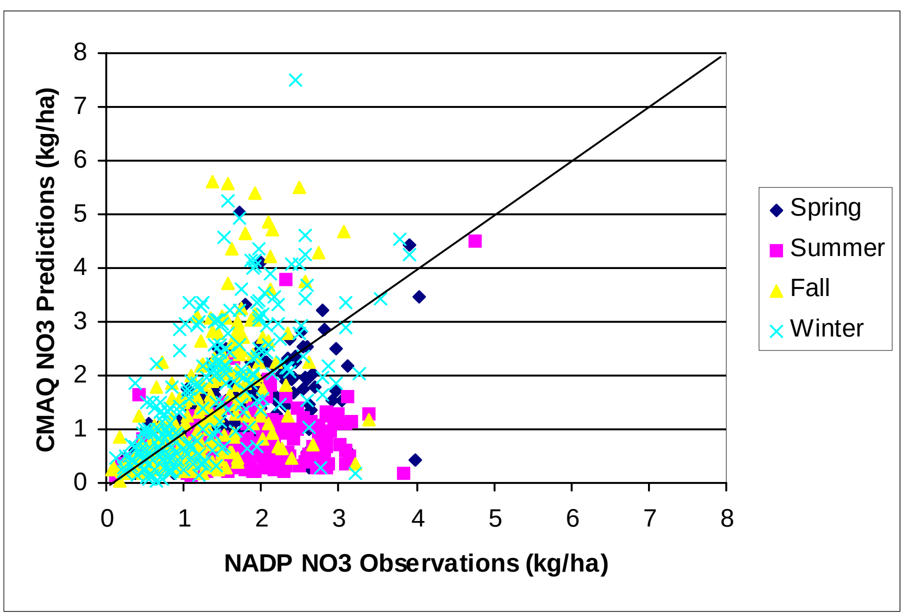


Figure 49. Seasonal total nitrate wet deposition: NADP observations versus CMAQ predictions**.**

3. Wet Ammonium Deposition Performance at NADP Sites

Table 21 lists the performance annual statistics for wet ammonium deposition at the NADP sites. Nationally, the model underpredicted ammonium wet deposition by 7%. In the East, model performance for wet ammonium deposition shows an overprediction of 7%, whereas, in the West, CMAQ underpredicted by 46%. The fractional bias is approximately 0.8% in the East, while the fractional error is 63%. In the West, the fractional bias and error is higher, approximately -39% and 88% respectively.

Table 21. Annual mean wet ammonium deposition performance at NADP sites.

	No. of Obs.	Mean CMAQ Predictions (kg/ha)	Mean Observations (kg/ha)	Ratio of Means (pred/obs)	Bias (kg/ha)	Fractional Bias (%)	Error (kg/ha)	Fractional Error (%)	Correlation Coefficient
National	7619	0.35	0.38	0.93	-0.02	-11.20	0.28	70.70	0.10
East	5299	0.43	0.40	1.07	0.03	0.76	0.29	63.17	0.11
West	2320	0.17	0.32	0.54	-0.15	-38.53	0.25	87.90	0.07

The annual and seasonal NADP observations versus CMAQ predictions for total ammonium wet deposition are shown in Figures 50 and 51. The annual and seasonal scatter plots showed some scatter, with correlations: annual R^2 = 0.30; summer R^2 = 0.07; fall R^2 = 0.22; spring R^2 = 0.15; and winter R^2 = 0.41.

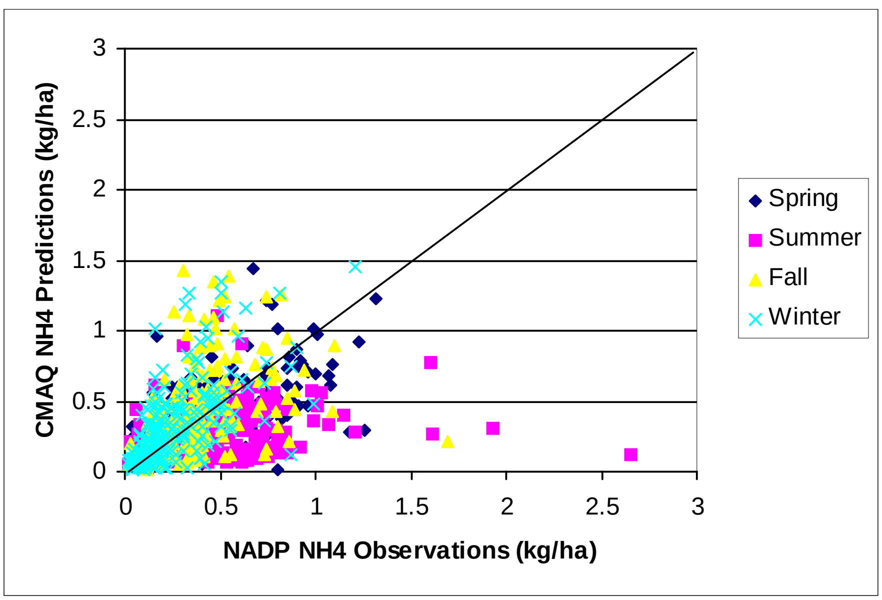


Figure 50. Annual total ammonium wet deposition: NADP observations versus CMAQ predictions.

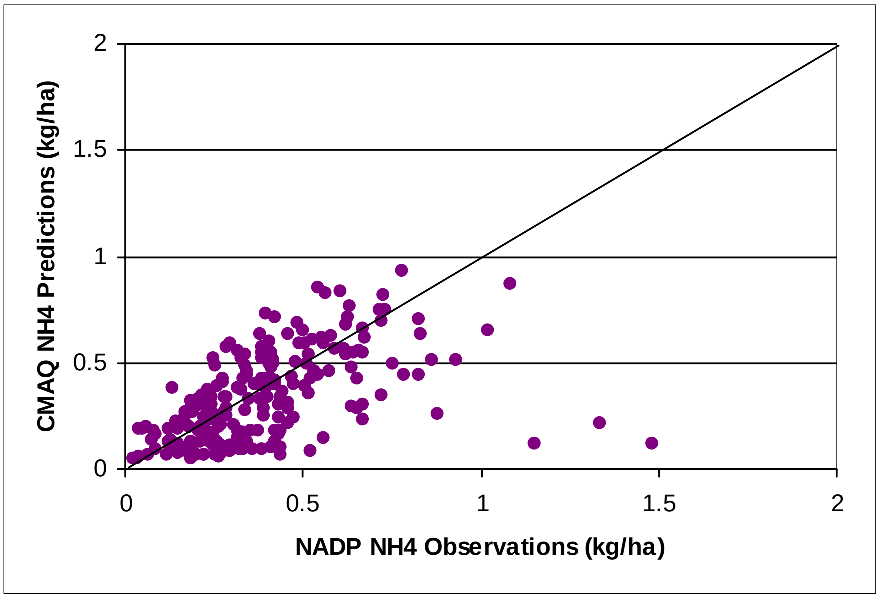


Figure 51. Seasonal total ammonium wet deposition: NADP observations versus CMAQ predictions**.**

D. Visibility

For the purpose of this model performance evaluation, visibility was calculated in a manner similar to recommendations for the Regional Haze rule. EPA has released a draft version of guidance that details the calculation of base period visibility (EPA, 2001) for the 20% best days and 20% worst days in each Class I area..

We are evaluating visibility in terms of light extinction. The daily average extinction coefficient (b_{ext}) values are calculated using the following formula:

b_{ext} = 10.0 + [3.0 * f(RH) * (1.375 * sulfate) + 3.0 * f(RH) * (1.29 * nitrate)+
4.0 * (organic aerosols) + 10.0 * (elemental carbon) + 1.0 * (crustal) + 0.6 * (coarse PM)]

B_{ext} is in units of inverse megameters (Mm^{-1}). The 10.0 initial value accounts for atmospheric background (i.e., Rayleigh) scattering. F(RH) refers to the relative humidity correction function as defined by IMPROVE (2000). The relative humidity correction factor was derived from historical climatological meteorological data. There is a published f(rh) value for each month of the year for each Class I area (SAIC, 2001). The climatological f(rh) values will be used to calculate bext for the Regional Haze rule.

The formula to calculate b_{ext} from CMAQ output species is as follows:

b_{ext} = 10.0 + [3.0 * f(RH) * (1.375 * (ASO4I + ASO4J)) + 3.0 * f(RH) * ((1.29 * (ANO3I + ANO3J)) + 4.0 * (PM_ORG_TOT) + 10.0 * (PM_EC) + 1.0 * (PM_OTH) + 0.6 * (PMCOARS)]

For the purpose of this model performance evaluation, we have calculated the 20% best and worst days from 2001 (the meteorological year we are using) at each IMPROVE site with complete data. The following scatter plots (Figures 52 and 53) show the observed vs. predicted b_{ext} values at the IMPROVE sites on the 20% best and worst days.

CMAQ was generally able to predict the highest b_{ext} values on the observed worst days in the East. The 20% worst days in the East show little bias, but a large amount of scatter. The 20% best days in the East are generally overpredicted. The 20% worst days in the West are equally dispersed around the 1:1 line. CMAQ rarely predicted high b_{ext} values (greater than 100-150 M m^{-1}) in the West. The model predictions on the 20% best and worst days are similar for both Eastern and Western US.

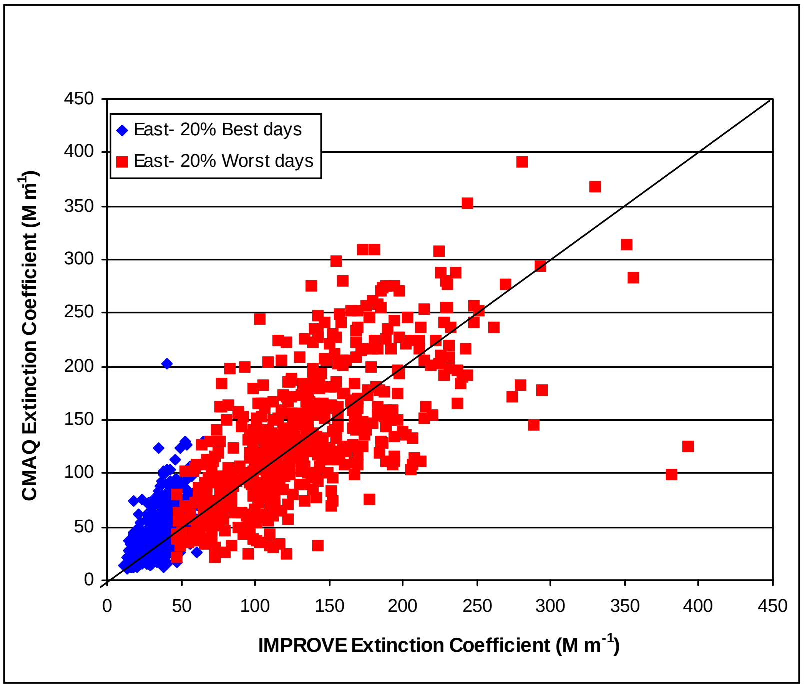


Figure 52. IMPROVE observed versus CMAQ predicted light extinction coefficient values on the 20% best and worst days in the East.

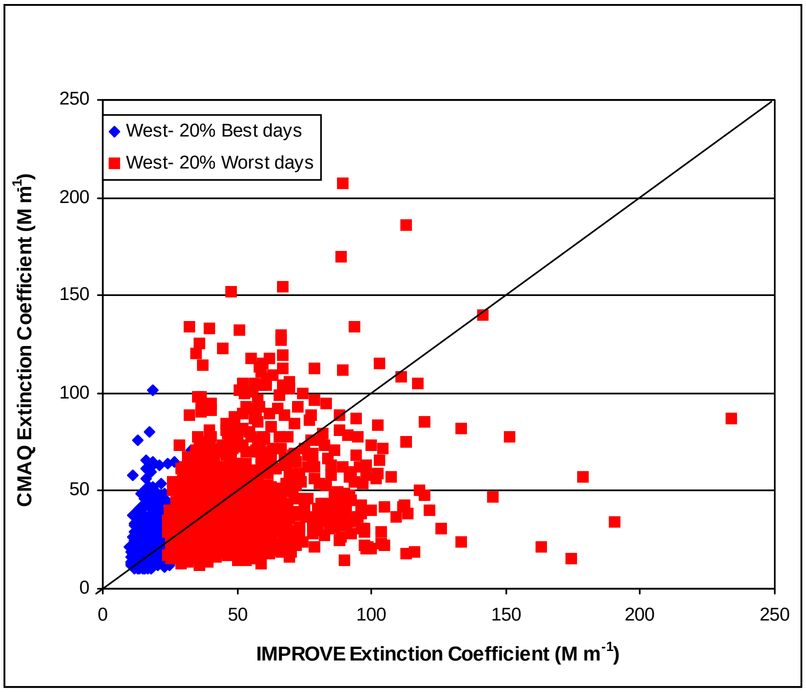


Figure 53. IMPROVE observed versus CMAQ predicted light extinction coefficient values on the 20% best and worst days in the West.

IV. Evaluation Analysis for Precursor Gases

A. Sulfur Dioxide Analysis

1. Time-series Analysis of Sulfur Dioxide (CASTNet and SEARCH)

As described in Section II, we analyzed gaseous precursor species (sulfur dioxide will be discussed here pertaining to Appendix E, Figures E- 1-7) at six SEARCH sites based on daily, weekly, and monthly averages, namely, Birmingham, Alabama (urban); Centreville, Alabama (rural); Gulfport Mississippi (urban); Jefferson Street, Atlanta, Georgia (urban); Oak Grove, Mississippi (rural); and Yorkville, Georgia (rural). In addition to these six rural and urban sites, a sulfur dioxide (SO2) time-series analysis was performed at selected rural/suburban CASTNet sites (Figure E-1). Overall, when comparing SO2 time-series analysis at both rural and urban sites, CMAQ performed fairly well, following the daily, weekly, and monthly trends and variations. At the selected CASTNet sites, CMAQ tended to overpredict SO2 in the East, although the model performed better (closer to observations) during the spring and summer. The model was able to delineate the differences between SO2 and sulfate PM concentrations, which are seasonally opposite, with SO2 exhibiting a maximum in winter and a minimum in summer. One would expect higher SO2 in the colder months due to the lower mixing height and possibly higher consumption of fossil fuels. The lower SO2 concentrations in the summer may also be indicative of an increase in the SO2 oxidation rate during the warmer period of the year, corresponding to an enhanced photochemical activity. In addition, SO2 time-series analysis showed very good model performance at the SEARCH sites, especially Suburban Pensacola, FL; Oak Grove, MS; Gulfport, MS; Centreville, AL; and Birmingham, AL. At these sites, CMAQ consistently performed well to capture the magnitude of the observations during the spring and summer on a daily, weekly, and monthly timescale. Although the model tended to overpredict SO2 at Jefferson Street, Atlanta, GA and Yorkville, GA, the model followed seasonal trends and variations at these sites. Overpredictions of these two GA sites and overpredictions in the colder months at other Eastern sites is possibly attributed to characterization of vertical mixing in the model at nighttime. It is well known that the SO2 concentrations decreases rapidly with height above the ground surface and is strongly influenced by the vertical stability of the atmosphere and the presence of inversion layers, especially at night.

B. Ozone Analysis

1. Statistical Analysis of Ozone (AIRS)

Figures 54 and 55 show the annual 2001 AIRS observations versus CMAQ predictions for 8-hour maximum ozone (O3) and 1-hour maximum ozone, respectively. The scatter plot and linear regression of 8-hour and 1-hour maximum ozone observations versus CMAQ ozone predictions showed good agreement. Correlations of 8-hour O3: annual: R^2 = 0.59; summer: R^2 = 0.49; fall: R^2 = 0.51; spring: R^2 = 0.39; winter: R^2 = 0.41. Correlations of 1-hour O_3: annual: R^2 = 0.60; summer: R^2 = 0.48; fall: R^2 = 0.54; spring: R^2 = 0.39; winter: R^2 = 0.49.

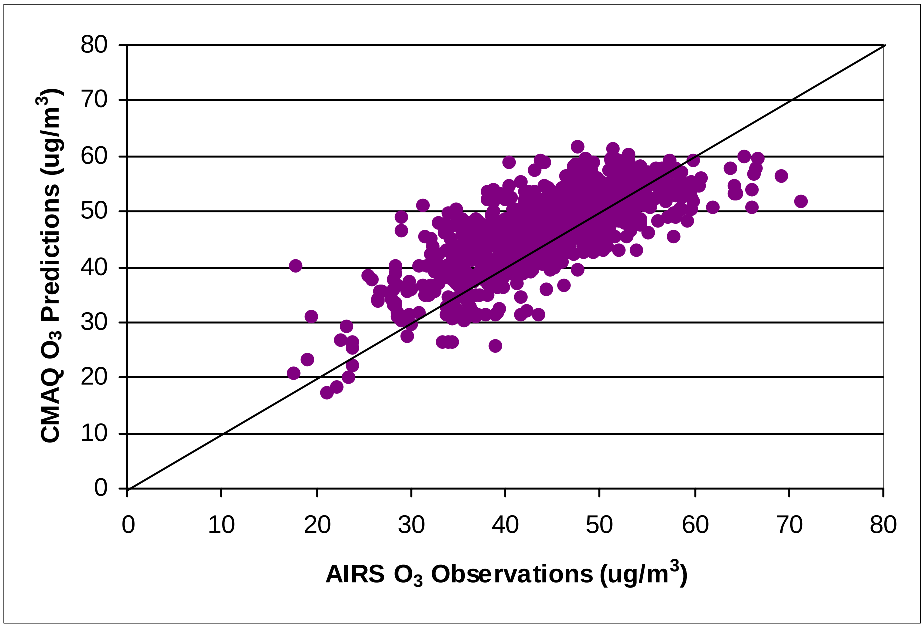


Figure 54. Annual 8-hour maximum average ozone 2001 AIRS observations versus CMAQ predictions.

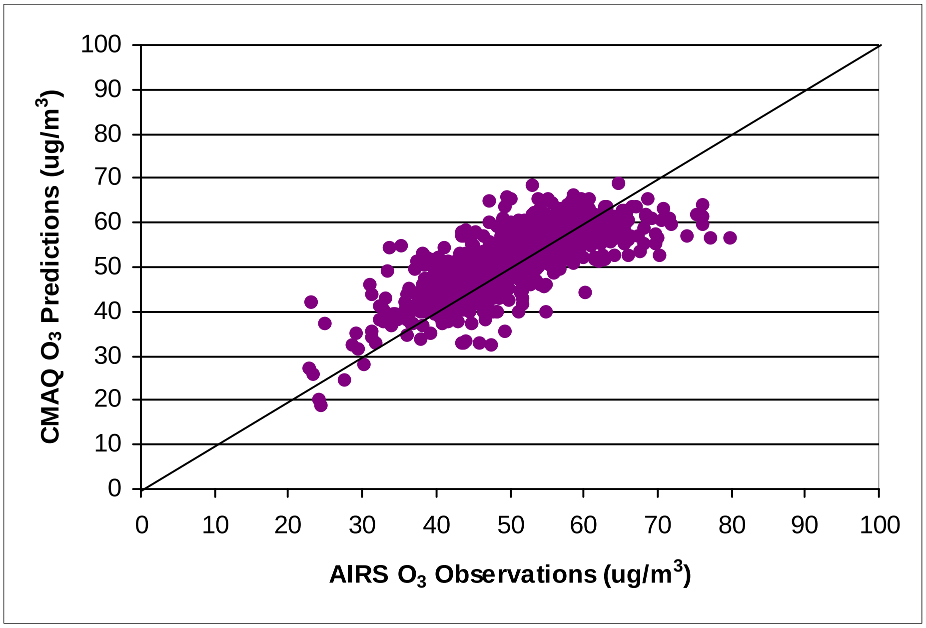


Figure 55. Annual 1-hour maximum average ozone 2001 AIRS observations versus CMAQ predictions.

2. Time-series Analysis of Ozone (SEARCH)

In general, ozone time-series analysis showed acceptable performance at the six SEARCH sites (Figures E- 8-13), although similar to SO2 performance, there are also issues of slight overprediction. The CMAQ tended to slightly overpredict ozone at all SEARCH urban and rural sites, significantly overpredicted the Brimingham, AL site. However, CMAQ performance follows the seasonal patterns of observed daily, weekly, and monthly ozone concentrations. Over the six SEARCH sites, CMAQ seemed to perform better during the fall and winter seasons. During the peak ozone season (May-October), the model follows the daily and weekly patterns, although the predicted magnitude of ozone is greater than observations. It is anticipated that a coarser grid resolution of 36-km may not be able to capture the magnitude of ozone concentrations over urban and suburban sites. A plausible explanation of ozone overprediction is that the model may not adequately resolve the vertical mixing at night and thus overestimate ozone concentration at night, similar to the SO2 performance. Both the analyses of O3 and SO2 performance suggest that the model simulation of vertical mixing, especially under lower vertical mixing conditions at night and in the colder months, need to be improved.

C. Nitric Acid Analysis: **Time-series Analysis of Nitric Acid (SEARCH)**

Time-series plots of predicted nitric acid (HNO3) by the CMAQ versus observed data was compared at four available SEARCH sites, with the exception of Oak Grove, Mississippi (Figures E- 14-18). Recognizing that gaseous nitric acid can coexist in the atmosphere with nitrate bound to aerosol particles has led to filter technique applications for the sampling of particulate nitrate. These monitoring techniques of separating nitrogen compounds such as gaseous nitric acid from aerosol nitrate are used by the SEARCH monitoring network. The model was able to capture the daily/weekly diurnal variation featuring a minimum at night and a maximum at midday. CMAQ was also able to predict the pronounced seasonal variations of HNO3 high concentrations during the warmer months and low concentrations during the colder months, which is opposite of particulate nitrate. These variations both diurnal and seasonal are attributed to the fact that at lower temperature, HNO3 condenses onto aerosol particles at night or during colder months, followed by a partial reevaporation during the day or warmer season when the temperature rises and relative humidity declines. In addition, the abundance of nitrogen pentoxide (N2O5), nitrogen dioxide (NO2), and nitrate (NO3) results in higher HNO3 at night via homogeneous and heterogeneous chemical reactions and then these species either photochemically dissociate and volatilize after the sun rises and leads to the diurnal variations of HNO3. Generally, the model performed well or slightly overpredicted HNO3 throughout the 2001 year at three sites (North Birmingham, AL, Centreville, AL, and Yorkville, GA), but overpredicted for the other two sites (Gulfport, MS and Jefferson Street, Atlanta, GA). The overprediction could be due to the characterization of vertical mixing at night, similar to the ozone and SO2 performance issue.

D. Nitric Oxide: Time-series Analysis of Nitric Oxide (SEARCH)

Time-series analysis of nitric oxide (NO) was conducted at three SEARCH sites due to data adequacy and availability, including Centreville, AL, Yorkville, GA, and Oak Grove, MS (Figures E- 19-21). The model performed well or slightly underpredicted NO at the three sites. CMAQ was able to capture the diurnal and seasonal patterns at these sites, with an increase in NO during the colder months due to the lower vertical mixing and increase in combustion of fossil fuels and a decrease in NO during the warmer months.

V. References

Carlson, R. E., Foley, T. A., 1991: Radial Basis Interpolation Methods on Track Data, Lawrence Livermore National Laboratory, UCRL-JC-1074238.

EPA, 2001: Guidance for Demonstrating Attainment of Air Quality Goals for PM2.5 and Regional Haze; Draft 1.1, Office of Air Quality Planning and Standards, Research Triangle Park, NC.

EPA, 2002: Clean Air Status and Trends Network (CASTNet), 2001 annual report.

EPA, 2005a: Technical Support Document for the Final Clean Air Interstate Rule, Emission Inventories, United States Environmental Protection Agency, Research Triangle Park, 27711, March 2005. Docket No. OAR-2003-0053.

EPA, 2005b: Technical Support Document for the Final Clean Air Interstate Rule, Air Quality Modeling, United States Environmental Protection Agency, Research Triangle Park, 27711, March 2005. Docket No. OAR-2003-0053.

Hardy, R. L., 1990: Theory and Applications of Multiquadric-Biharmonic Method, Computers Math Applications 19, 163-208.

IMPROVE, 2001: Spatial and Seasonal Patterns and Temporal Variability of Haze and its Constituents in the United States: Report III. Cooperative Institute for Research in the Atmosphere, ISSN: 0737-5352-47. IMPROVE Web Site: http://vista.cira.colostate.edu/improve/.

NADP, 2002: National Acid Deposition Program 2002 Annual Summary.

Surfer® 8, 2002: User's Guide: Contouring and 3D Surface Mapping for Scientists and Engineers, Golden Software, Inc., 809 14th Street, Golden, Colorado 80401-1866, USA.

CMAQ Model Performance Evaluation for 2001: Updated March 2005

Appendix A

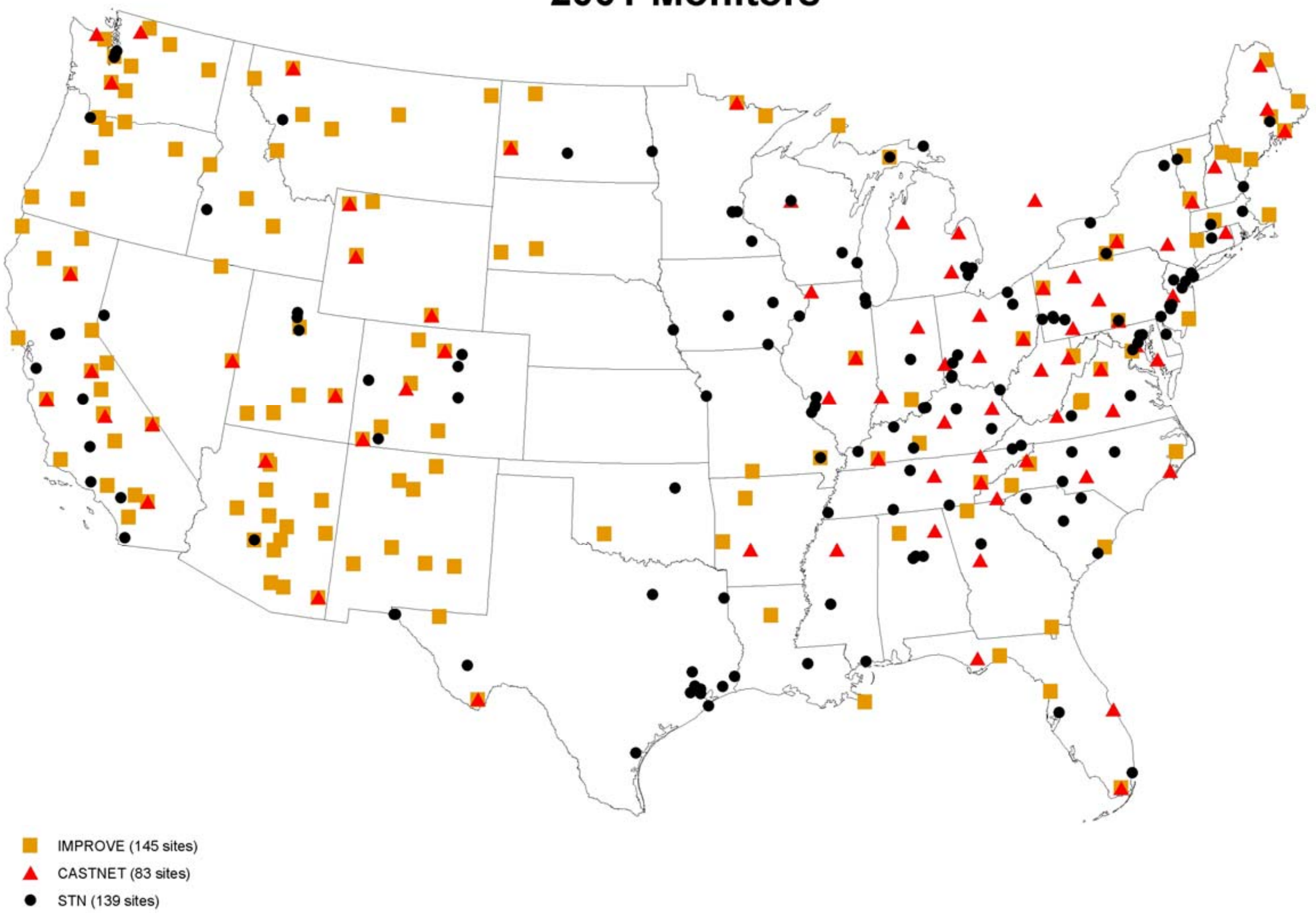
2001 Monitoring Networks:

IMPROVE, STN, CASTNet, NADP, AIRS, and SEARCH

conducted by

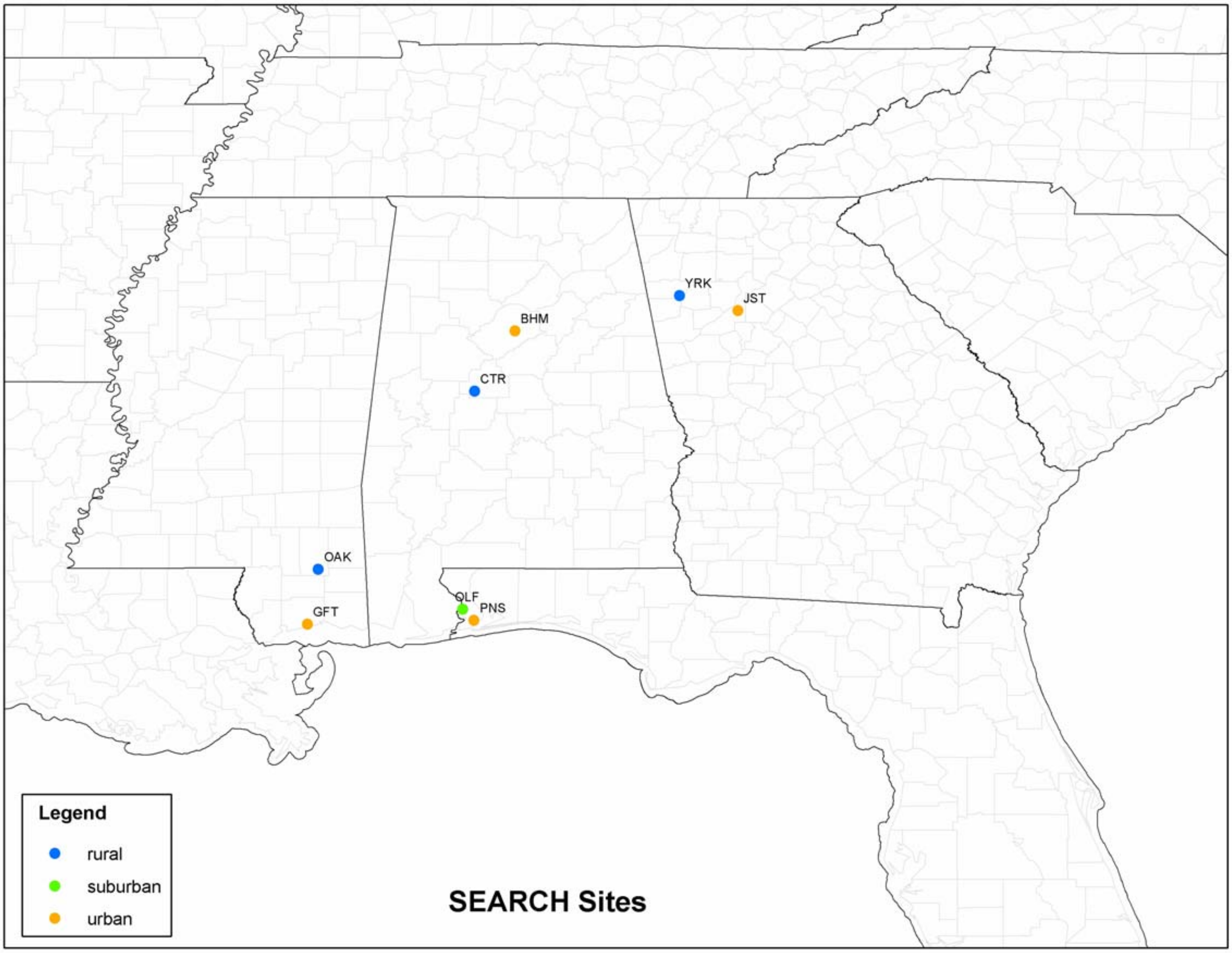
U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Emissions Analysis and Monitoring Division
Air Quality Modeling Group
Research Triangle Park, NC 27711

2001 Monitors



2001 NADP Monitors

2001 AIRS Monitors


YRK
JST
BHM
CTR
OAK
OLF
PNS
GFT
Legend
rural
suburban
urban
SEARCH Sites

CMAQ Model Performance Evaluation for 2001: Updated March 2005

Appendix B

2001 CMAQ Statistical Assessments based on:

IMPROVE, STN, CASTNet, NADP, and AIRS monitoring networks

conducted by

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Emissions Analysis and Monitoring Division
Air Quality Modeling Group
Research Triangle Park, NC 27711

Description and notes about statistics calculated

- Statistics were performed for all non-zero observations.
- **n_obs** refers to the total number of observations plotted and used in calculating pred, obs, and
- **obs** is the average observed value.
- **nzero_obs** is the number of observations used to calculate bias, nbias, err, and nerr.
- **pred** is the average model value.
- **bias** is the mean bias.
- **nbias** is the normalized bias percentage.
- **fbias** is the fractional bias percentage.
- **err** is the mean error.
- **nerr** is the normalized error percentage.
- **ferror** is the fractional error percentage.
- **r2** is the correlation coefficient r sqare.
- **nmb** is the normalized mean bias.
- **nme** is the normalized mean error.

Table 1. Comparison of IMPROVE elemental carbon observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	13492	13441	13492	0.24	0.23	0.98	-0.01	51.41	-16.26	0.15	105.60	60.77	0.22	-2.27	61.73
	east	4765	4759	4765	0.35	0.31	0.87	-0.04	0.08	-22.57	0.16	53.40	50.74	0.28	-12.63	46.71
	west	8727	8682	8727	0.17	0.19	1.09	0.02	79.55	-12.81	0.13	134.21	66.25	0.14	9.34	78.56

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3367	3363	3367	0.20	0.18	0.91	-0.02	-4.31	-30.42	0.11	58.12	58.45	0.25	-9.36	56.73
	east	1190	1190	1190	0.32	0.31	0.98	-0.01	8.03	-17.52	0.17	57.17	49.97	0.17	-2.01	52.78
	west	2177	2173	2177	0.14	0.11	0.81	-0.03	-11.07	-37.47	0.09	58.64	63.08	0.16	-18.55	61.66

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3411	3385	3411	0.26	0.28	1.10	0.03	156.60	1.40	0.19	201.37	62.86	0.10	10.44	73.62
	east	1273	1267	1273	0.36	0.25	0.68	-0.12	-12.08	-39.47	0.16	58.17	57.56	0.43	-32.31	44.77
	west	2138	2118	2138	0.19	0.30	1.59	0.11	257.50	25.73	0.20	287.04	66.01	0.09	58.94	106.34

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3751	3740	3751	0.27	0.24	0.89	-0.03	16.30	-17.87	0.14	68.85	56.73	0.33	-11.49	51.83
	east	1379	1379	1379	0.37	0.31	0.84	-0.06	-8.39	-25.16	0.16	45.40	48.75	0.38	-16.49	41.93
	west	2372	2361	2372	0.20	0.19	0.94	-0.01	30.72	-13.63	0.13	82.55	61.36	0.23	-6.14	62.39

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2963	2953	2963	0.21	0.22	1.02	0.00	38.77	-18.46	0.14	96.43	66.13	0.30	2.35	66.31
	east	923	923	923	0.35	0.38	1.10	0.03	19.17	-1.92	0.17	53.94	45.29	0.33	9.58	50.09
	west	2040	2030	2040	0.15	0.14	0.95	-0.01	47.68	-25.95	0.12	115.75	75.56	0.14	-5.30	83.47

Table 2. Comparison of STN elemental carbon observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	7108	7108	7108	0.65	0.85	1.30	0.20	103.63	20.24	0.52	134.47	64.22	0.09	30.15	79.12
	east	5483	5483	5483	0.59	0.91	1.53	0.31	128.17	32.06	0.51	150.91	63.35	0.15	52.70	86.47
	west	1625	1625	1625	0.85	0.65	0.77	-0.20	20.81	-19.63	0.52	78.99	67.16	0.08	-23.18	61.74

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1424	1424	1424	0.50	0.81	1.61	0.31	132.02	33.70	0.50	157.06	69.17	0.11	60.76	98.49
	east	1082	1082	1082	0.49	0.89	1.82	0.40	163.39	46.11	0.55	181.54	70.99	0.14	82.06	110.96
	west	342	342	342	0.54	0.54	1.00	0.00	32.79	-5.54	0.34	79.64	63.41	0.05	-0.19	62.78

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2147	2147	2147	0.53	0.81	1.52	0.28	113.93	31.74	0.44	135.88	61.78	0.11	52.48	83.21
	east	1698	1698	1698	0.52	0.84	1.61	0.32	128.80	36.54	0.45	147.42	61.47	0.13	60.54	86.09
	west	449	449	449	0.55	0.68	1.24	0.13	57.70	13.57	0.40	92.22	62.95	0.05	23.70	72.93

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2201	2201	2201	0.80	0.83	1.04	0.04	47.27	-0.70	0.49	88.62	58.68	0.15	4.43	62.10
	east	1691	1691	1691	0.73	0.88	1.21	0.15	62.57	11.03	0.47	94.59	55.63	0.20	20.83	64.43
	west	510	510	510	1.02	0.66	0.65	-0.35	-3.47	-39.59	0.57	68.82	68.77	0.13	-34.67	56.54

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1336	1336	1336	0.77	0.99	1.28	0.22	149.66	21.92	0.69	183.65	72.01	0.04	28.03	90.10
	east	1012	1012	1012	0.60	1.08	1.81	0.48	199.10	44.65	0.66	218.13	71.25	0.14	80.51	110.51
	west	324	324	324	1.31	0.70	0.53	-0.61	-4.76	-49.11	0.80	75.96	74.41	0.08	-46.54	61.09

Table 3. Comparison of CASTNet NH4 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3736	3736	3736	1.16	1.24	1.07	0.08	20.66	5.85	0.39	45.67	37.97	0.67	6.88	33.82
	east	2639	2639	2639	1.49	1.63	1.09	0.14	25.77	13.91	0.48	41.50	32.94	0.54	9.40	32.28
	west	1097	1097	1097	0.38	0.32	0.83	-0.06	8.37	-13.54	0.18	55.70	50.06	0.12	-16.84	48.31

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	953	953	953	1.12	1.25	1.11	0.13	23.09	9.27	0.36	42.66	33.93	0.68	11.41	32.28
	east	676	676	676	1.42	1.61	1.14	0.19	28.86	16.67	0.43	40.25	30.13	0.57	13.63	30.62
	west	277	277	277	0.40	0.37	0.92	-0.03	9.01	-8.79	0.19	48.53	43.20	0.05	-7.67	46.55

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	937	937	937	1.51	1.26	0.83	-0.26	-17.87	-26.92	0.42	31.75	38.04	0.75	-16.94	27.77
	east	654	654	654	1.97	1.69	0.86	-0.28	-7.90	-13.62	0.50	25.80	27.97	0.60	-13.96	25.58
	west	283	283	283	0.46	0.25	0.54	-0.21	-40.91	-57.66	0.23	45.49	61.32	0.20	-46.23	49.29

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	980	980	980	0.93	1.18	1.27	0.25	36.93	19.68	0.42	53.88	41.12	0.64	27.01	44.84
	east	687	687	687	1.17	1.54	1.31	0.37	44.36	28.64	0.52	53.33	39.42	0.53	31.48	44.88
	west	293	293	293	0.36	0.34	0.93	-0.02	19.52	-1.33	0.16	55.17	45.12	0.18	-6.61	44.57

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	866	866	866	1.09	1.29	1.18	0.20	41.27	21.88	0.37	54.75	38.77	0.74	18.20	34.04
	east	622	622	622	1.40	1.67	1.19	0.27	37.28	23.57	0.45	46.30	34.07	0.63	18.95	32.39
	west	244	244	244	0.28	0.30	1.09	0.02	51.42	17.56	0.15	76.30	50.74	0.25	8.64	55.14

Table 4. Comparison of IMPROVE NH4 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	330	330	330	1.38	1.72	1.25	0.35	177.10	26.19	0.69	193.07	47.10	0.36	25.15	50.15
	east	326	326	326	1.38	1.74	1.26	0.36	175.68	26.93	0.69	190.65	46.19	0.36	25.65	49.71
	west	4	4	4	0.82	0.46	0.57	-0.36	292.66	-34.31	0.92	390.27	121.54	0.22	-43.49	111.70

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	90	90	90	1.35	1.67	1.24	0.32	39.58	20.52	0.61	54.75	39.74	0.34	23.73	45.44
	east	90	90	90	1.35	1.67	1.24	0.32	39.58	20.52	0.61	54.75	39.74	0.34	23.73	45.44

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	84	84	84	1.89	1.93	1.02	0.04	507.18	10.82	0.77	532.39	43.59	0.29	2.1176	40.7390
	east	84	84	84	1.89	1.93	1.02	0.04	507.18	10.82	0.77	532.39	43.59	0.29	2.1176	40.7390

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	94	94	94	1.23	1.69	1.38	0.47	58.86	33.18	0.66	69.98	47.06	0.52	38.07	53.76
	east	93	93	93	1.24	1.71	1.38	0.47	59.93	34.10	0.67	70.29	47.00	0.51	38.17	53.77
	west	1	1	1	0.14	0.08	0.59	-0.06	-41.35	-52.13	0.06	41.35	52.13		-41.35	41.35

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	62	62	62	0.96	1.58	1.65	0.62	108.78	44.65	0.75	120.74	62.63	0.38	64.56	77.98
	east	59	59	59	0.95	1.63	1.71	0.67	93.76	48.36	0.72	101.12	58.45	0.50	70.61	75.92
	west	3	3	3	1.05	0.59	0.56	-0.46	404.00	-28.37	1.20	506.57	144.67	0.93	-43.58	114.74

Table 5. Comparison of NADP NH4 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	7619	7619	7619	0.38	0.35	0.93	-0.02	56.22	-11.20	0.28	110.06	70.70	0.10	-6.54	74.36
	east	5299	5299	5299	0.40	0.43	1.07	0.03	64.67	0.76	0.29	107.53	63.17	0.11	7.13	73.44
	west	2320	2320	2320	0.32	0.17	0.54	-0.15	36.93	-38.53	0.25	115.86	87.90	0.07	-45.67	77.01

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1955	1955	1955	0.44	0.38	0.88	-0.05	41.37	-11.96	0.29	93.14	65.65	0.16	-12.38	65.23
	east	1304	1304	1304	0.47	0.46	0.97	-0.01	41.01	-3.24	0.29	83.80	58.70	0.19	-2.62	61.82
	west	651	651	651	0.37	0.23	0.63	-0.14	42.08	-29.42	0.27	111.86	79.58	0.09	-37.36	73.96

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1949	1949	1949	0.45	0.28	0.61	-0.18	8.23	-40.07	0.29	82.54	72.46	0.02	-39.47	64.19
	east	1441	1441	1441	0.44	0.31	0.71	-0.13	8.40	-27.17	0.25	69.36	60.99	0.05	-28.58	57.48
	west	508	508	508	0.50	0.16	0.33	-0.33	7.73	-76.63	0.40	119.93	105.00	0.00	-66.90	81.10

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1805	1805	1805	0.36	0.43	1.17	0.06	89.60	3.64	0.31	133.65	70.76	0.10	16.84	85.94
	east	1255	1255	1255	0.40	0.54	1.34	0.14	107.45	18.46	0.36	139.44	65.22	0.11	33.93	89.39
	west	550	550	550	0.28	0.17	0.61	-0.11	48.87	-30.16	0.21	120.43	83.42	0.08	-38.90	74.70

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1910	1910	1910	0.25	0.33	1.34	0.08	88.87	4.99	0.23	133.18	74.00	0.18	33.57	94.00
	east	1299	1299	1299	0.29	0.42	1.48	0.14	109.53	18.67	0.28	142.86	68.08	0.16	47.77	98.21
	west	611	611	611	0.16	0.12	0.78	-0.03	44.97	-24.08	0.12	112.62	86.57	0.22	-21.67	77.60

Table 6. Comparison of STN NH4 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	6970	6970	6970	1.26	1.58	1.25	0.32	412.61	35.50	0.84	436.05	68.24	0.34	25.30	66.20
	east	5414	5414	5414	1.36	1.87	1.37	0.51	467.21	44.10	0.89	484.36	67.16	0.43	37.31	65.28
	west	1556	1556	1556	0.94	0.61	0.65	-0.33	222.61	5.57	0.66	267.95	72.01	0.20	-35.28	70.80

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1378	1378	1378	1.24	1.54	1.24	0.30	224.94	29.99	0.71	245.21	57.25	0.46	24.41	57.01
	east	1051	1051	1051	1.43	1.83	1.28	0.40	272.77	34.42	0.81	289.98	57.03	0.43	27.89	56.32
	west	327	327	327	0.62	0.61	0.99	-0.01	71.21	15.74	0.38	101.32	57.96	0.31	-1.40	62.15

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2106	2106	2106	1.51	1.64	1.08	0.13	162.95	13.50	0.78	193.46	55.38	0.44	8.38	51.23
	east	1677	1677	1677	1.69	1.95	1.15	0.26	198.79	22.90	0.84	222.02	53.70	0.47	15.21	49.42
	west	429	429	429	0.82	0.44	0.54	-0.38	22.85	-23.22	0.54	81.83	61.92	0.22	-46.40	65.79

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2155	2155	2155	1.01	1.57	1.55	0.56	588.07	61.04	0.95	604.87	84.78	0.26	55.18	94.12
	east	1671	1671	1671	1.00	1.82	1.82	0.82	630.56	71.52	1.00	641.13	85.80	0.48	82.24	99.73
	west	484	484	484	1.05	0.70	0.66	-0.36	441.38	24.86	0.80	479.66	81.26	0.20	-33.78	75.67

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1331	1331	1331	1.31	1.57	1.20	0.26	717.84	34.65	0.88	744.14	73.18	0.23	19.74	67.62
	east	1015	1015	1015	1.33	1.84	1.39	0.51	843.13	44.02	0.87	860.99	69.16	0.41	38.55	65.91
	west	316	316	316	1.24	0.69	0.55	-0.56	315.41	4.57	0.91	368.81	86.10	0.18	-44.67	73.47

Table 7. Comparison of CASTNet NO3 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3735	3735	3735	0.99	1.25	1.26	0.26	98.13	-6.40	0.75	154.67	88.11	0.53	26.11	75.95
	east	2638	2638	2638	1.20	1.64	1.36	0.43	131.73	15.84	0.90	172.52	81.14	0.53	36.07	75.09
	west	1097	1097	1097	0.48	0.32	0.66	-0.16	17.31	-59.89	0.39	111.73	104.87	0.09	-33.92	81.09

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	953	953	953	1.10	1.35	1.22	0.25	95.35	-4.36	0.82	149.15	81.05	0.48	22.20	73.97
	east	676	676	676	1.31	1.72	1.32	0.41	133.56	15.81	0.98	174.34	78.60	0.47	31.51	74.69
	west	277	277	277	0.60	0.44	0.73	-0.16	2.10	-53.57	0.42	87.69	87.01	0.12	-27.40	70.16

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	937	937	937	0.37	0.23	0.60	-0.15	17.36	-62.21	0.33	115.82	111.87	0.01	-39.68	89.60
	east	654	654	654	0.34	0.29	0.86	-0.05	52.05	-25.47	0.29	122.58	91.18	0.04	-14.07	86.87
	west	283	283	283	0.45	0.07	0.16	-0.38	-62.79	-147.11	0.43	100.20	159.70	0.00	-83.79	94.31

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	980	980	980	0.86	1.13	1.32	0.27	109.86	6.39	0.73	156.78	84.37	0.37	31.97	84.72
	east	687	687	687	1.04	1.47	1.42	0.43	138.72	24.15	0.87	172.92	79.84	0.36	41.72	83.81
	west	293	293	293	0.43	0.34	0.77	-0.10	42.19	-35.26	0.39	118.93	95.00	0.03	-22.67	89.83

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	865	865	865	1.68	2.38	1.41	0.70	175.38	37.31	1.16	200.42	74.37	0.55	41.36	69.04
	east	621	621	621	2.18	3.14	1.44	0.96	205.94	50.18	1.50	222.68	74.75	0.47	44.29	68.84
	west	244	244	244	0.43	0.44	1.03	0.01	97.61	4.54	0.31	143.77	73.41	0.29	3.38	71.61

Table 8. Comparison of IMPROVE NO3 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	13458	13398	13443	0.48	0.61	1.27	0.13	90.46	-39.71	0.49	176.87	112.04	0.35	27.04	102.54
	east	4771	4755	4767	0.66	1.04	1.58	0.38	69.44	-31.90	0.74	149.28	107.04	0.44	57.63	111.57
	west	8687	8643	8676	0.38	0.37	0.98	-0.01	102.02	-44.01	0.36	192.05	114.79	0.23	-2.03	93.95

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3374	3356	3372	0.52	0.74	1.43	0.22	118.82	-19.24	0.53	189.24	100.89	0.46	42.71	101.99
	east	1194	1191	1194	0.79	1.24	1.58	0.45	86.91	-18.28	0.86	157.33	101.65	0.45	57.79	108.95
	west	2180	2165	2178	0.38	0.47	1.25	0.09	136.38	-19.76	0.35	206.80	100.47	0.41	25.43	94.00

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3390	3378	3385	0.27	0.14	0.53	-0.13	-34.92	-115.96	0.24	104.45	139.10	0.16	-47.22	89.67
	east	1273	1263	1269	0.29	0.19	0.67	-0.10	-33.43	-97.79	0.26	92.29	124.48	0.09	-33.30	88.75
	west	2117	2115	2116	0.25	0.11	0.43	-0.14	-35.80	-126.86	0.23	111.71	147.87	0.20	-56.78	90.30

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3712	3706	3709	0.40	0.60	1.48	0.20	110.08	-25.74	0.50	187.44	109.92	0.24	48.43	123.56
	east	1380	1380	1380	0.55	0.99	1.79	0.44	93.21	-18.66	0.74	164.15	105.64	0.35	79.35	132.62
	west	2332	2326	2329	0.32	0.37	1.16	0.05	120.09	-29.93	0.36	201.26	112.45	0.13	16.34	114.14

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2982	2958	2977	0.77	1.01	1.30	0.23	176.86	6.38	0.73	232.27	96.57	0.32	30.29	94.28
	east	924	921	924	1.17	2.02	1.73	0.85	152.30	21.24	1.25	194.72	92.16	0.41	73.09	106.69
	west	2058	2037	2053	0.59	0.55	0.93	-0.05	187.96	-0.30	0.50	249.25	98.55	0.23	-7.46	83.34

Table 9. Comparison of NADP NO3 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	7619	7619	7619	1.52	1.31	0.86	-0.21	31.47	-33.47	1.13	101.41	74.92	0.11	-13.79	74.07
	east	5299	5299	5299	1.68	1.66	0.99	-0.02	43.44	-21.23	1.25	103.50	69.43	0.12	-0.91	74.40
	west	2320	2320	2320	1.16	0.51	0.44	-0.65	4.14	-61.41	0.85	96.65	87.47	0.05	-56.27	72.96

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1955	1955	1955	1.57	1.23	0.78	-0.34	6.28	-36.27	0.94	73.84	64.50	0.20	-21.53	60.12
	east	1304	1304	1304	1.76	1.55	0.88	-0.21	18.02	-27.25	1.02	77.68	59.56	0.22	-11.97	58.09
	west	651	651	651	1.18	0.59	0.50	-0.59	-17.25	-54.36	0.78	66.15	74.38	0.12	-50.15	66.19

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1949	1949	1949	1.79	0.71	0.40	-1.08	-42.49	-80.80	1.24	66.77	91.83	0.03	-60.24	69.20
	east	1441	1441	1441	1.78	0.82	0.46	-0.96	-39.85	-72.50	1.15	61.37	83.04	0.04	-53.99	64.74
	west	508	508	508	1.80	0.40	0.22	-1.40	-49.99	-104.36	1.47	82.09	116.79	0.01	-77.75	81.69

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1805	1805	1805	1.32	1.55	1.18	0.24	115.09	-6.73	1.11	165.20	69.94	0.16	17.87	83.94
	east	1255	1255	1255	1.49	2.02	1.36	0.53	131.20	9.87	1.30	168.74	65.54	0.15	35.77	87.68
	west	550	550	550	0.94	0.50	0.53	-0.44	78.32	-44.60	0.66	157.13	79.97	0.05	-46.82	70.40

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1910	1910	1910	1.40	1.78	1.28	0.38	53.73	-7.55	1.22	104.70	73.06	0.20	27.52	87.64
	east	1299	1299	1299	1.67	2.37	1.42	0.70	76.58	11.62	1.53	113.11	68.01	0.17	42.18	91.72
	west	611	611	611	0.82	0.52	0.64	-0.29	5.15	-48.33	0.57	86.80	83.78	0.08	-36.03	69.98

Table 10. Comparison of STN NO3 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	6130	6130	6130	1.77	1.69	0.95	-0.08	180.38	-31.19	1.41	254.27	93.02	0.18	-4.64	79.72
	east	4662	4662	4662	1.52	1.94	1.28	0.42	248.66	-11.90	1.23	308.39	86.03	0.38	27.70	80.55
	west	1468	1468	1468	2.55	0.86	0.34	-1.68	-36.45	-92.44	1.99	82.38	115.22	0.21	-66.09	78.14

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1377	1377	1377	1.65	1.81	1.10	0.16	159.57	-23.18	1.27	227.74	90.44	0.37	9.61	76.52
	east	1050	1050	1050	1.73	2.12	1.23	0.39	215.00	-9.80	1.35	274.47	87.74	0.40	22.69	78.04
	west	327	327	327	1.41	0.81	0.58	-0.59	-18.41	-66.14	0.99	77.69	99.11	0.32	-42.08	70.50

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1662	1662	1662	0.99	0.64	0.65	-0.35	-7.77	-74.72	0.86	99.02	110.20	0.07	-35.41	87.53
	east	1268	1268	1268	0.81	0.74	0.92	-0.06	8.86	-55.49	0.69	100.66	98.18	0.13	-7.82	86.01
	west	394	394	394	1.57	0.30	0.19	-1.27	-61.28	-136.64	1.41	93.74	148.92	0.24	-81.01	90.03

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1856	1856	1856	1.82	1.86	1.02	0.04	204.55	-14.60	1.63	266.95	89.37	0.10	2.23	89.70
	east	1410	1410	1410	1.33	2.09	1.57	0.76	278.77	7.83	1.32	324.93	82.64	0.33	56.66	98.91
	west	446	446	446	3.37	1.14	0.34	-2.22	-30.10	-85.53	2.63	83.66	110.67	0.19	-65.99	78.15

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1235	1235	1235	2.86	2.69	0.94	-0.17	420.45	-6.47	1.96	473.70	78.26	0.15	-6.10	68.61
	east	934	934	934	2.55	3.16	1.24	0.61	566.58	15.11	1.67	603.58	72.74	0.38	23.91	65.59
	west	301	301	301	3.85	1.24	0.32	-2.61	-32.96	-73.42	2.88	70.70	95.39	0.18	-67.80	74.81

Table 11. Comparison of Ozone 8-hour maximum observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	310,546	310,431	310,546	44.67	47.16	1.06	2.48	15.41	6.77	8.87	28.27	21.79	0.58	5.56	19.85
	east	207,546	207,476	207,546	45.05	48.01	1.07	2.96	12.98	6.74	8.70	25.31	21.21	0.62	6.56	19.31
	west	103,000	102,955	103,000	43.92	45.47	1.04	1.53	20.29	6.84	9.21	34.23	22.98	0.51	3.49	20.97

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	83,969	83,956	83,969	48.39	50.83	1.05	2.44	11.54	6.09	8.18	21.95	17.88	0.46	5.03	16.91
	east	58,348	58,339	58,348	48.13	50.81	1.06	2.68	10.90	6.54	8.04	20.90	17.87	0.50	5.57	16.71
	west	25,621	25,617	25,621	48.98	50.87	1.04	1.88	13.01	5.08	8.50	24.37	17.90	0.37	3.83	17.35

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	102,147	102,140	102,147	52.17	55.68	1.07	3.50	13.99	8.26	10.47	25.11	21.01	0.49	6.71	20.07
	east	73,095	73,094	73,095	51.98	57.73	1.11	5.75	18.96	12.74	10.50	26.43	21.09	0.54	11.07	20.21
	west	29,052	29,046	29,052	52.66	50.50	0.96	-2.16	1.46	-3.01	10.40	21.77	20.81	0.45	-4.11	19.75

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	79,239	79,220	79,239	40.02	42.02	1.05	1.99	15.51	6.93	8.28	28.70	22.18	0.50	4.97	20.69
	east	52,971	52,957	52,971	39.57	41.14	1.04	1.57	11.81	5.51	7.70	25.17	20.87	0.54	3.96	19.45
	west	26,268	26,263	26,268	40.93	43.78	1.07	2.84	22.96	9.80	9.46	35.81	24.81	0.44	6.94	23.10

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	45,191	45,115	45,191	28.98	30.14	1.04	1.13	25.63	4.38	7.54	46.42	30.15	0.33	3.90	26.01
	east	23,132	23,086	23,132	27.92	25.92	0.93	-2.03	1.99	-8.90	6.94	33.25	30.73	0.46	-7.26	24.85
	west	22,059	22,029	22,059	30.09	34.57	1.15	4.45	50.40	18.31	8.17	60.22	29.54	0.23	14.76	27.15

Table 12. Comparison of Ozone 1-hour maximum observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	310684	310556	310684	50.93	51.83	1.02	0.89	8.36	2.76	9.33	22.97	19.74	0.58	1.75	18.33
	east	207618	207545	207618	51.10	52.80	1.03	1.69	8.13	3.56	9.01	21.60	19.20	0.63	3.30	17.63
	west	103066	103011	103066	50.58	49.89	0.99	-0.72	8.83	1.17	9.98	25.74	20.83	0.49	-1.42	19.73

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	84014	83997	84014	53.66	54.91	1.02	1.25	7.05	3.21	8.45	18.78	16.46	0.47	2.32	15.75
	east	58376	58367	58376	53.19	54.90	1.03	1.70	7.20	3.96	8.17	18.13	16.27	0.52	3.20	15.36
	west	25638	25630	25638	54.72	54.95	1.00	0.21	6.70	1.51	9.09	20.27	16.90	0.39	0.39	16.61

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	102204	102198	102204	59.65	61.07	1.02	1.41	8.55	3.95	11.37	22.33	19.80	0.47	2.37	19.06
	east	73129	73128	73129	59.30	63.22	1.07	3.93	12.98	8.38	10.87	22.47	19.00	0.53	6.62	18.34
	west	29075	29070	29075	60.56	55.65	0.92	-4.91	-2.60	-7.21	12.63	21.95	21.82	0.43	-8.11	20.85

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	79251	79232	79251	46.57	47.10	1.01	0.53	8.60	2.82	8.75	23.32	19.76	0.51	1.14	18.79
	east	52971	52956	52971	45.67	46.29	1.01	0.62	7.09	2.68	8.08	21.17	18.76	0.55	1.35	17.70
	west	26280	26276	26280	48.38	48.74	1.01	0.36	11.65	3.10	10.09	27.65	21.78	0.42	0.75	20.86

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	45215	45129	45215	33.79	33.50	0.99	-0.33	9.95	-0.84	7.39	31.65	25.66	0.35	-0.98	21.87
	east	23142	23094	23142	32.38	29.44	0.91	-2.98	-2.51	-10.70	7.38	28.60	28.24	0.47	-9.18	22.79
	west	22073	22035	22073	35.26	37.76	1.07	2.44	23.01	9.50	7.40	34.83	22.97	0.20	6.90	20.98

Table 13. Comparison of CASTNET HNO3 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3738	3738	3738	1.49	1.67	1.12	0.18	42.78	10.30	0.68	70.85	47.58	0.50	11.98	45.82
	east	2640	2640	2640	1.76	2.02	1.15	0.26	41.41	10.58	0.81	68.36	46.89	0.41	14.57	46.00
	west	1098	1098	1098	0.83	0.82	0.99	-0.01	46.08	9.62	0.37	76.83	49.25	0.57	-1.24	44.87

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	952	952	952	1.47	1.44	0.98	-0.03	27.55	2.18	0.59	59.36	44.36	0.48	-2.02	40.20
	east	675	675	675	1.79	1.72	0.96	-0.07	22.16	-2.41	0.70	56.58	43.83	0.35	-3.73	39.37
	west	277	277	277	0.68	0.74	1.09	0.06	40.67	13.36	0.31	66.13	45.67	0.61	8.98	45.51

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	938	938	938	1.87	2.29	1.22	0.41	39.34	14.94	0.78	59.75	40.68	0.64	22.12	41.78
	east	654	654	654	2.14	2.82	1.32	0.68	58.04	29.31	0.90	66.27	38.88	0.61	31.78	41.89
	west	284	284	284	1.26	1.06	0.84	-0.20	-3.73	-18.16	0.52	44.72	44.82	0.57	-15.71	41.33

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	980	980	980	1.35	1.82	1.35	0.47	73.68	28.70	0.74	90.53	49.83	0.48	34.70	55.00
	east	687	687	687	1.57	2.22	1.42	0.66	79.22	34.52	0.90	91.73	50.09	0.39	41.86	57.44
	west	293	293	293	0.84	0.87	1.03	0.03	60.69	15.04	0.37	87.73	49.20	0.56	3.39	44.32

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	868	868	868	1.26	1.08	0.86	-0.18	28.34	-6.59	0.61	73.22	56.04	0.29	-14.00	48.36
	east	624	624	624	1.56	1.28	0.82	-0.28	3.18	-21.37	0.74	57.55	55.06	0.18	-17.77	47.47
	west	244	244	244	0.49	0.57	1.16	0.08	92.67	31.20	0.27	113.29	58.54	0.33	16.38	55.56

Table 14. Comparison of IMPROVE OC observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	13492	13427	13492	1.11	1.50	1.35	0.39	132.57	29.72	0.92	159.76	67.68	0.11	34.77	82.84
	east	4765	4764	4765	1.56	1.45	0.93	-0.10	15.03	-9.73	0.77	58.97	51.78	0.23	-6.66	49.35
	west	8727	8663	8727	0.87	1.52	1.75	0.65	197.20	51.26	1.00	215.18	76.37	0.09	75.44	115.71

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3367	3360	3367	0.95	1.21	1.27	0.25	86.55	24.78	0.67	112.35	60.42	0.14	26.77	70.04
	east	1190	1190	1190	1.39	1.52	1.09	0.13	34.08	0.77	0.78	70.95	51.64	0.21	9.01	56.34
	west	2177	2170	2177	0.71	1.04	1.46	0.32	115.32	37.91	0.60	135.06	65.22	0.05	45.76	84.70

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3411	3395	3411	1.38	1.81	1.31	0.43	106.56	15.94	1.24	145.35	71.25	0.04	31.35	90.23
	east	1273	1273	1273	1.77	1.17	0.66	-0.60	-25.13	-43.50	0.83	46.55	58.94	0.23	-34.08	46.80
	west	2138	2122	2138	1.15	2.20	1.92	1.05	185.56	51.34	1.49	204.62	78.59	0.06	91.62	130.23

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3751	3727	3751	1.27	1.73	1.36	0.45	151.34	35.26	1.04	175.52	68.77	0.13	35.69	82.04
	east	1379	1378	1379	1.64	1.53	0.93	-0.12	13.92	-5.26	0.71	51.77	46.93	0.32	-7.00	43.32
	west	2372	2349	2372	1.06	1.84	1.74	0.79	231.95	58.82	1.24	248.11	81.46	0.10	74.33	117.07

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2963	2945	2963	0.78	1.18	1.51	0.40	191.30	44.19	0.68	210.50	70.45	0.25	50.90	87.18
	east	923	923	923	1.35	1.66	1.23	0.31	47.53	16.64	0.75	71.43	49.31	0.35	22.72	55.63
	west	2040	2022	2040	0.52	0.96	1.84	0.44	256.93	56.65	0.65	273.98	80.02	0.10	83.95	124.18

Table 15. Comparison of STN OC observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	7108	6947	7093	3.20	2.40	0.75	-0.86	34.84	-9.58	1.75	93.93	73.13	0.11	-24.98	54.66
	east	5483	5339	5470	2.93	2.39	0.82	-0.60	47.14	-3.21	1.55	103.79	75.11	0.13	-18.36	52.98
	west	1625	1608	1623	4.12	2.44	0.59	-1.72	-6.02	-31.05	2.42	61.17	66.44	0.11	-40.86	58.69

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	7108	6947	7093	3.20	2.40	0.82	-0.86	34.84	-9.58	1.75	93.93	73.13	0.11	-18.10	50.66
	east	5483	5339	5470	2.93	2.39	0.86	-0.60	47.14	-3.21	1.55	103.79	75.11	0.13	-13.66	50.92
	west	1625	1608	1623	4.12	2.44	0.69	-1.72	-6.02	-31.05	2.42	61.17	66.44	0.11	-31.36	49.87

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2147	2118	2146	2.94	1.98	0.67	-0.99	-1.64	-32.74	1.49	67.79	65.07	0.17	-32.50	50.73
	east	1698	1670	1697	2.94	1.84	0.62	-1.15	-4.25	-38.08	1.49	70.84	67.80	0.16	-37.61	50.76
	west	449	448	449	2.91	2.53	0.87	-0.38	8.09	-12.56	1.47	56.42	54.72	0.19	-12.96	50.62

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2201	2137	2190	3.39	2.54	0.75	-0.92	29.96	9.38	1.71	85.45	85.72	0.18	-25.04	50.62
	east	1691	1631	1681	3.13	2.49	0.80	-0.72	41.64	21.95	1.52	93.37	91.88	0.20	-20.44	48.51
	west	510	506	509	4.23	2.69	0.64	-1.57	-7.72	-32.13	2.36	59.93	65.37	0.11	-36.32	55.79

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1336	1295	1334	3.79	3.00	0.79	-0.91	114.54	-1.27	2.60	169.14	76.75	0.03	-20.89	68.61
	east	1012	976	1011	2.79	3.20	1.15	0.32	161.69	19.01	1.88	201.28	72.77	0.11	14.78	67.47
	west	324	319	323	6.94	2.39	0.34	-4.66	-29.71	-64.74	4.86	70.80	89.20	0.18	-65.58	70.04

Table 16. Comparison of IMPROVE PM2.5 versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	13317	13217	13317	5.77	6.32	1.09	0.54	43.41	11.94	2.89	73.03	51.93	0.47	9.48	50.05
	east	4729	4724	4729	9.04	9.86	1.09	0.82	27.32	8.32	3.80	53.46	43.27	0.48	9.04	41.96
	west	8588	8493	8588	3.96	4.36	1.10	0.38	52.36	13.94	2.39	83.92	56.70	0.17	10.03	60.22

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3281	3271	3281	5.85	5.71	0.98	-0.14	16.51	-3.62	2.69	54.50	48.20	0.44	-2.37	45.98
	east	1174	1172	1174	8.68	9.36	1.08	0.68	21.69	6.19	3.54	47.73	40.61	0.42	7.85	40.75
	west	2107	2099	2107	4.28	3.69	0.86	-0.60	13.62	-9.09	2.22	58.28	52.43	0.15	-13.92	51.88

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3379	3377	3379	7.77	6.96	0.90	-0.81	9.68	-10.50	3.16	51.32	45.89	0.53	-10.37	40.69
	east	1263	1262	1263	12.42	10.12	0.81	-2.31	-10.95	-20.54	3.84	32.62	37.69	0.64	-18.54	30.89
	west	2116	2115	2116	4.99	5.08	1.02	0.09	21.99	-4.51	2.76	62.48	50.78	0.10	1.79	55.26

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3717	3700	3717	5.51	6.75	1.23	1.24	46.36	19.91	2.80	67.99	48.89	0.53	22.54	50.82
	east	1369	1367	1369	7.90	9.81	1.24	1.92	35.29	17.85	3.44	54.23	43.06	0.65	24.27	43.57
	west	2348	2333	2348	4.12	4.97	1.21	0.85	52.85	21.11	2.43	76.05	52.28	0.20	20.61	58.92

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2940	2869	2940	3.70	5.69	1.54	1.99	109.98	45.04	2.90	126.22	66.89	0.46	53.67	78.38
	east	923	923	923	6.59	10.23	1.55	3.63	74.99	36.37	4.59	88.09	54.60	0.39	55.12	69.68
	west	2017	1946	2017	2.38	3.61	1.52	1.21	126.57	49.00	2.13	144.30	72.52	0.23	51.83	89.41

Table 17. Comparison of STN PM25 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	6420	6419	6420	12.89	10.79	0.84	-2.10	1.71	-21.11	5.48	51.73	48.54	0.29	-16.32	42.48
	east	4944	4944	4944	13.07	12.13	0.93	-0.94	11.45	-12.08	5.03	52.78	43.90	0.41	-7.17	38.52
	west	1476	1475	1476	12.30	6.29	0.51	-6.02	-30.95	-51.33	6.96	48.22	64.09	0.19	-48.88	56.58

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1309	1308	1309	11.49	9.93	0.86	-1.56	-1.75	-19.81	4.83	47.41	48.49	0.30	-13.59	42.00
	east	995	995	995	12.29	11.31	0.92	-0.98	5.47	-12.99	4.96	48.30	45.65	0.30	-7.97	40.35
	west	314	313	314	8.96	5.55	0.62	-3.42	-24.71	-41.44	4.41	44.55	57.50	0.13	-38.00	49.20

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1922	1922	1922	13.75	10.77	0.78	-2.98	-8.84	-29.20	5.29	47.36	47.98	0.46	-21.64	38.48
	east	1489	1489	1489	14.98	12.22	0.82	-2.76	-4.36	-24.94	5.37	46.99	44.27	0.47	-18.42	35.88
	west	433	433	433	9.53	5.81	0.61	-3.72	-24.25	-43.84	5.01	48.65	60.77	0.17	-39.07	52.51

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2005	2005	2005	12.61	10.91	0.87	-1.70	-1.80	-17.62	5.24	44.08	45.81	0.31	-13.48	41.55
	east	1541	1541	1541	12.20	12.07	0.99	-0.13	7.86	-6.68	4.46	43.13	40.36	0.52	-1.04	36.57
	west	464	464	464	13.99	7.07	0.50	-6.93	-33.92	-53.98	7.83	47.24	63.92	0.20	-49.50	55.99

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1184	1184	1184	13.51	11.55	0.85	-1.97	28.62	-15.30	6.89	76.55	54.12	0.11	-14.56	50.98
	east	919	919	919	12.28	12.98	1.06	0.70	49.58	0.66	5.52	83.18	47.35	0.32	5.73	44.98
	west	265	265	265	17.80	6.57	0.37	-11.23	-44.07	-70.63	11.63	53.55	77.62	0.26	-63.08	65.34

Table 18. Comparison of CASTNet SO4 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3736	3736	3736	3.21	3.09	0.96	-0.12	-2.31	-11.61	0.77	31.22	31.43	0.85	-3.71	23.91
	east	2639	2639	2639	4.11	4.10	1.00	-0.01	5.17	-2.09	0.89	26.72	23.77	0.81	-0.29	21.74
	west	1097	1097	1097	1.04	0.66	0.64	-0.38	-20.29	-34.51	0.46	42.03	49.84	0.34	-36.26	44.64

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	953	953	953	3.01	2.64	0.88	-0.37	-5.67	-18.48	0.71	33.08	30.65	0.77	-12.38	23.74
	east	676	676	676	3.77	3.43	0.91	-0.34	4.62	-7.79	0.80	30.08	22.18	0.68	-8.98	21.13
	west	277	277	277	1.16	0.70	0.61	-0.46	-30.79	-44.58	0.52	40.40	51.33	0.16	-39.36	44.53

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	937	937	937	5.05	5.00	0.99	-0.05	-7.30	-17.11	1.10	31.74	35.70	0.87	-0.94	21.72
	east	654	654	654	6.65	6.88	1.03	0.23	8.82	3.19	1.26	24.01	21.83	0.81	3.38	19.00
	west	283	283	283	1.35	0.67	0.50	-0.68	-44.54	-64.01	0.71	49.60	67.77	0.29	-50.40	52.76

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	980	980	980	2.58	2.85	1.10	0.27	8.21	0.59	0.68	30.79	29.40	0.83	10.40	26.43
	east	687	687	687	3.27	3.75	1.15	0.49	16.78	10.99	0.82	27.51	24.01	0.77	14.97	25.13
	west	293	293	293	0.96	0.71	0.74	-0.25	-11.86	-23.80	0.35	38.48	42.04	0.59	-26.01	36.73

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	866	866	866	2.14	1.78	0.83	-0.36	-5.10	-11.89	0.56	29.09	29.95	0.71	-16.62	26.36
	east	622	622	622	2.73	2.27	0.83	-0.46	-10.87	-15.88	0.69	25.06	27.30	0.44	-16.88	25.17
	west	244	244	244	0.64	0.55	0.86	-0.09	9.62	-1.72	0.25	39.36	36.73	0.34	-13.82	39.34

Table 19. Comparison of IMPROVE SO4 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	13458	13447	13458	1.68	1.72	1.02	0.04	45.01	0.94	0.67	78.29	45.67	0.74	2.16	39.59
	east	4771	4771	4771	3.34	3.62	1.09	0.29	24.78	7.00	1.22	49.14	39.56	0.68	8.55	36.55
	west	8687	8676	8687	0.77	0.67	0.87	-0.10	56.13	-2.39	0.36	94.31	49.02	0.28	-12.95	46.79

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3374	3372	3374	1.61	1.54	0.96	-0.07	61.95	-3.79	0.58	95.72	40.81	0.72	-4.44	36.03
	east	1194	1194	1194	3.07	3.03	0.99	-0.04	11.43	-0.88	0.99	38.57	34.54	0.62	-1.35	32.30
	west	2180	2178	2180	0.80	0.72	0.89	-0.09	89.65	-5.38	0.35	127.05	44.24	0.21	-10.90	43.85

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3390	3384	3390	2.54	2.51	0.99	-0.03	8.70	-11.58	0.97	52.15	47.56	0.76	-1.06	38.09
	east	1273	1273	1273	5.09	5.50	1.08	0.41	30.92	9.53	1.79	54.43	41.93	0.67	8.12	35.15
	west	2117	2111	2117	1.01	0.72	0.71	-0.29	-4.70	-24.28	0.47	50.77	50.94	0.22	-28.96	47.05

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3712	3711	3712	1.51	1.73	1.14	0.22	33.43	8.94	0.65	60.24	44.75	0.77	14.34	42.82
	east	1380	1380	1380	2.78	3.44	1.23	0.65	35.06	16.08	1.15	53.13	40.03	0.73	23.45	41.32
	west	2332	2331	2332	0.76	0.72	0.95	-0.04	32.47	4.72	0.35	64.44	47.55	0.33	-5.35	46.06

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2982	2980	2982	1.01	1.01	1.01	0.01	81.47	10.56	0.45	110.72	50.16	0.51	0.56	44.26
	east	924	924	924	2.10	2.08	0.99	-0.02	18.21	0.12	0.84	49.56	42.09	0.28	-0.80	39.84
	west	2058	2056	2058	0.52	0.53	1.03	0.02	109.90	15.25	0.27	138.21	53.78	0.32	3.02	52.29

Table 20. Comparison of NADP SO4 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	7619	7619	7619	1.46	1.68	1.15	0.22	42.05	-4.40	1.02	87.13	63.09	0.17	15.27	70.24
	east	5299	5299	5299	1.77	2.21	1.25	0.44	52.46	8.61	1.24	86.17	57.51	0.12	24.57	69.91
	west	2320	2320	2320	0.74	0.47	0.64	-0.26	18.27	-34.13	0.53	89.32	75.85	0.03	-35.91	72.03

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1955	1955	1955	1.47	1.60	1.09	0.13	26.98	-8.80	0.94	73.38	59.99	0.18	8.56	64.08
	east	1304	1304	1304	1.80	2.12	1.18	0.33	38.94	5.33	1.12	72.63	53.76	0.14	18.21	62.36
	west	651	651	651	0.82	0.55	0.66	-0.28	3.03	-37.10	0.59	74.88	72.49	0.02	-33.56	71.56

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1949	1949	1949	1.83	1.61	0.88	-0.22	19.07	-23.00	1.09	77.31	62.42	0.15	-11.83	59.60
	east	1441	1441	1441	2.10	2.00	0.95	-0.10	22.14	-10.66	1.20	68.62	55.06	0.12	-4.98	57.02
	west	508	508	508	1.04	0.51	0.49	-0.53	10.36	-57.99	0.77	101.94	83.32	0.00	-51.20	74.42

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1805	1805	1805	1.35	2.01	1.48	0.65	78.82	12.33	1.26	114.93	67.74	0.17	48.23	93.02
	east	1255	1255	1255	1.65	2.69	1.63	1.04	103.88	29.17	1.60	127.43	64.59	0.11	63.02	97.19
	west	550	550	550	0.68	0.45	0.66	-0.23	21.63	-26.08	0.48	86.42	74.93	0.12	-33.61	69.94

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1910	1910	1910	1.17	1.53	1.31	0.36	46.19	3.26	0.82	84.97	62.55	0.35	31.07	70.19
	east	1299	1299	1299	1.51	2.07	1.37	0.56	50.00	13.43	1.06	79.39	57.14	0.27	37.26	70.05
	west	611	611	611	0.44	0.38	0.86	-0.06	38.07	-18.38	0.31	96.83	74.05	0.14	-13.85	71.18

Table 21. Comparison of STN SO4 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	6970	6970	6970	3.40	3.62	1.06	0.22	55.36	-0.54	1.47	89.70	46.15	0.61	6.33	43.24
	east	5414	5414	5414	3.93	4.37	1.11	0.44	75.58	8.43	1.67	102.51	44.53	0.59	11.09	42.48
	west	1556	1556	1556	1.56	1.00	0.64	-0.55	-14.97	-31.74	0.78	45.16	51.78	0.16	-35.56	49.94

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1378	1378	1378	3.22	2.96	0.92	-0.26	35.33	-11.79	1.23	75.85	42.44	0.48	-8.10	38.32
	east	1051	1051	1051	3.78	3.56	0.94	-0.21	50.37	-6.94	1.42	86.49	41.24	0.39	-5.63	37.72
	west	327	327	327	1.43	1.01	0.71	-0.42	-13.04	-27.39	0.62	41.64	46.27	0.20	-29.14	43.42

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2106	2106	2106	4.76	5.28	1.11	0.52	54.69	0.97	2.05	88.61	47.42	0.63	10.81	42.93
	east	1677	1677	1677	5.50	6.37	1.16	0.86	76.43	13.81	2.31	99.30	44.27	0.60	15.68	41.98
	west	429	429	429	1.87	1.03	0.55	-0.85	-30.31	-49.25	1.01	46.80	59.75	0.15	-45.12	53.88

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	2155	2155	2155	2.81	3.25	1.16	0.44	53.84	6.14	1.27	82.51	44.83	0.62	15.72	45.27
	east	1671	1671	1671	3.15	3.88	1.23	0.73	73.65	16.59	1.41	93.96	43.50	0.63	23.20	44.74
	west	484	484	484	1.62	1.06	0.65	-0.56	-14.57	-29.92	0.79	42.96	49.39	0.17	-34.53	48.82

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	1331	1331	1331	2.40	2.27	0.95	-0.13	79.65	-2.08	1.13	117.44	50.14	0.28	-5.44	47.20
	east	1015	1015	1015	2.79	2.71	0.97	-0.08	103.43	2.02	1.30	138.45	50.08	0.19	-2.94	46.59
	west	316	316	316	1.15	0.87	0.75	-0.29	3.24	-15.26	0.60	49.96	50.34	0.12	-24.88	51.99

Table 22. Comparison of CASTNet SO2 observations versus CMAQ predictions.

ANNUAL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	3748	3748	3748	3.85	5.57	1.45	1.72	71.00	31.35	2.12	86.71	53.09	0.76	44.60	54.90
	east	2648	2648	2648	5.19	7.63	1.47	2.43	78.67	42.08	2.83	84.87	49.88	0.70	46.86	54.44
	west	1100	1100	1100	0.63	0.63	1.00	0.00	52.54	5.52	0.40	91.13	60.84	0.15	-0.46	63.95

SPRING																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	955	955	955	3.41	4.75	1.39	1.34	61.61	27.18	1.74	78.29	50.75	0.73	39.40	51.09
	east	678	678	678	4.57	6.49	1.42	1.92	72.65	40.40	2.30	77.34	46.03	0.65	42.04	50.40
	west	277	277	277	0.58	0.51	0.88	-0.07	34.57	-5.19	0.37	80.64	62.31	0.06	-11.72	64.41

SUMMER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	941	941	941	2.56	3.38	1.32	0.82	43.78	15.40	1.36	70.05	52.21	0.65	32.20	53.27
	east	657	657	657	3.34	4.59	1.38	1.25	59.16	31.09	1.77	72.05	47.99	0.58	37.52	52.92
	west	284	284	284	0.75	0.58	0.78	-0.17	8.19	-20.89	0.43	65.45	61.96	0.20	-22.46	56.83

FALL																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	983	983	983	3.61	6.12	1.69	2.50	105.85	46.31	2.71	116.32	60.08	0.72	69.23	74.91
	east	688	688	688	4.91	8.42	1.71	3.51	117.04	57.09	3.70	120.78	61.76	0.64	71.49	75.33
	west	295	295	295	0.60	0.75	1.26	0.15	79.74	21.18	0.40	105.92	56.16	0.29	25.75	66.82

WINTER																
	region	**n_obs**	**nzero_obs**	**nzero_sum**	**obs**	**pred**	**means_ratio**	**bias**	**nbias**	**fbias**	**err**	**nerr**	**ferr**	**r2**	**nmb**	**nme**
	nation	869	869	869	6.02	8.23	1.37	2.21	71.38	36.27	2.67	80.50	48.72	0.80	36.81	44.42
	east	625	625	625	8.14	11.19	1.37	3.05	63.45	38.93	3.55	67.01	42.95	0.74	37.48	43.68
	west	244	244	244	0.58	0.66	1.13	0.07	91.69	29.47	0.41	115.04	63.51	0.12	12.82	70.60

CMAQ Model Performance Evaluation for 2001: Updated March 2005

Appendix C

Model Performance Evaluations

conducted by

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Emissions Analysis and Monitoring Division
Air Quality Modeling Group
Research Triangle Park, NC 27711

Table 1: Summary of recent model performance evaluations conducted by other modeling groups

1. Boylan, J., VISTAS, "PM Model Performance Goal and Criteria", National RPO Modeling Meeting, Denver, CO, 2004a.

- Based on benchmarking with a combination of data from a number of PM modeling studies (SAMI, VISTAS, WRAP, EPA, MANE-NU, EPRI, and Midwest RPO). Proposed performance goals (close to best achievable) and performance criteria (acceptable) for these metrics and showed where the modeling studies fall for the various components of PM.
- Proposed to use mean fractional bias (MFB) and mean fractional error (MFE) as the standard performance metrics.
  Goal: MFE <= 50%, MFB <= +-30%
  Criteria: MFE <= 75%, MFB <= +-60%
  Less abundant species should have
  less stringent goal & criteria
- Proposed to use asymptotically approaching goals & criteria when data are greater than 2.5 um, approaching +200% MFE and +-200% MFB for extreme small model & observed data (forumla of logrithmic MFB & MFE are proposed)
- Based on combined modeling studies described above, for more abundant conditions, MFE and MFB are typical in the range of
  Sulfate: MFE = 30%~77%, MFB = -45%~+51% (> 2 ug/m3)
  Nitrate: MFE = 55%~125%, MFB = +3%~+82% (> 1 ug/m3)
  Organic: MFE = 35%~95%, MFB = -70%~+35% (> 1.5 ug/m3)
  EC: MFE = 50%~95%, MFB = -45%~+50% (> 0.5 ug/m3)
  PM 2.5:   MFE = 50%~85%, MFB = -55%~+60% (> 5 ug/m3)
- Suggested to conduct performance evaluation on episode-by-episode basis or month-by-month for annual modeling
- Different performance goals & criteria may be needed for gaseous precursors and wet depositions.
- Benchmarking should be done for the entire modeling system (meteorology, emissions inventory, and model).

2. Morris, R., et al., "Application of Multiple Models to Simulation Fine Particulate in the Southeastern US", National RPO Modeling Meeting, Denver, CO, 2004a.

- Based on model multiple model applications over VISTAS modeling:
  a. July 1999 & July 2001: CMAQ and CMAQ 36-km & 12-km
  b. January 2002 & July 2001: CMAQ and CMAQ MADRID 36-km only
  c. Used same horizontal & vertical grids, CMAQ-to-CAMx emissions, ICs/BCs, but different MM5 interface (MCIP vs. MM5CAMx).
- Both models performed reasonably well, with CMAQ performing better for SO4 and CAMx performing better for OM. Both models did not perform well for NO3, soil, and coarse PM, but CAMx seemed to have much higher positive bias in winter nitrate

than CMAQ

- Used fractional bias and fractional error (instead of normalized ones) to illustrate model performance because these statistics do not exhibit such extreme fluctuation.
- Demonstrated the usefulness of "soccer goal" plots for MFB & MFE. Suggested 15%/35% (MFB/MFE) for O3, and illustrated 50%/75% for PM2.5 species and bounded at 100%/200%
- Based on modeling studies described above (July 1999 & 2001), MFE and MFB are typical in the range of
  Sulfate: MFE = 25%~70%, MFB = -25%~+51%
  Organic: MFE = 30%~75%, MFB = -50%~+45%
  EC: MFE = 35%~65%, MFB = -30%~+40%
- CMAQ performance improved for OM when they adjusted the Kz min value to 1.0 m^2/sec (from 0.1m^2/sec).
- Indicated that in running multiple models, the set-up time for running a second model are minimal because there are available utility programs for converting CMAQ inputs to CAMx format and vice versa.
- Also illustrated CMAQ & CAMx vs. SEARCH hourly data (July 2001) of SO4 and total carbon mass (TCM). Both models seemed to captured the diurnal and daily trends well for both SO4 & TCM, but the magnitude can be significantly off for some of the days.

3. Boylan, J. and Baker, K., "Photochemical Model Performance and Consistency", National RPO Modeling Meeting, Denver, CO, 2004.

- Illustrated model performance comparisons of 36-km daily modeling results by MRPO (CAMx4), VISTAS (CMAQ-CB4), and MANE-VU (CMAQ-SARPC99) for two episodes (July 1999 and January 2002) at three IMPROVE sites; and by MRPO (CAMx4) and VISTAS (CMAQ-CB4 for one episode (July 1999) for the Pittsburgh supersite.
- Indicated that in some cases there was good agreement among the models and selected IMPROVE sites, but in others cases there were noticeable variations (even between the two RPOs running CMAQ).
- Sulfate were more consistent among the three models; nitrate and OM have higher discrepancies; All three models overpredicted nitrate and underpredicted OM (based on model vs. observed scatter plots comparisons)
- Suggested that where models diverge, they may show a different response to control strategies. Reasons for the model variations may include differences between CB4 and SAPRC99, and potential differences in emissions inventories, differences in Kz_min values, differences in met. & land use/soil methodologies, etc.
- Also described a comparison of hourly modeling results by MRPO and VISTAS for a July 1999 episode at the Pittsburgh super site. In some cases these hourly results were better than daily results and generally captured the diurnal patterns for PM2.5 species and gaseous species (O3, NOx, HNO3, SO2, etc.), although the magnitude was considerably off in some cases.

4. Seigneru, C., “Review of CMAQ and REMSAD Performance for Regional PM Modeling”, AER Report for UARG, Doc# CP163-03-01b, March 2003.

- Describe a review of summary performance of CMAQ, CMAQ-MADRID 1, CMAQ-MADRID 2, and REMSAD. Based on the comparison studies by others given below:
  a. BRAVO 1999 studay: CMAQ-MADRID 1 & REMSAD
  b. WRAP 1996 studies: CMAQ & REMSAD
  c. WRAP Aug. 1999 & Jan. 2000 studies: CMAQ & REMSAD
  d. EPA/ORD July 1999 studies: CMAQ & REMSAD
  e. Southeast PM - July 1999 study (Nashville/Altanta):CMAQ, CMAQ-MADRID1,2 & REMSAD
- AER Suggested normalized errors of 50% as the benchmark for sulfate and PM2.5 (note: this suggestion was not agreed by other modeling groups, see references #2, #5, #7: the MNE is most biased metrics and has high fluctuations). The review showed only SE PM study meets this criteria for sulfate and PM2.5, and all the rest of species failed. No model showed consistently better performance than the others. Suggested that the model inputs has more effect on performance than model formulations.
- Indicated that “the current performance of air quality models for PM is poor”...”There is a dire need for improving model inputs and model formulations in order to obtain acceptable model performance”... “3-D air quality models are the best tools available to address the PM source-receptors relationships because they take into account the non-linearities that affect the formation of secondary PM”.

5. Boylan, J., VISTAS, “Calculating Statistics: Concentration Related Performanc Goals”, PM Model Performance Workshop, RTP, NC, 2004b.

- Illustrated a set of standard bias and errors calculations commonly used for model performance statistics and proposed model performance goal.
- Indicated Mean Normalized Bias and Errors (MNBE) are most biased and least useful among “MNBE”, “NMBE” and “MFBE”. The Mean Fractional Bias and Errors (MFBE) is least biased and most useful among the three metrics.
- Recommended MFB & MBE and proposed performance goal: MFE<=50% and MFB <=+-30% for more abundant species (eg., sulfate & PM2.5) and less stringent for less abundant species (eg., nitrate, OC, EC, soil, etc.). Performance goal is not criteria and should be prohibit the modeling from being used if it fails to meet the goal.
- Proposed to use “2.5ug/m3" as the “graytline” for 50% MFE & +-30% MFB and asymmetrically approaching 200% MFE & +-200% MFB to extremely small concentrations.
- Recommended to use monthly avg. for annual modeling.

6. Morris, R., et al., “Model and Chemistry Intercomparison: CMAQ with CB4, CB4-2002, SAPRC99”, National RPO Modeling Meeting, Denver, CO, 2004b.

- Based on US (36-km) and VISTAS (12-km) January 2002 modeling, conducted chemistry mechanisms intercomparisons for CMAQ with CB4, CB4-2002,and SAPRC99.

- The performance of CB4 and CB4-2002 was similar for PM, and superior to SAPRC99 overall (for the Jan02 case).
- The model performance for CMAQ/CB4, US 36-km domain is in the range of:
  Sulfate: MFE = 42%~73%, MFB = -21%~+14%
  Nitrate: MFE = 62%~105%, MFB = -21%~+46%
  Organic: MFE = 50%~77%, MFB = +3%~+59%
  EC: MFE = 59%~88%, MFB = +2%~+70%
  Soil: MFE = 165%~180%,MFB =+164%~+180%
  PM 2.5: MFE = 48%~88%, MFB = +25%~+81%
- Given that the computational cost of SAPRC99 is twice that of CB4, suggested to use 36 and 12 km grids with CB4 chemistry for PM modeling for the time being.
- Noted that both CB4 and SAPRC underpredicted winter O3 significantly.

7. Tonnesen, G., et al., "Regional Haze Modeling: Recent Modeling Results for VISTAS and WRAP", CMAS Annual workshop, RTP, NC, 2003.

- Illustrated the WRAP 1996 CMAQ 36-km modeling and performance evaluation in the Western U.S. and VISTAS CMAQ 12-km modeling for 3 episodes: January 2002, July 1999, July 2001. Recommended to use the performance metrics of Mean Fractional Bias (MFB)and Mean Fractional errors (MFE) over mean normalized bias & errors (used in earlier WRAP model evaluation).
  Sulfate: MFB = -47%~+48% (1996 WRAP domain)
  Nitrate: MFB = -95%~+30% (1996 WRAP domain)
  Organic: MFB = -20%~+70% (1996 WRAP domain)
  OC: MFB = -45%~ +3% (1996 WRAP domain)
- VISTAS modeling key findings (1) sulfate performance reasonably well (2) nitrate overpredictions in the winter, underpredictions in summer, may need better NH3 emissions (3) Kv min =1 improved performance, mixing height is important (4) minor differences in 19 vs. 34 layers

8. Zhang, Y., et al., "Performance Evaluation of CMAQ and PM-CAMx for July 1999 SOS Episode", AER Report for CRC, Doc# CP131-03-01, Apirl 2003.

- Conducted CMAQ (2002 version) and PM-CAMx performance evaluation based on July 1999 SOS episode (6/29-7/11) modeling study (32-km nested w/ 8-km in the SE U.S., including Atlanta & Nashville)
- Ozone performance: use MNB & MNE w/ 60 ppb threshold for O3 (CMAQ performed better):
  CMAQ:MNB < 1%, MNE = 18%
  CAMx:MNB =27%, MNE = 33%
- PM performance: CMAQ & PM-CAMx are generally consistent in the rural areas (vs. IMPROVE); differs significantly over urban/suburban; in general, CMAQ performs

much better than PM-CMAx

PM 2.5: CMAQ:MNB = 38%, MNE = -7%

CAMx:MNB =55%, MNE = 35%

Sulfate: CMAQ:MNB = 9%, MNE = 45%

CAMx:MNB =44%, MNE = 63%

Nitrate: CMAQ:MNB = -50%, MNE = 98%

CAMx:MNB =137%, MNE = 158%

- The performance of CMAQ for PM and O3 is consistent with the performance expected for air quality models (however, nitrate issue existed); the performance of CAMx does not generally meet current expectations for AQM.

9. Morris. R., et al.,"Evaluation of CAMx: Issues Related to Section Models ", PM Model Performance Workshop,RTP, NC, 2004c.

- Illustrated a WRAP comparison of CMAQ (v4.3), REMSAD (v7), CAMx (bimodal PM), and CAMx (4-section PM) based on January and July 1996 and annual 1996 over the 36-km WRAP domain.
- Indicated that all models exhibited variations in performance, but no clear winner across all species and periods. Sulfate predictions were reasonable, but nitrate was significantly overprected. For all three models,

  Sulfate: MFE = 40%~60%, MFB = -40%~+14% (July 96)

  Nitrate: MFE =105%~200%, MFB = +45%~>+100% (Jan. 96)

  Organic: MFE = 50%~75%, MFB = -65%~+5% (July 96)

  EC: MFE = 47%~105%, MFB = -48%~+25% (Jan. 96)
- The 1996 model performance is less than stellar, indicating potential issues in 1996 MM5 and emissioins.
- Showed the effects of sectional PM distribution on PM Modeling in the Western US. Based on a study in the South Coast Air Basin using CAMx4+, which allows side-by-side comparisons of aqueous-phase chemistry modules (bulk vs. variable size resolution) and of PM size distribution treatments (bimodal vs. sectional).

10. Tonnesen, G., et al..,"Model Performance Metrics, Ambient Data Sets and Evaluation Tools", PM Model Performance Workshop, RTP, NC, 2004a.

- Illustrated model performance metrics, available PM2.5 and O3 data, and evaluation software tool. Suggested that air quality modeling should include model evaluation as part of the system.
- Comparing performance metrics may not be enough since performance metrics often show mixed response and it is possible for a better model to have poorer metrics (e.g., bias in met & emissions inputs). Diagnostic evaluation is needed to judge finer grid performance since coarser grid may have compensating errors. But should we assume that finer grid modeling always gives better simulations/physics?
- An example of VISTAS modeling (July 1999) showed differences of hourly sulfate and its wet deposition between CMAQ results using 12-km and 36-km grids, possible due to regional transport (wind speed & direction), precipitations/clouds, and numerical

diffusion. • Recommended bias factor as the best metric for evaluating haze.
11. Wang, Z., et al.," Comparison and Diagnostic Evaluation of Air Quality Models for Particulate Matter: CAMx, CMAQ, CMAQ-MADRID", National RPO Modeling Meeting, 2004. • Conducted model evaluation based on 1999 SOS episode (6/29-7/10) EPRI modeling study, • CAMx has higher positive bias than CMAQ and CMAQ-Madrid in predicting sulfate; CMAQ underestimated nitrate and CAMx and CMAQ-MADRID overestimated nitrate. • All three models underestimated OM. However, there was no clear winner in model performance. • The three models responded differently to a 50% increase in ammonia emissions, indicating a need to further look at the models' responsiveness to changes in emissions.
12. Ku, C., CENRAP, "CMAQ and CAMx Simulations for January and July 2002", National RPO Modeling Meeting, Denver, CO, 2004. • Compared CMAQ and CAMx 36-km simulations Based on January and July 2002 (basB) over a continental US domain. • Indicated that the results were mixed for the models over CENRAP generally. Both models performed acceptably for PM2.5 and sulfate in the summer (when sulfate is abundant) but they were overpredicted in the winter compared against IMPROVE network. • CAMx significantly overpredicted nitrate in the winter (higher prediction than CMAQ), but has better performance in OM (lower prediction than CMAQ), based on performance measures of normalized bias and errors. • The study also showed mixed results for the models in three climatically different regions in CENRAP that contain Class I areas, with varying performance depending on region and season. This finding points up the difficulty in improving model performance over the whole CENRAP domain.
13. Eder B. and Yu S., "An Evulation of the 2003 Release of Models-3/CMAQ", CMAS Annual workshop, RTP, NC, 2003. • Illustrated CMAQ 2003 evaluation for two episodes (winter 2002 and Summer 1999) for O3 and PM 2.5 species against AIRS, CASNTE, IMPROVE, and STN. Suggested the use of the performance metrics of Normalized Mean Bias (NMB)and Normalized Mean errors (NMB) (and correlation coefficient, R). • Ozone is fairly unbiased and accurate (NMB<10%) and NME=~20%); sulfate performance is quite well, even for STN. NO3 was the worst in the winter (NME ~67% for STN and ~96% for IMPROVE)
14. Frank, N.,"Use of National PM2.5 and Speciation Network Measurements for Model

Evaluation ", PM Model Performance Workshop, RTP, NC, 2004.

- Compared correlated speciated monitoring sites (e.g., IMPROVE, CASTNet, STN) for ambient PM species measurements.
- The sulfate agrees very well, but nitrate has both positive & negative bias site-by-site.
- OM is more uncertain than other species, but is still somewhat robust for model evaluation (ie., uncertainty is relatively small compared to current range of uncertainty in modeling). OM is about 50%-80% of urban excess of PM2.5.

15. Hu, Y., et.al., "Evaluation of CMAQ with FAQS Episode of August 11th-20th", 2000, CMAS Annual workshop, RTP, NC, 2003.

- Conducted CMAQ (36/12/4 km nesting) performance evaluation for O3 based on Fall Line Air Quality Study (FAQS) 8/11-20.
- Indicated that CMAQ had a good O3 performance, but has a nighttime problem, which could be due to min Kz used. Analysis suggested that an optimal of min Kz may lie between 0.1~1 m^2/s.
- The Isoprene emissions may be overestimated in the rural area and CO emissions may be underestimated.

16. Tonnesen, G., et al., "Prelim Preliminary Results CMAQ and CMAQ-AIM with SAPRC99", National RPO Modeling Meeting, 2004b.

- Compared CMAQ and CMAQ-AIM with SAPRC99 based on 2001 VISTAS modeling study. CMAQ-AIM with SAPRC99 has larger negative bias and lower predictions of Sulfate PM than standard released CMAQ.
- Conducted model & chemistry intercomparisons: CMAQ with CB4, CB4-2002, SAPRC99. Some chemistry differences were observed in the models based on the 36-km U.S. and the 12-km VISTAS modeling; the performance of CB4 and CB4-2002 was similar, and superior to SAPRC99 overall.
- Given that the computational cost of SAPRC99 is twice that of CB4, suggested to use 36 and 12 km grids with CB4 chemistry for current VISTAS modeling study.

17. Yu, S., et al., "Simulation of Primary and Secondary Organic Aerosols over the US by CMAQ: Evaluation and Analysis", CMAS Annual workshop, RTP, NC, 2003.

- Evaluated CMAQ w/ SAPRC99 performance of Primary Organic Aerosols (POA), EC, and secondary Organic Aerosols (SOA) based on IMPROVE, SEARCH, and SOS data.

- Suggested that model captured general trends & patterns of most EC & POA within a factor of two (based on IMPROVE & SEARCH).
- Slight underprediction in the Eastern U.S., likely due to underprediction in biogenic SOA.

18. Chien, C. Y., et al., “CMAQ Model Performance Evaluation with the Updated CB4-2002", CMAS Annual workshop, RTP, NC, 2003. • Evaluated CMAQ w/ CB4 vs. CB4-2002 (and CB4-2002 with removed N2O5 gaseous reaction) against IMPROVE, CASTNet and AQS based on January & July 1996 cases. Described the key updates of CB4-2002 (HNO3, N2O5 & PAN rxns). • CB4-2002 has lower O3, lower N2O5, lower PAN, higher HNO3, higher nitrate, slightly higher sulfate, and slightly lower SOA prediction than CB4. • The performance of CMAQ CB4 and CB4-2002 was similar for PM species. However, CB4-2002 has higher positive bias for winter nitrate (since it predicted higher nitrate).
19. Dennis, R.,”Time-Resolved and In-Depth Evaulation of PM and PM Precursors Using CMAQ ”, PM Model Performance Workshop, RTP, NC, 2004. • Evaluated the CMAQ (2003 version) performance of inorganic PM, EC, and gaseous precursors against Atlanta 1999 supersite summer data and 2002 Pittsburgh supersite winter data. • Suggested that collapse of evening PBL is too fast and rise of morning PBL too slow (based on higher modeled EC, NOy & CO against Atlanta data at sunrise & sunset) • Performance for sulfate & ammonium was fairly good; • Overprediction for nitrate, but updated chemistry in CMAQ (included in 2004 version) has improved the nitrate performance (updated reaction probability for HNO3 heterogeneous rxn and remove gaseous N2O5->HNO3 rxn) • Use ratio to define nitrate PM formation being HNO3- or NH3-limited: (NHx-2*SO4)/(HNO3+NO3) • Nitrate PM predictions are very sensitive to NHx, and thus the NH3 emissions need serious attention.
20. Kumar, N.,”PM2.5 Model Performance: Lessons Learned and Recommendations ”, PM Model Performance Workshop, RTP,NC, 2004. • Illustrated the use of model performance statistics based on two CMAQ-MADRID applications, SOS 1999 episode in the SE U.S. and 12-km BRAVO summer 1999 episode (nested within RESMAD BRAVO 36-km modeling results) • Indicated model evaluation issues regarding local vs. regional, daily/weekly vs. month/seasonal Sulfate: MNB= +20%/+51%,MNE = 51%/89% (SEARCH/IMPROVE) Nitrate: MNB= +72%/-25%,MNE = 72%/46% (SEARCH/IMPROVE) EC : MNB= +14%/-8%, MNE = 52%/54% (SEARCH/IMPROVE) PM 2.5 : MNB= -19%/-8%, MNE = 32%/49% (SEARCH/IMPROVE) • Described the available performance metrics and illustrated the use of logarithmic and fractional bias and errors as potential benchmarks

21. Baker K., Midwest RPO, “Fine Grid Model Performance”, National RPO Modeling Meeting, Denver, CO, 2004. • Based on the Midwest RPO 36-km and 12-km Modeling study using CAMx4 • Indicated that the model performance for PM2.5 species generally was similar for 36 and 12 km grids; there were some differences in running control scenarios for sulfate/nitrate, but we could not determine which one is better
22. Morris, R., et al., “VISTAS Grid Resolution Sensitivity”, National RPO Modeling Meeting, Denver, CO, 2004d. • Based on VISTAS Southeast U.S. modeling study for Phase I episode (Jan. 2002, July 1999, and July 2001), compared results for CMAQ w/ CB4 and SAPRC99 using the 36 km national RPO domain and the 12 km grid VISTAS domain • Effects of grid resolution on model performance was mixed (performance was not necessarily improving using 12-km) • CMAQ w/ SAPRC99 (mixed for sulfate, worse for nitrate) was not performing better than w/ CB4 • Compared July 1999 episode for ozone using 36-km & 12-km CMAQ and CAMx. CMAQ O3 performance degraded to underprediction with finer grid; CAMx is similar at 36-km and 12-km. • Examined the performance of the MM5 model configurations using various cloud schemes (including Kain-Fritsch and Reisner schemes) for the 12 km (WRAP) and 36 km domains. The results showed that cool and moist bias found in the West, overprediction of convective precipitation using KF.
23. Zhang, Y., et al., “Development and Application of MADRID: A New Aerosol Module in CMAQ”, CMAS Annual workshop, RTP, NC, 2003. • Evaluated CMAQ-MADRID against SCAQS 1987 episode. The performance of CMAQ-MADRID seemed to perform well in O3, PM2.5, and sulfates, and comparable in other PM 2.5 species to other models (UAM-IV/CALGRID/UAM-AERO, GATOR, SMOG, CIT, SAQM-AERO) • Described the development and sciences of MADRID aerosol module included in CMAQ. Key features: sectional (size bins), hybrid equilibrium, more sophisticated SOA treatment, CMU aqueous chemistry
24. Morris, R., et al., “WRAP Multi-Model Evaluation Using the 1996 36 km Section 309 Database”, National RPO Modeling Meeting, Denver, CO, 2004e. • Conducted WRAP 1996 multi-model evaluation. Compared CMAQ (v4.3), REMSAD (v7), CAMx (bimodal PM), and CAMx (4-section PM) using the 1996 36-km section 309 database. • Indicated that sulfate was the best performing species on an annual basis, with a winter overprediction compensating for a summer underprediction; NO3 was predicted poorly by all models; OC, EC, and CM were underpredicted by all models. concluded that

modeling is more challenging in the West than in the Midwest and Southeast.

CMAQ Model Performance Evaluation for 2001: Updated March 2005

Appendix D

Time Series Analysis of PM2.5 Species :

CASTNet, IMPROVE, STN, and SEARCH monitoring networks

conducted by

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Emissions Analysis and Monitoring Division
Air Quality Modeling Group
Research Triangle Park, NC 27711

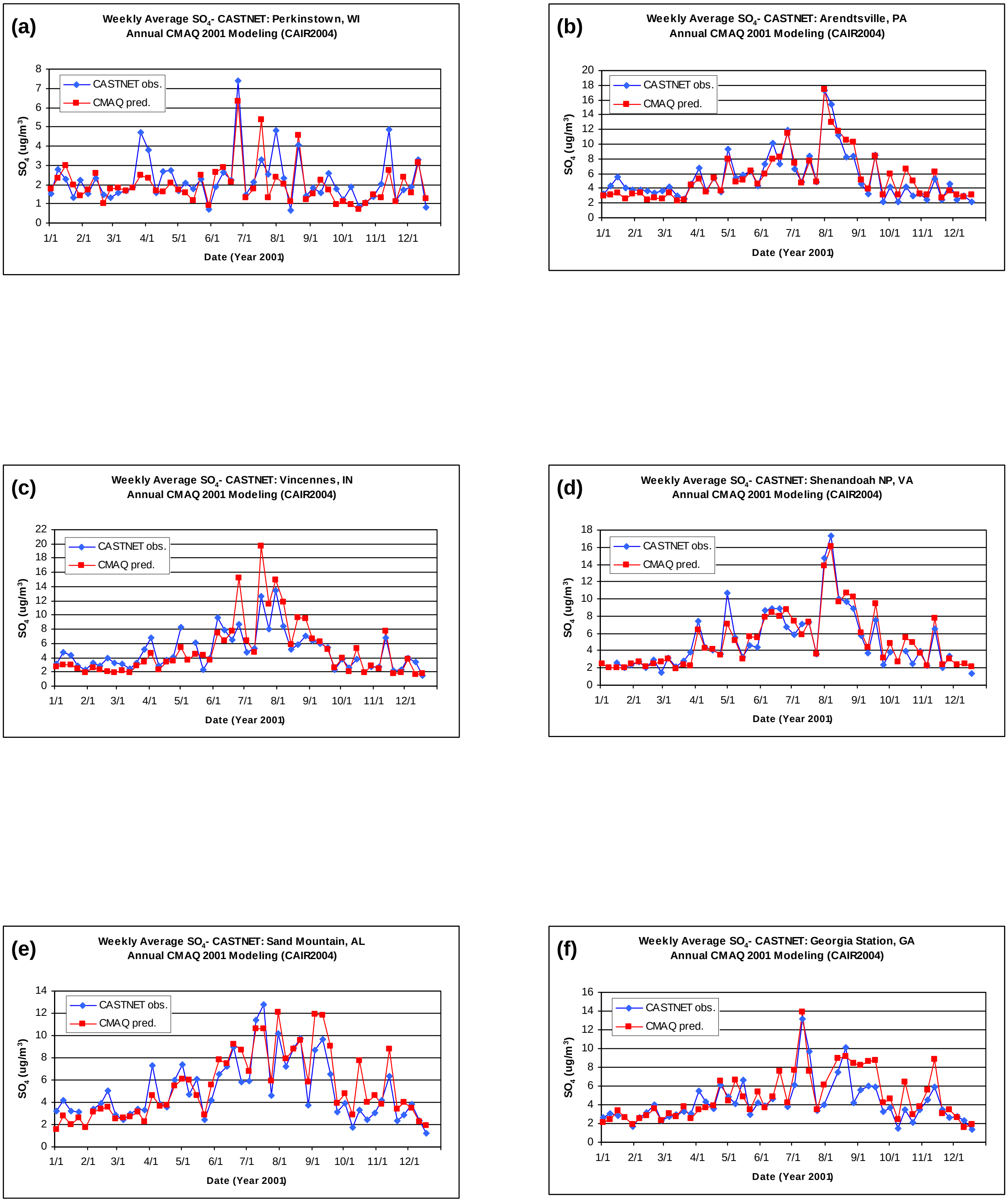


Figure D-1. Time-series analysis of annual sulfate (SO_4) 2001 CASTNet observations versus CMAQ predictions.

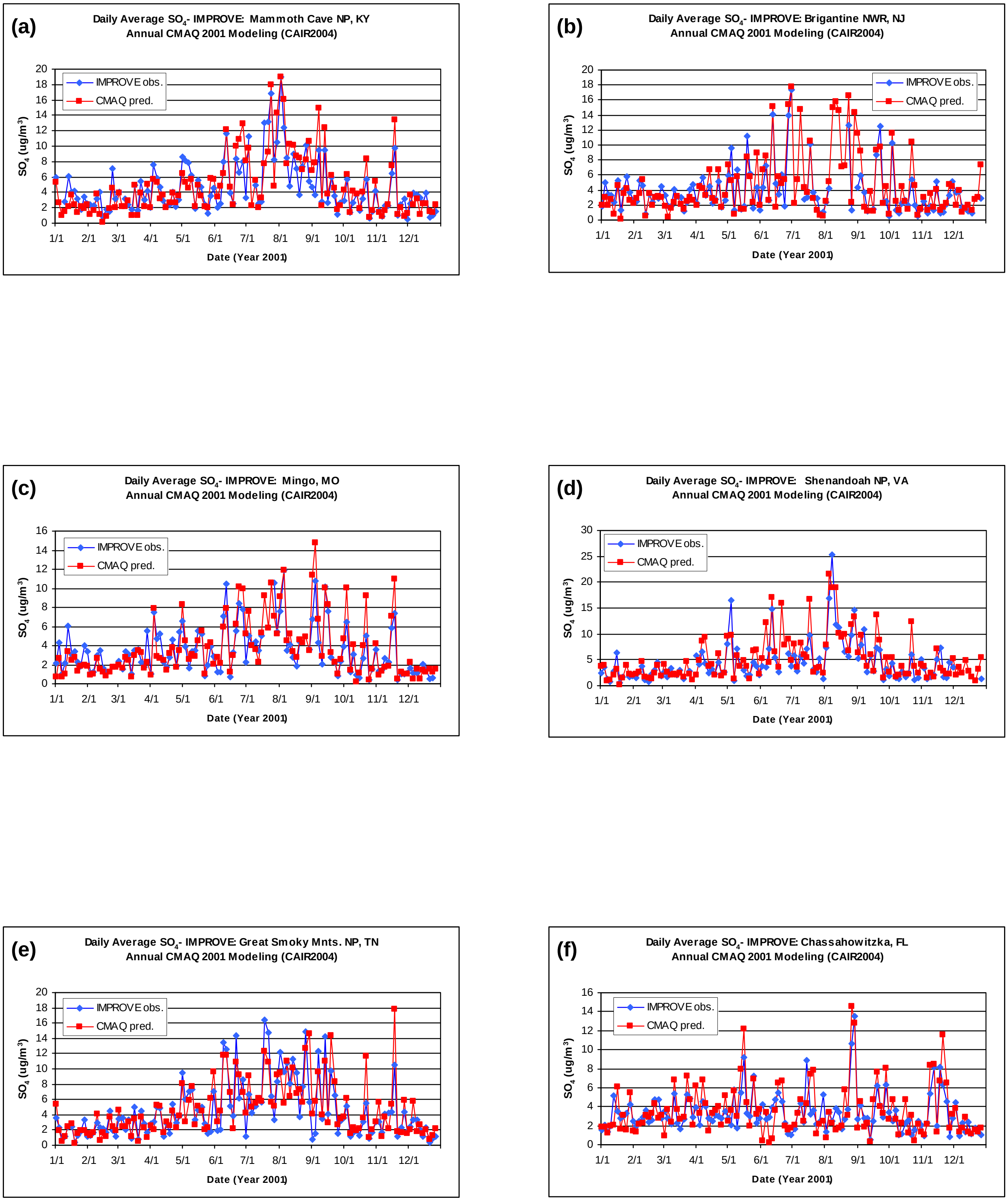


Figure D-2. Time-series analysis of annual sulfate (SO_4) 2001 IMPROVE observations versus CMAQ predictions.

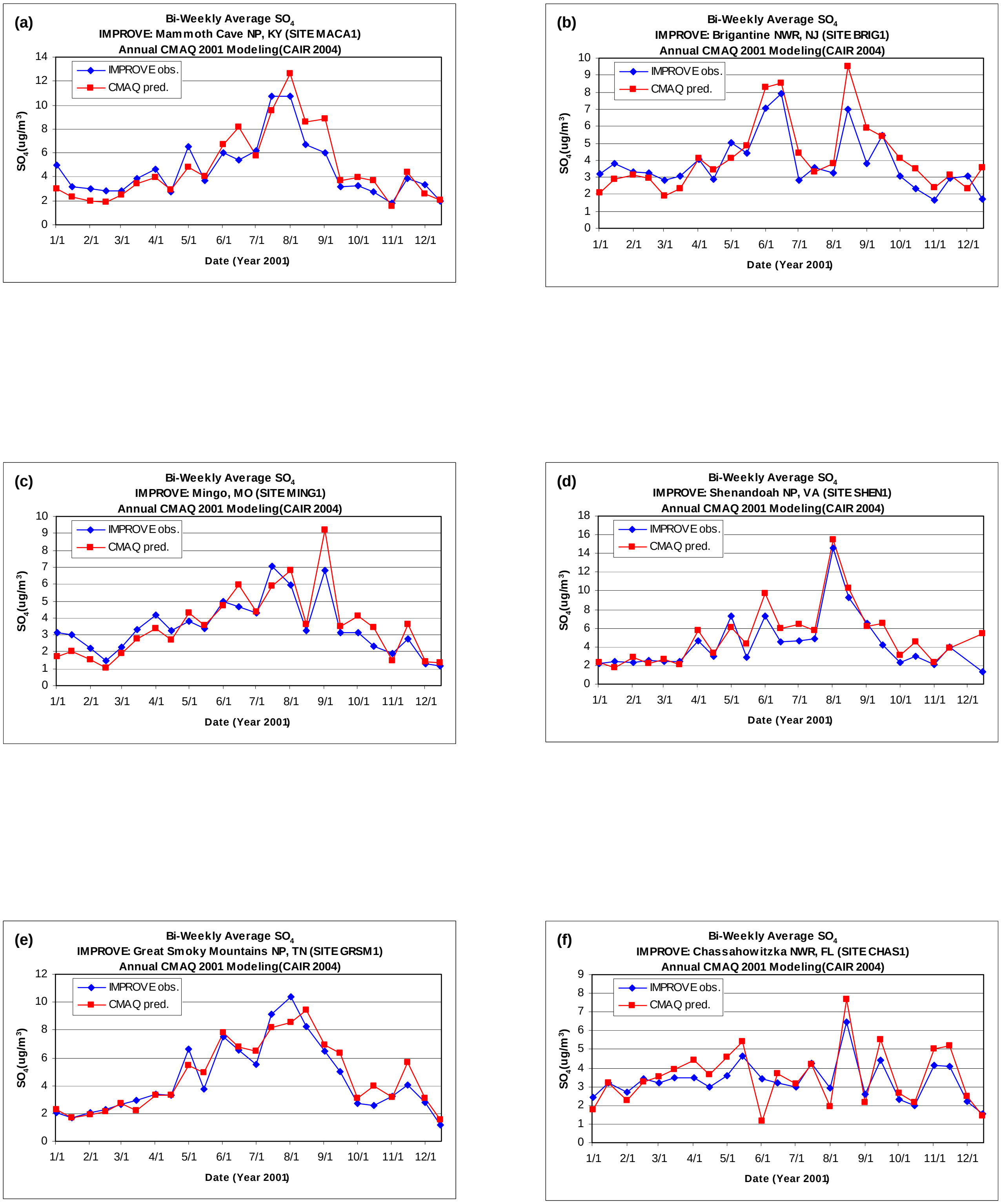


Figure D-3. Time-series analysis of annual sulfate (SO_4) 2001 IMPROVE observations versus CMAQ predictions.

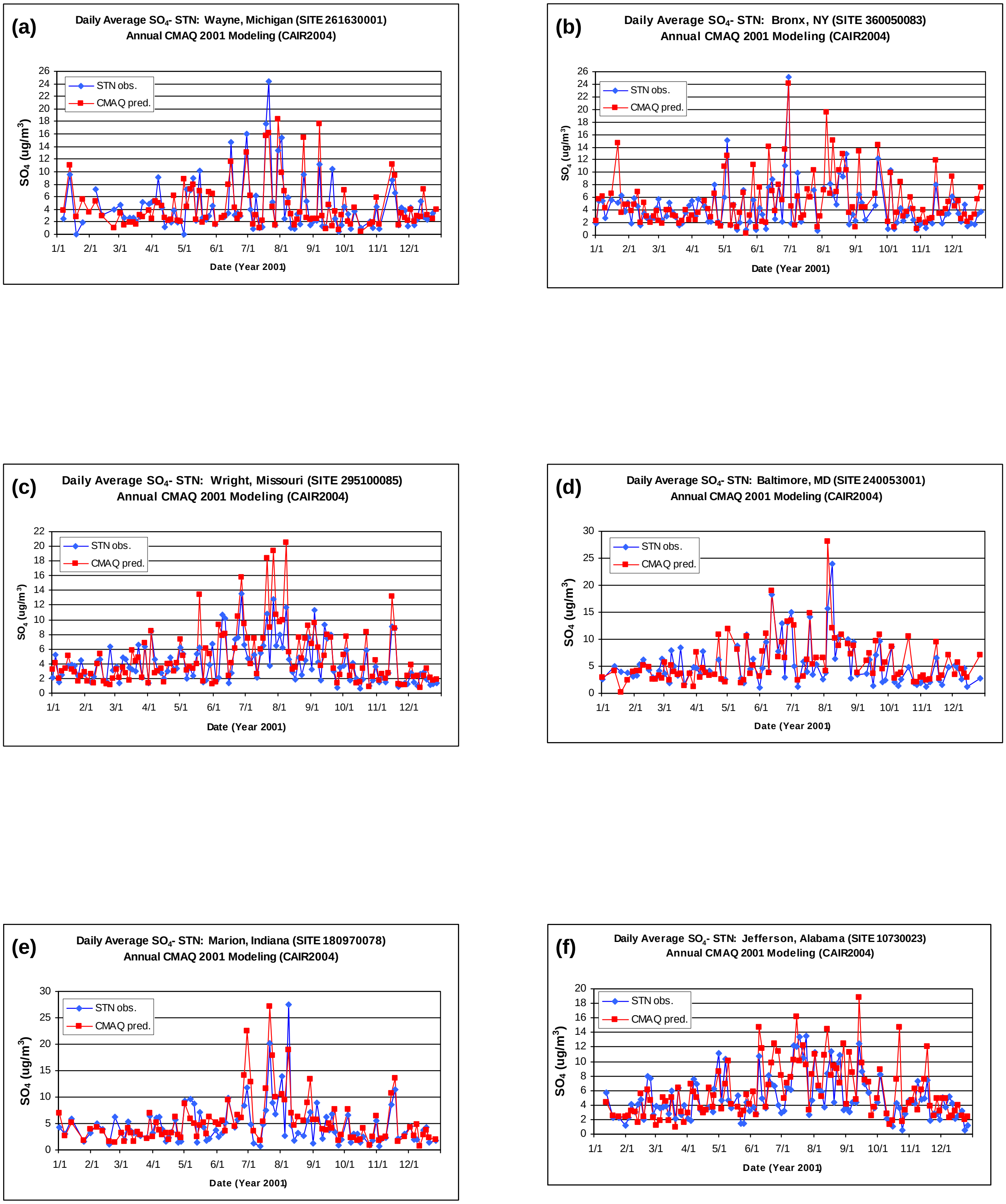


Figure D-4. Time-series analysis of annual sulfate (SO_4) 2001 STN observations versus CMAQ predictions.

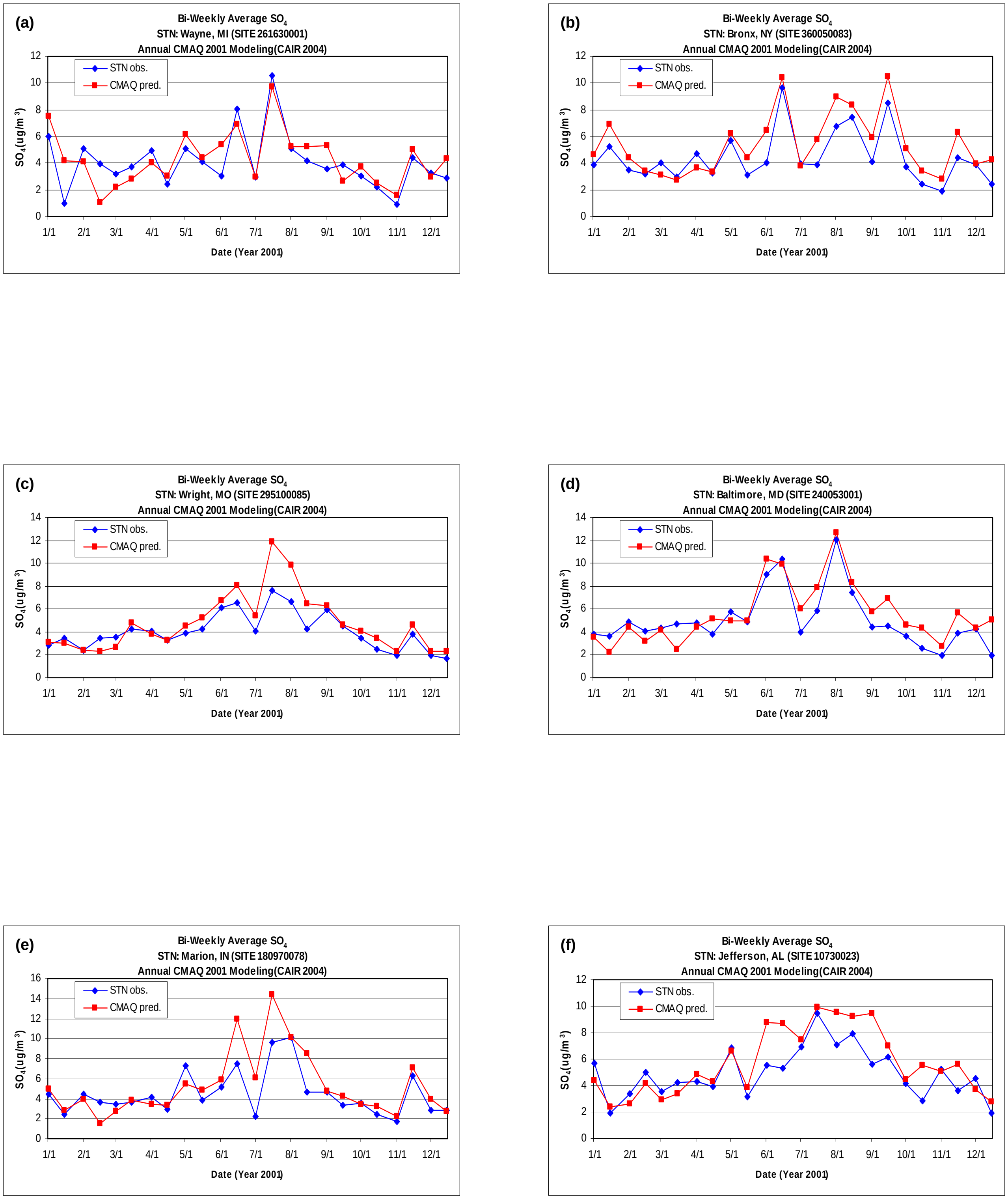
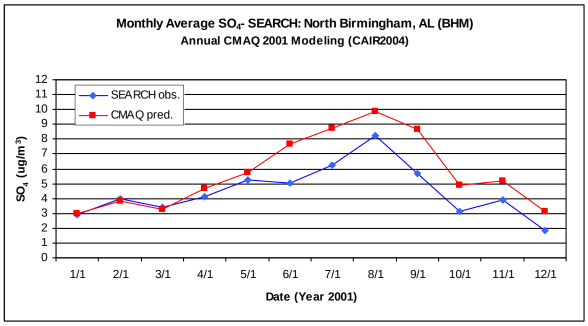
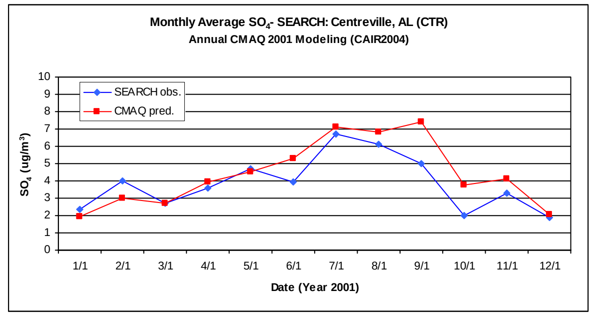
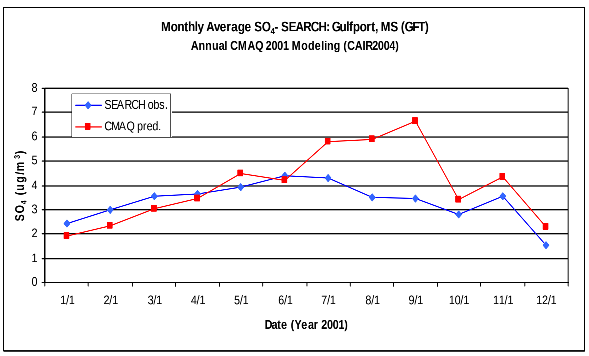
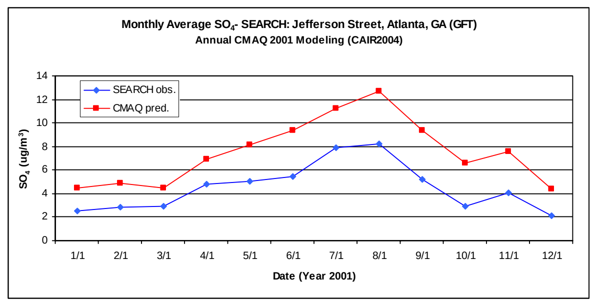


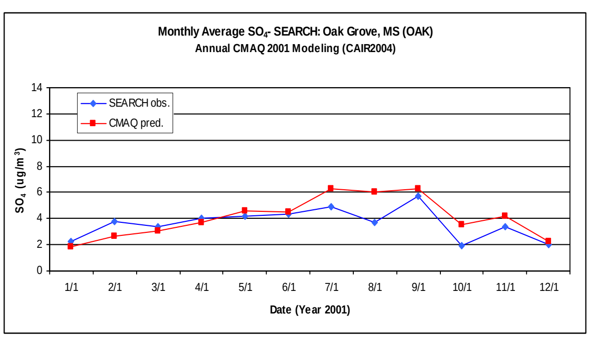
Figure D-5. Time-series analysis of annual sulfate (SO_4) 2001 STN observations versus CMAQ predictions.











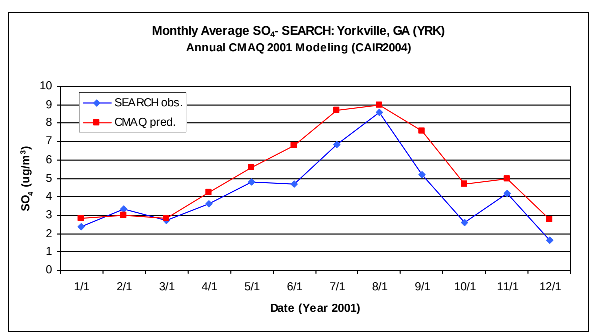


Figure D-6. Time-series analysis of annual sulfate (SO4) 2001 SEARCH observations versus CMAQ predictions.

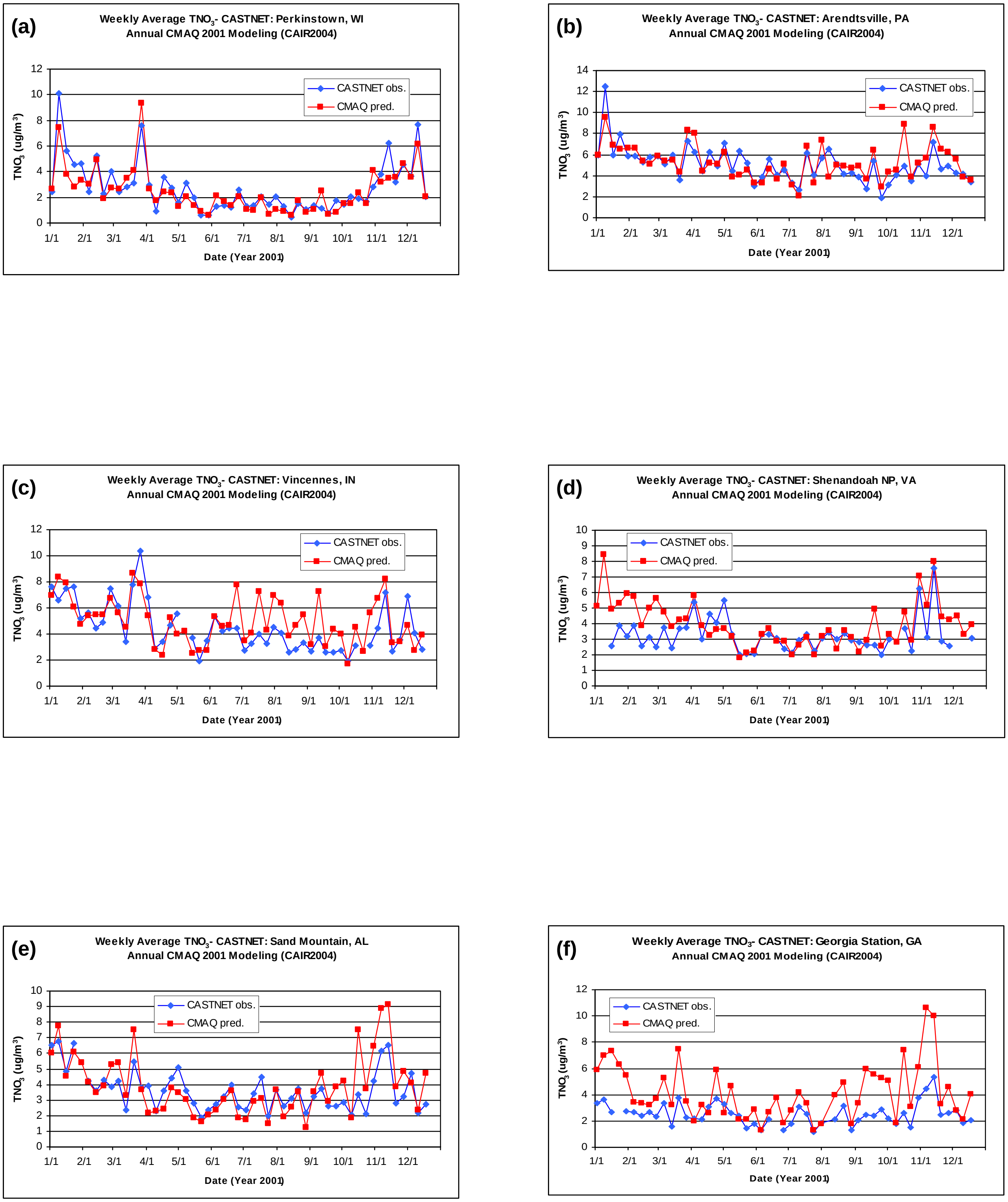


Figure D-7. Time-series analysis of annual total nitrate (NO_3+HNO_3) 2001 CASTNet observations versus CMAQ predictions.

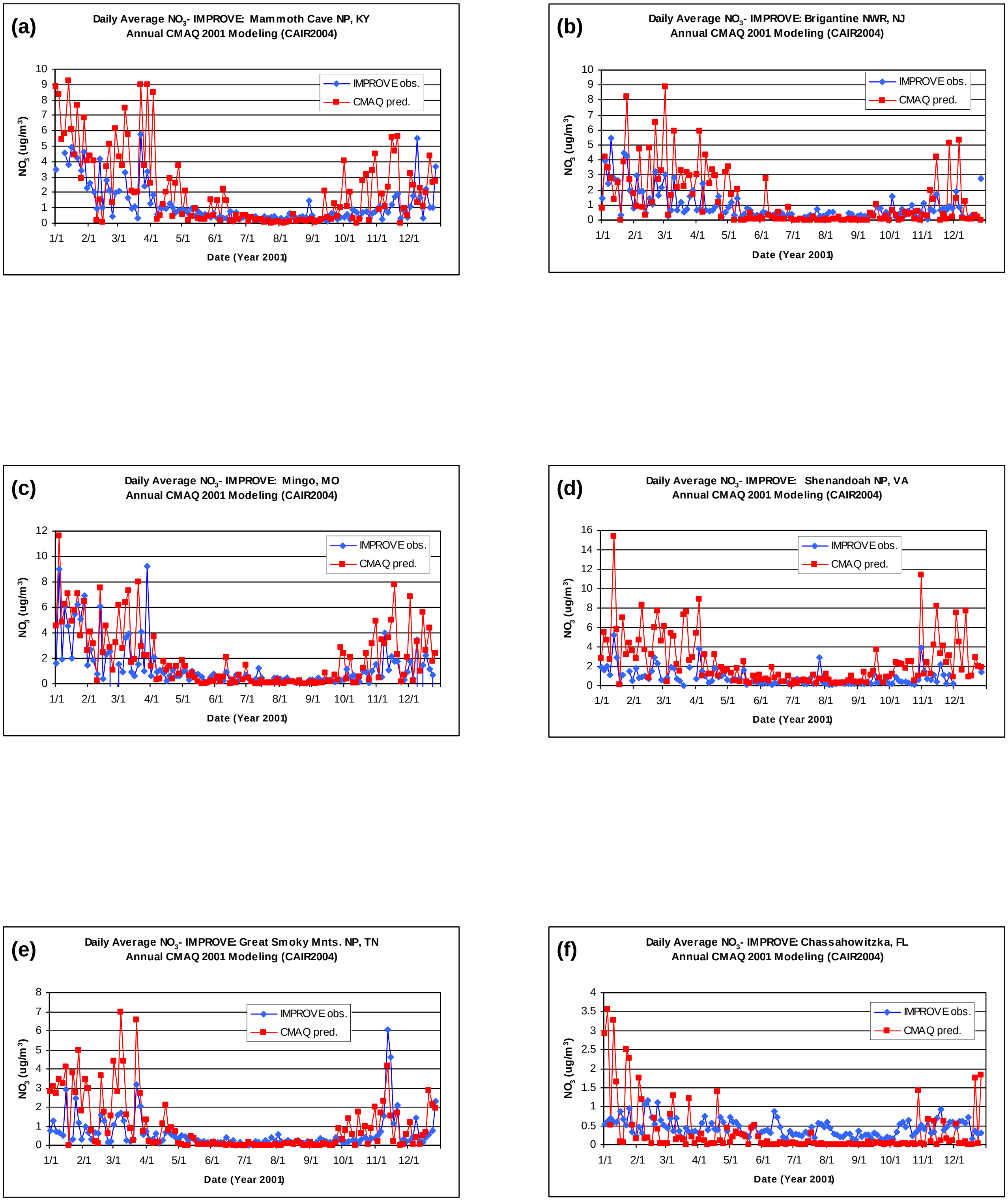
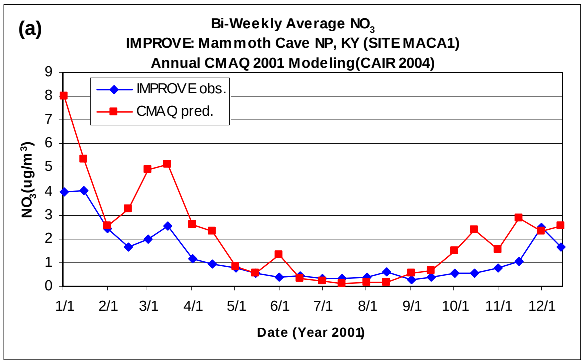
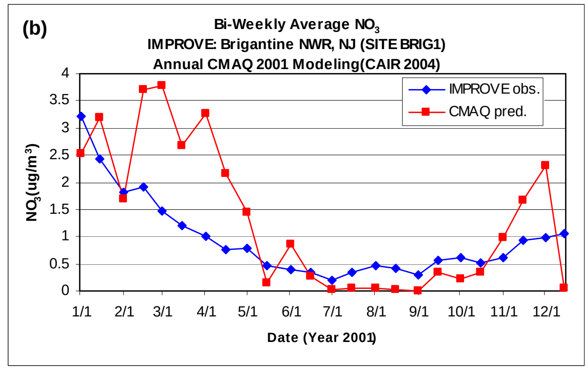
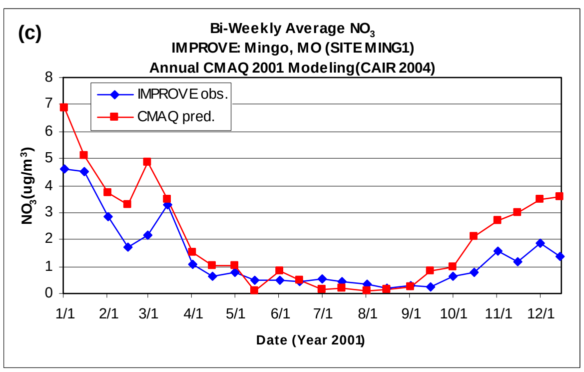
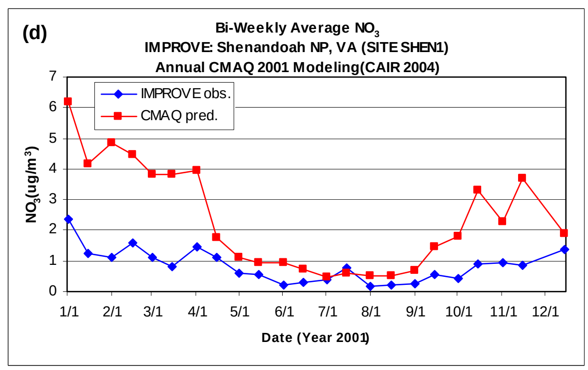


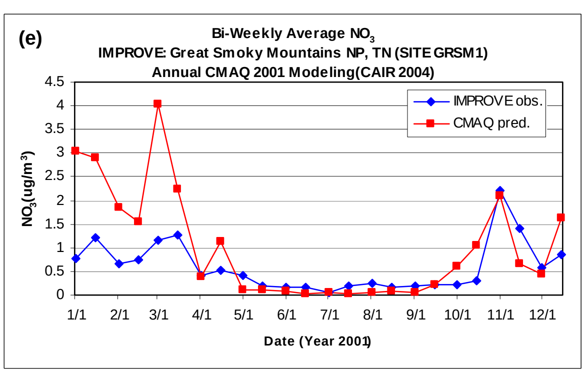
Figure D-8. Time-series analysis of annual nitrate (NO_3) 2001 IMPROVE observations versus CMAQ predictions.











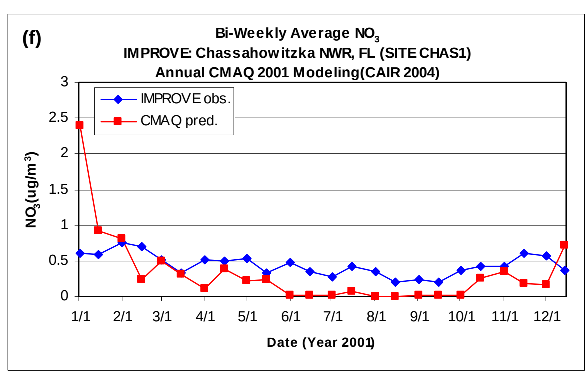


Figure D-9. Time-series analysis of annual nitrate PM (NO_3) 2001 IMPROVE observations versus CMAQ predictions.

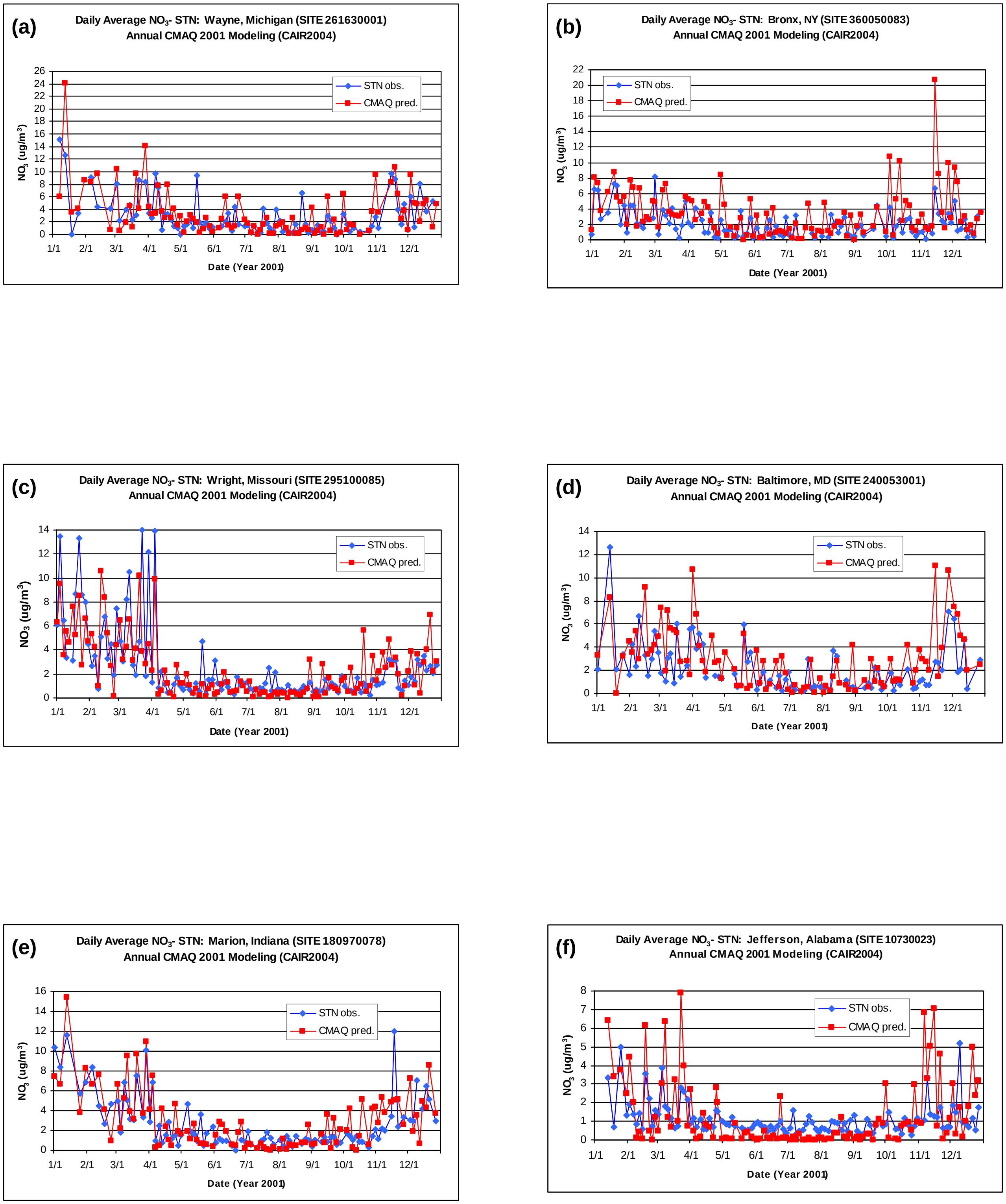


Figure D-10. Time-series analysis of annual nitrate (NO_3) 2001 STN observations versus CMAQ predictions.

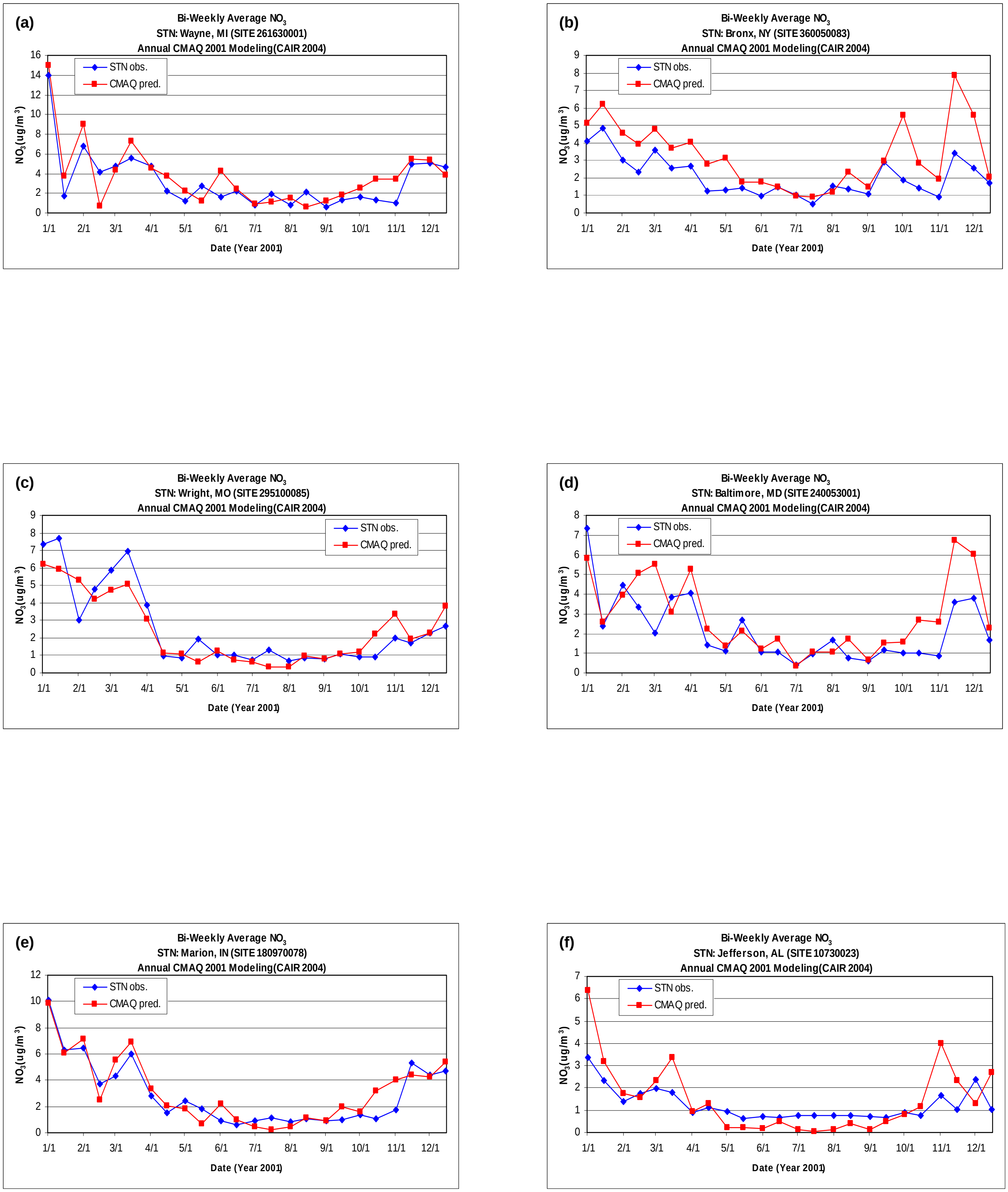
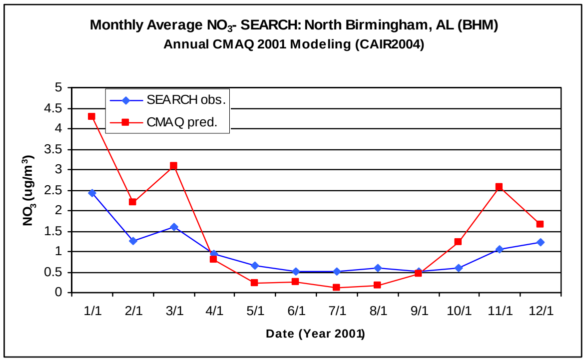
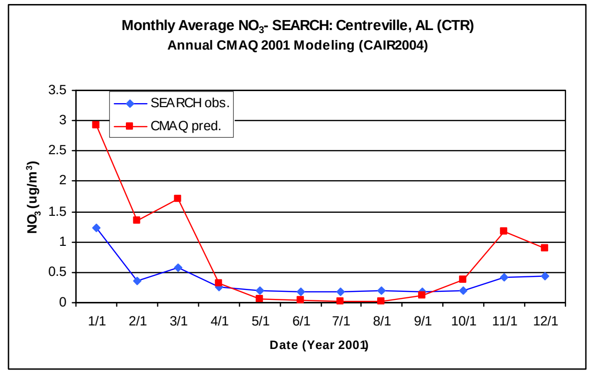
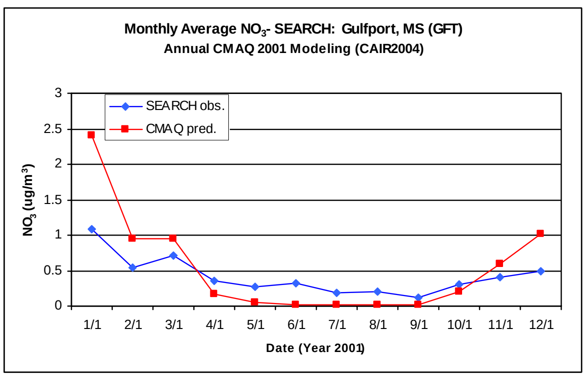
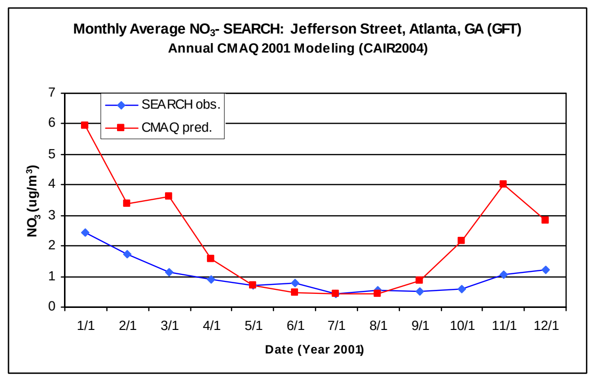


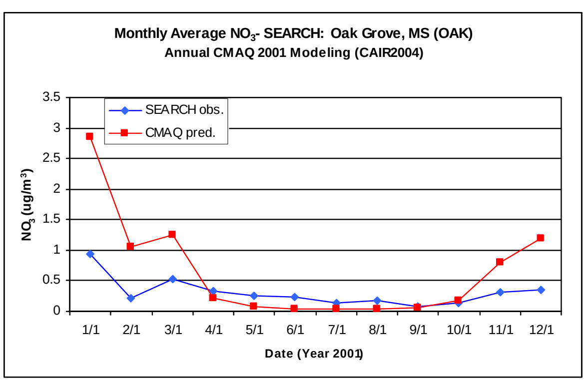
Figure D-11. Time-series analysis of annual nitrate PM (NO_3) 2001 STN observations versus CMAQ predictions.











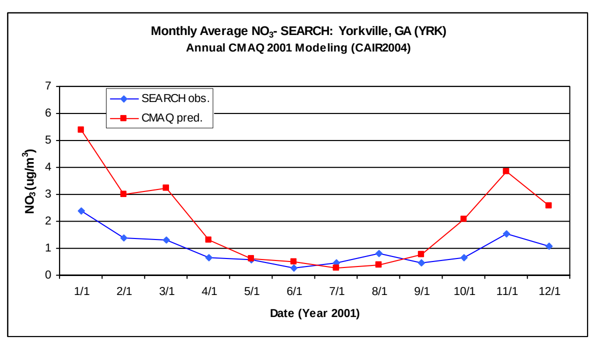


Figure D-12. Time-series analysis of annual nitrate (NO3) 2001 SEARCH observations versus CMAQ predictions.

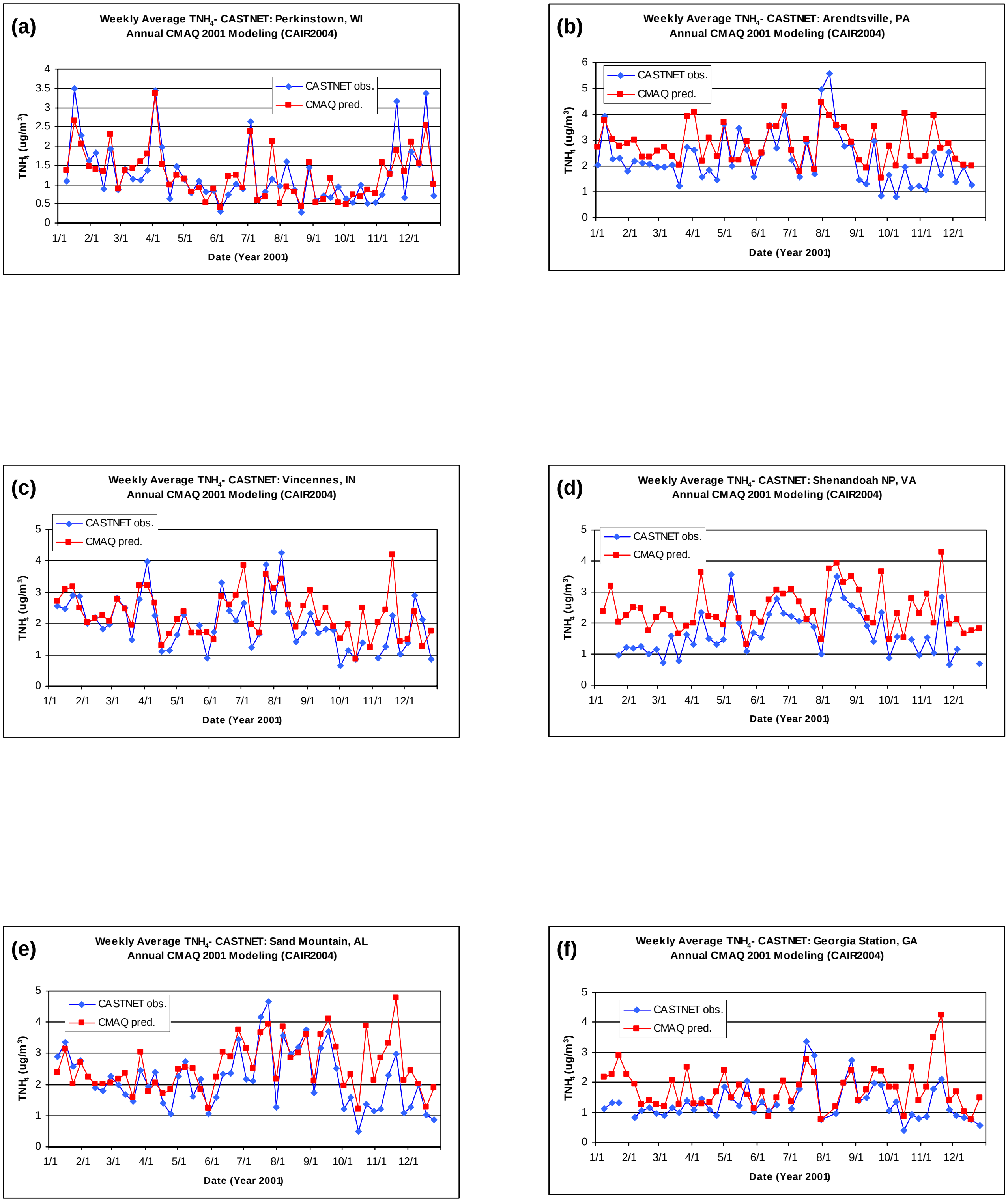


Figure D-13. Time-series analysis of annual ammonium PM (NH_4) 2001 CASTNet observations versus CMAQ predictions.

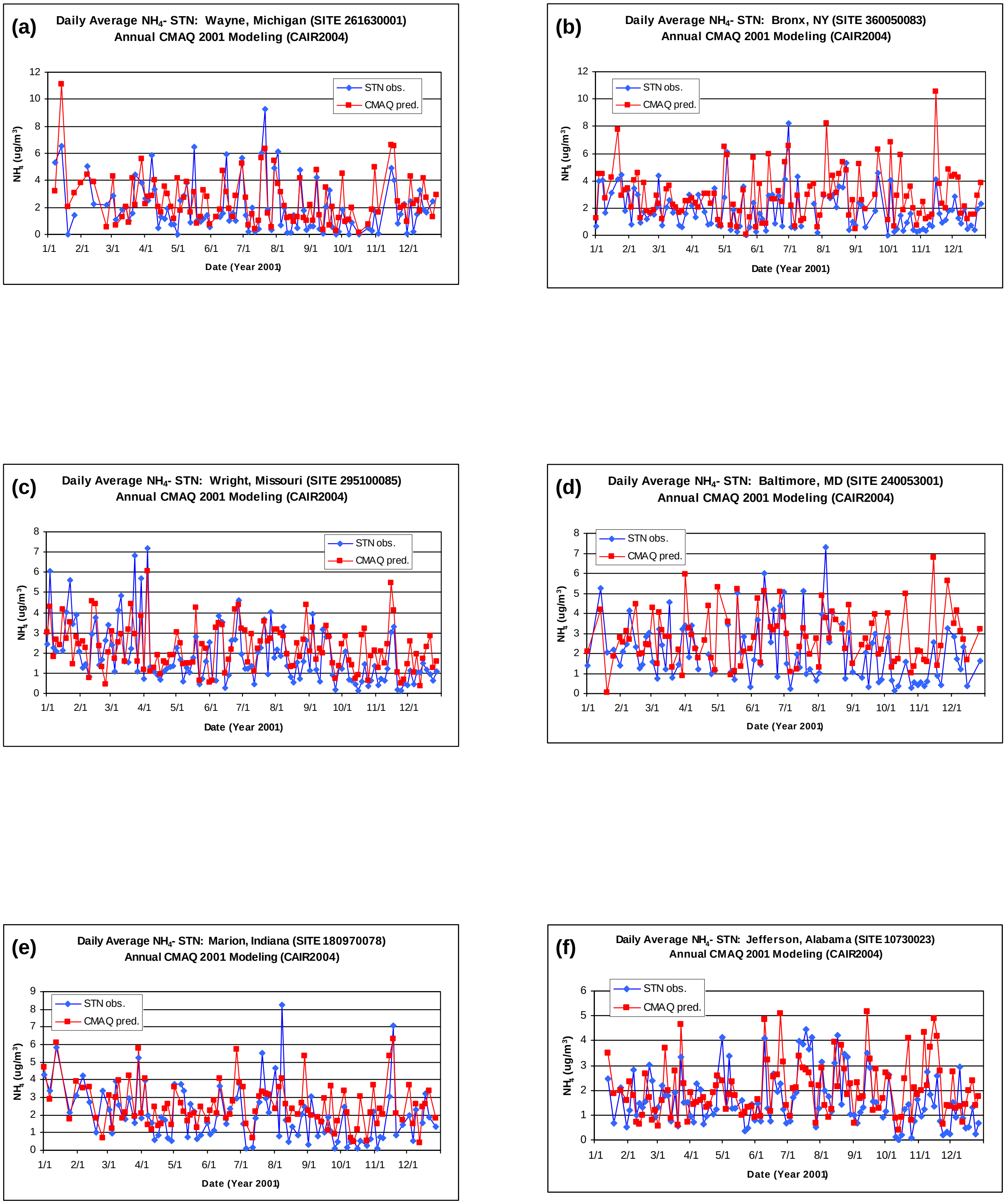
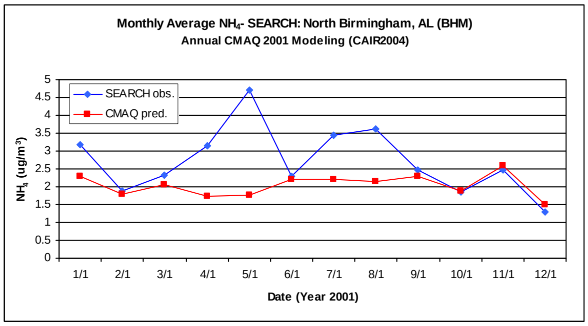
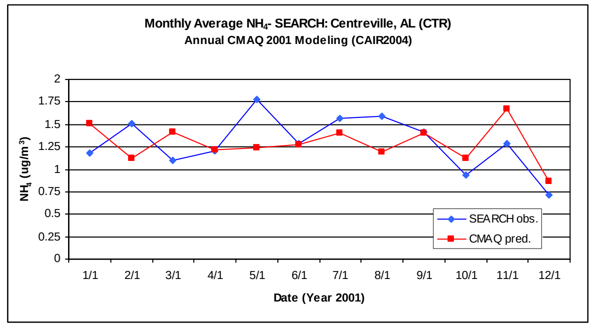
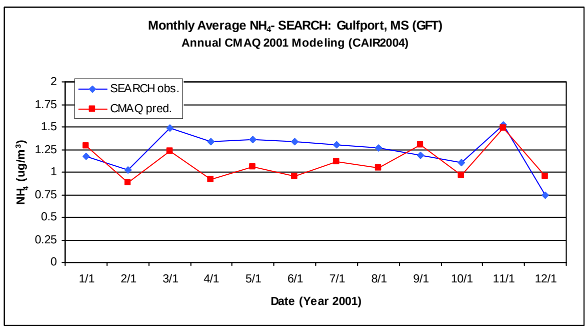


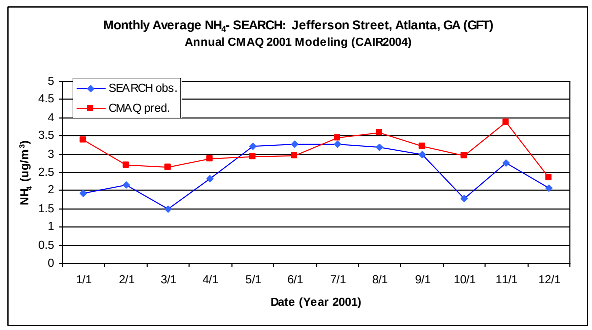
Figure D-14. Time-series analysis of annual ammonium (NH_4) 2001 STN observations versus CMAQ predictions.

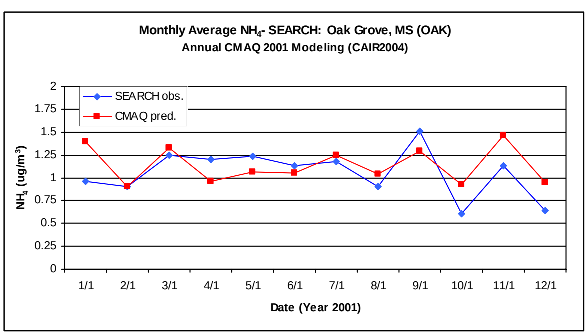
Figure D-15. Time-series analysis of annual ammonium PM (NH_4) 2001 STN observations versus CMAQ predictions.











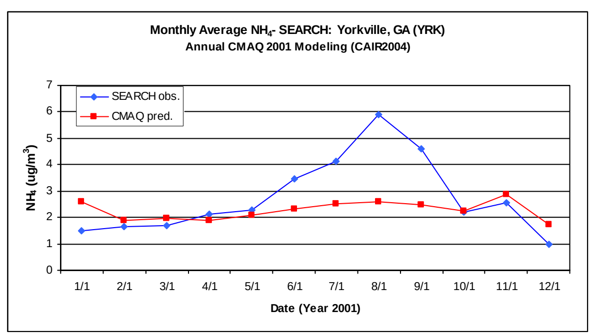


Figure D-16. Time-series analysis of annual nitrate (NO3) 2001 SEARCH observations versus CMAQ predictions.

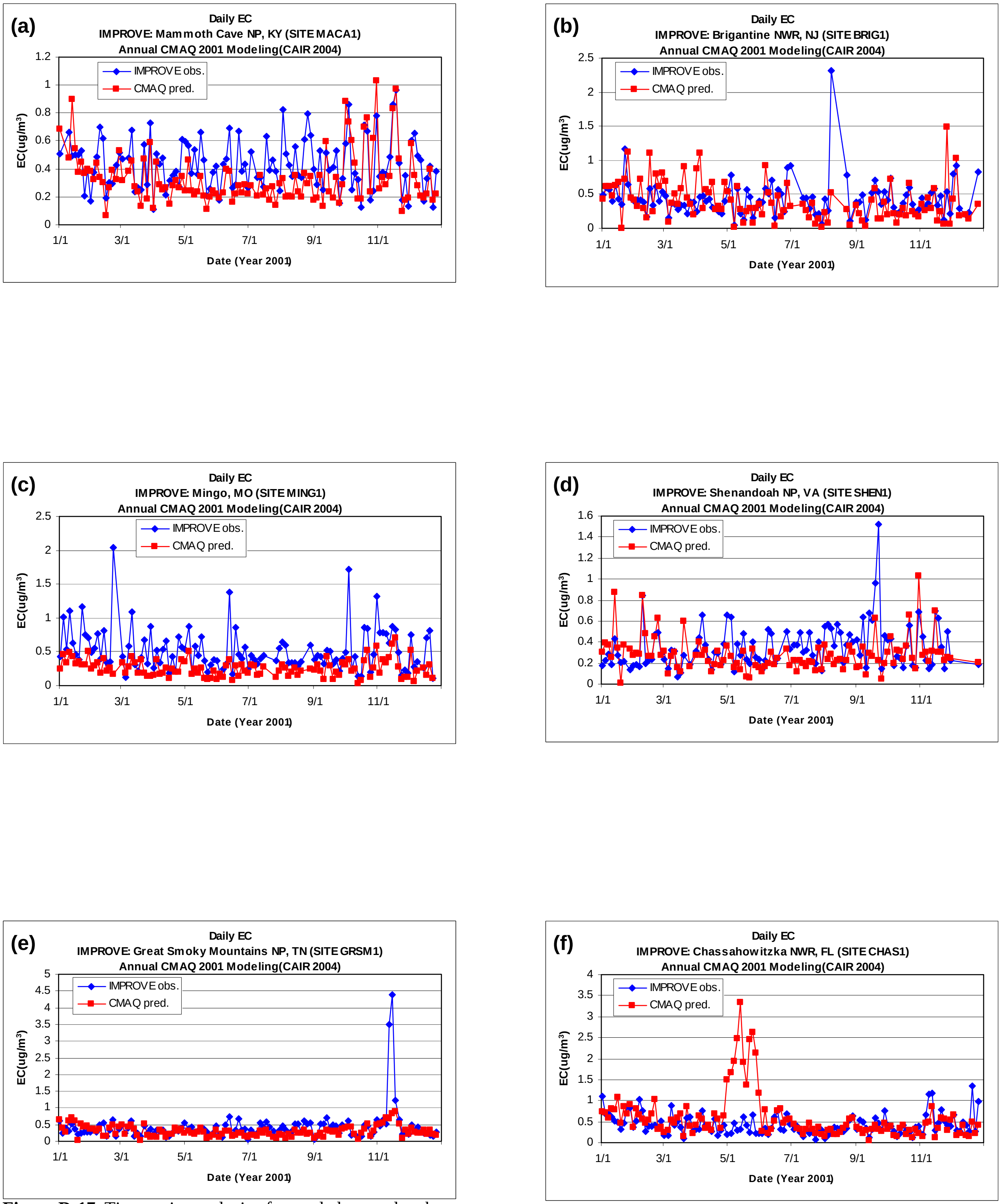


Figure D-17. Time-series analysis of annual elemental carbon (OC) 2001 IMPROVE observations versus CMAQ predictions.

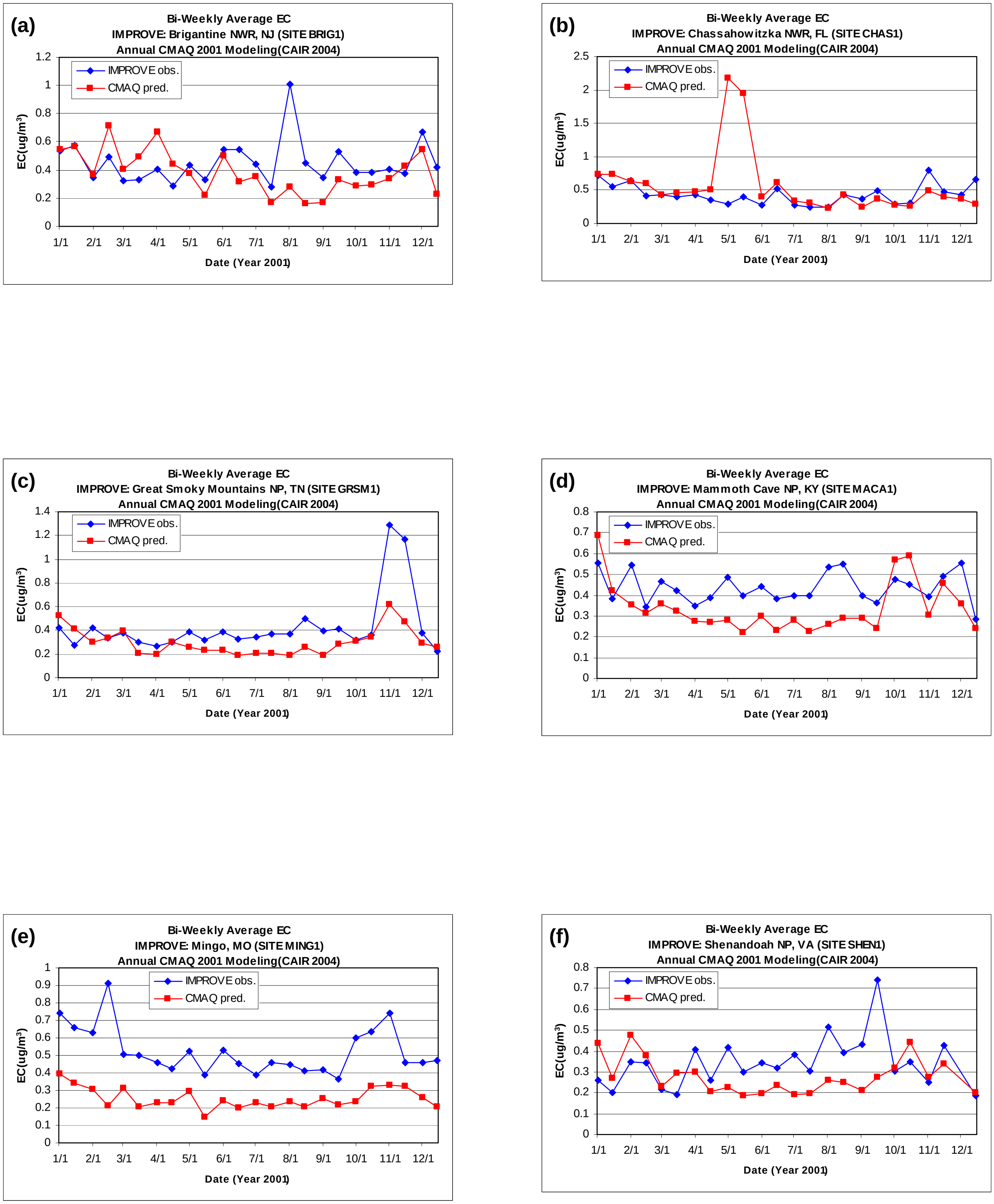
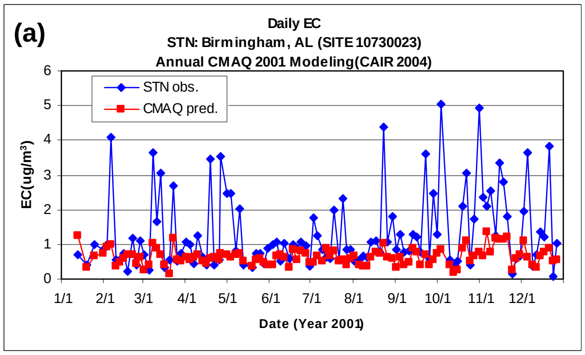
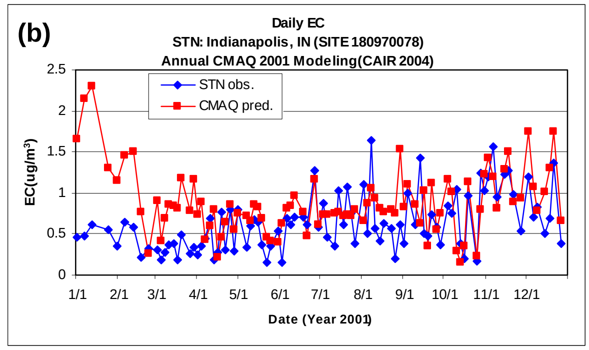
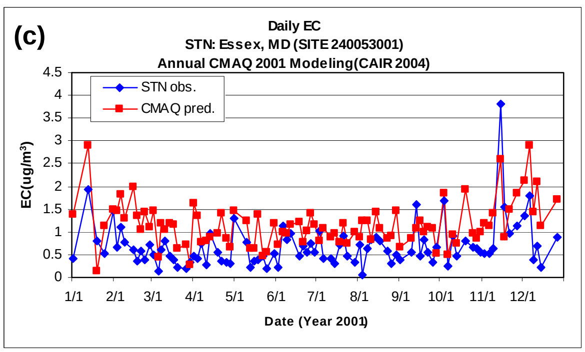
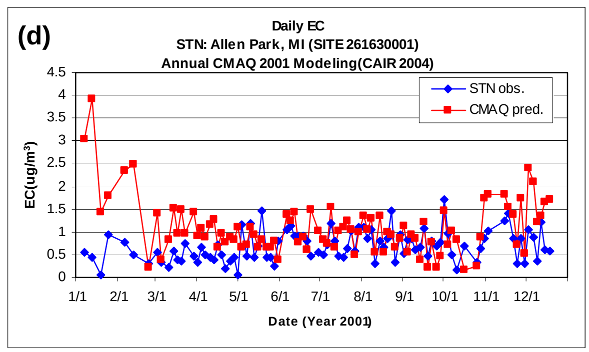


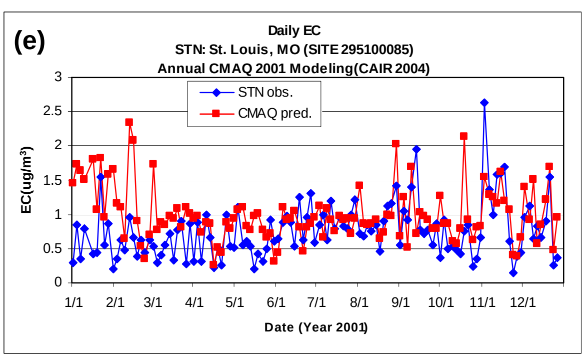
Figure D-18. Time-series analysis of annual elemental carbon 2001 IMPROVE observations versus CMAQ predictions.











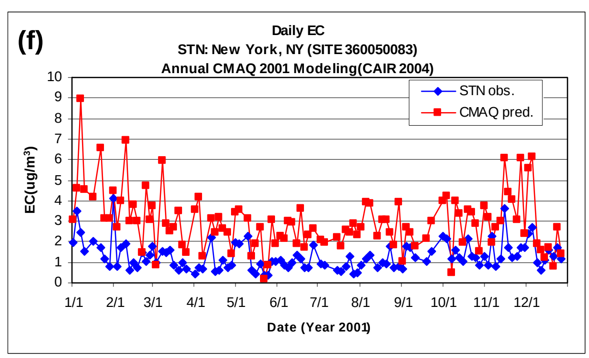
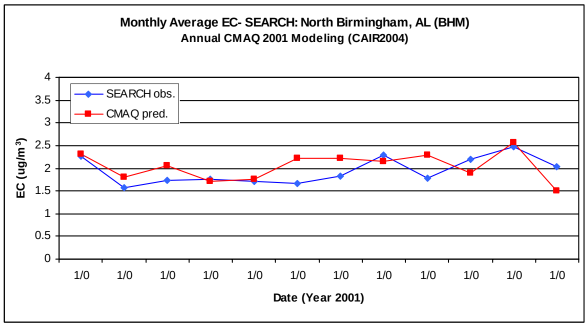
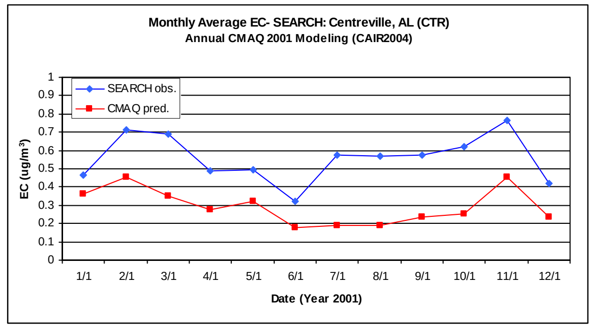
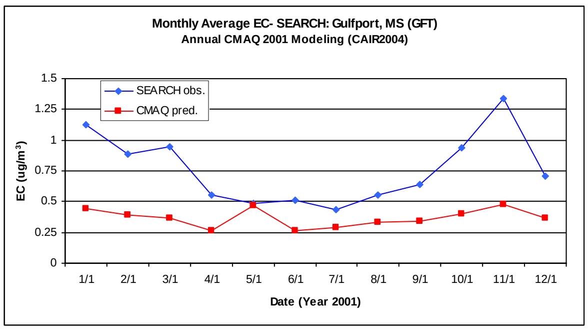


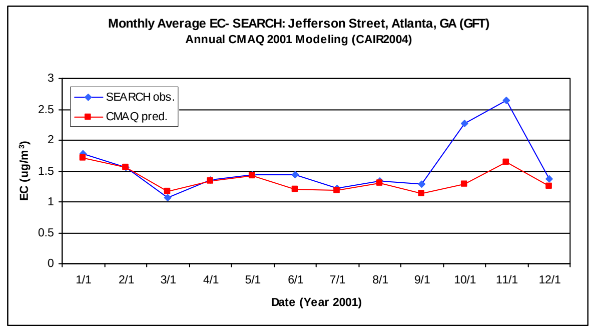
Figure D-19. Time-series analysis of annual elemental carbon (EC) 2001 IMPROVE observations versus CMAQ predictions.

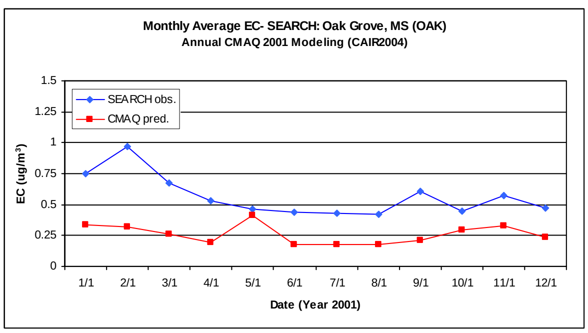
Figure D-20. Time-series analysis of annual elemental carbon (EC) 2001 IMPROVE observations versus CMAQ predictions.











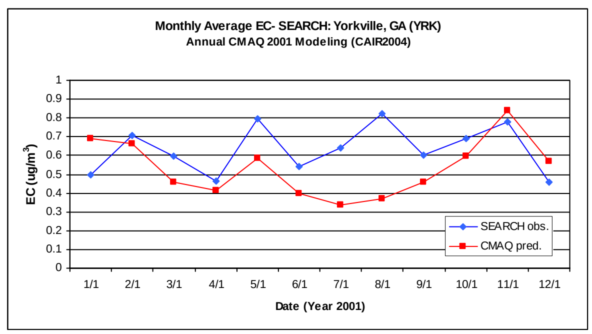


Figure D-21. Time-series analysis of annual nitrate (NO3) 2001 SEARCH observations versus CMAQ predictions.

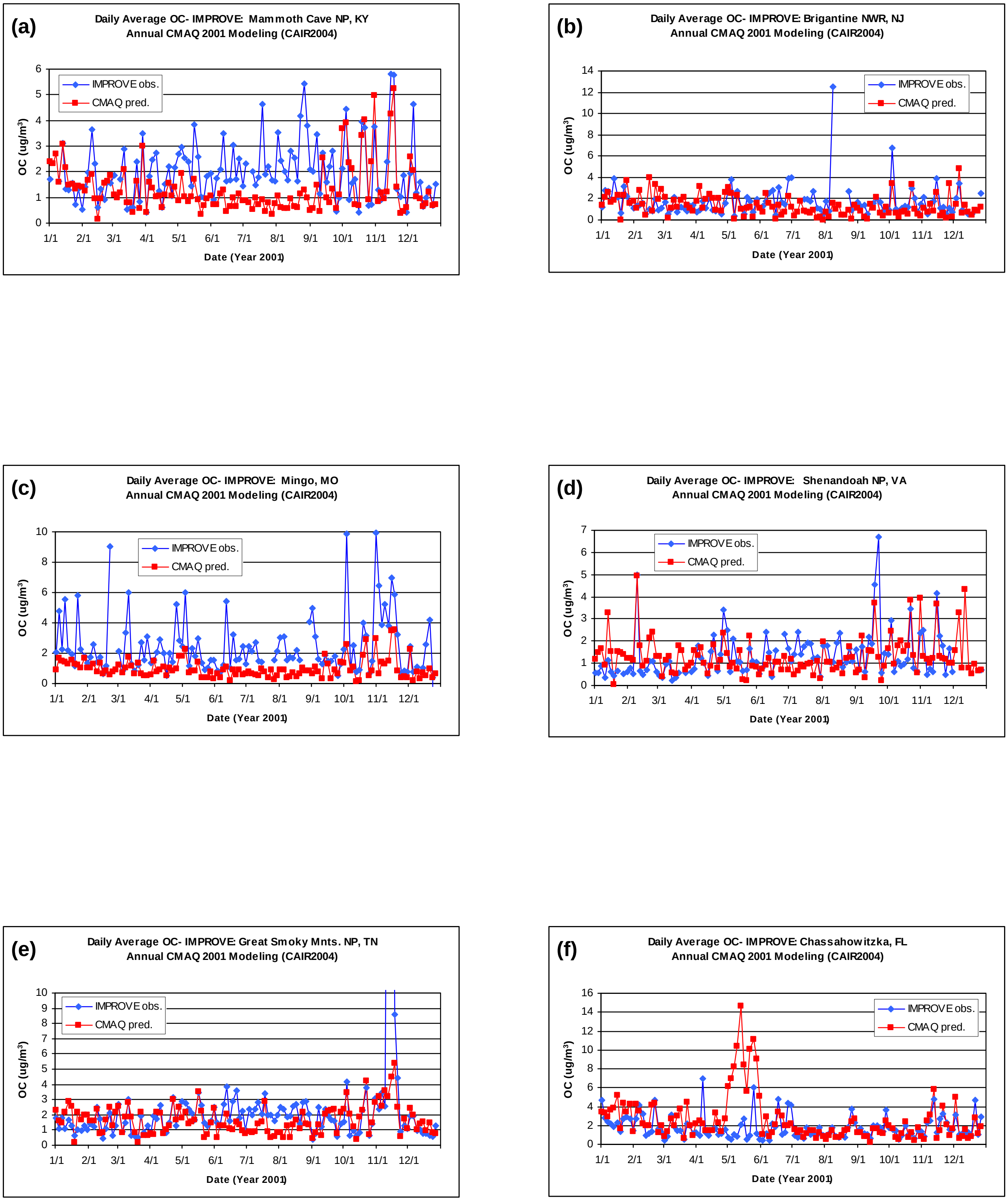


Figure D-22. Time-series analysis of annual organic carbon (OC) 2001 IMPROVE observations versus CMAQ predictions.

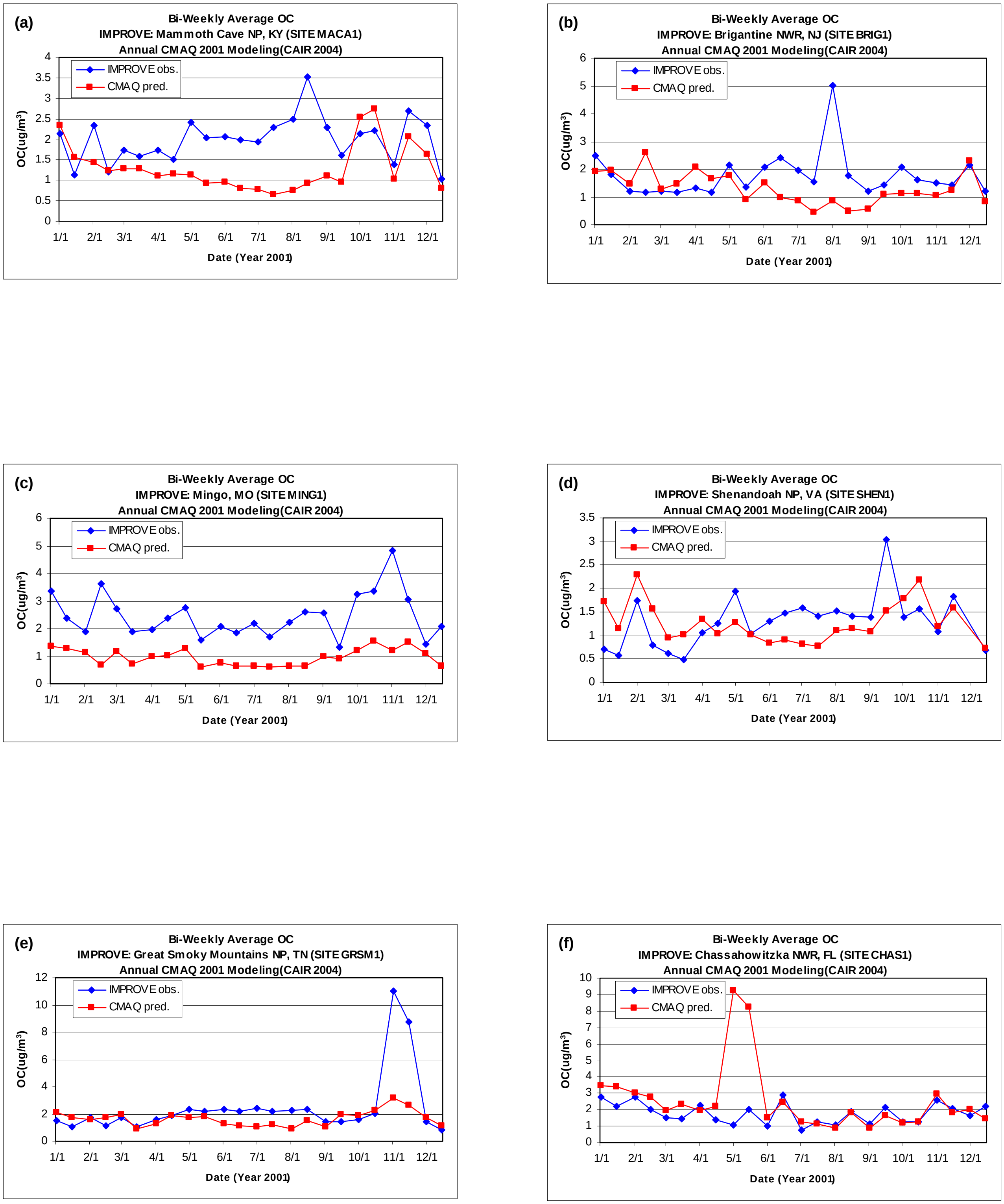


Figure D-23. Time-series analysis of annual organic carbon (OC) 2001 IMPROVE observations versus CMAQ predictions.

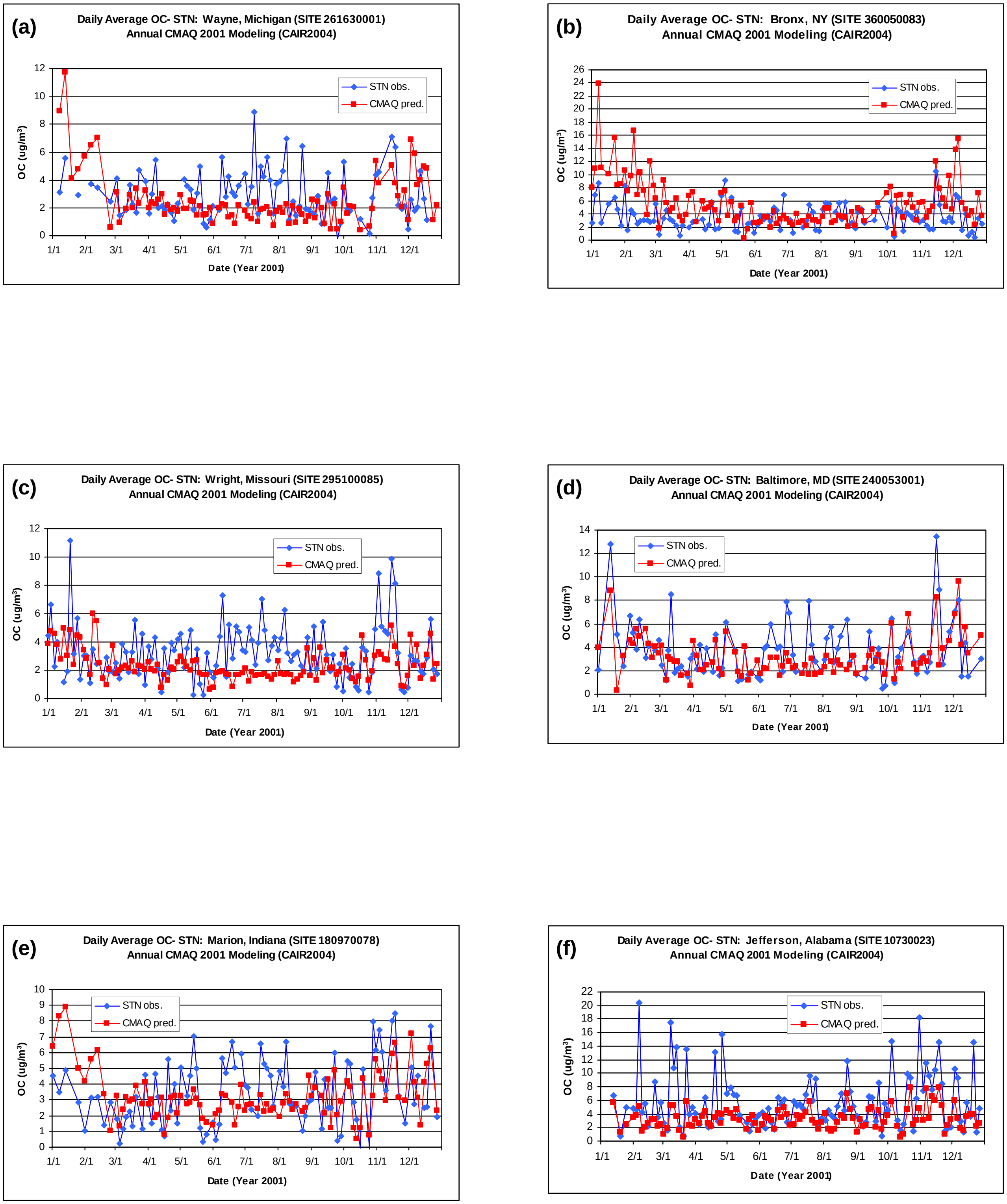


Figure D-24. Time-series analysis of annual organic carbon (OC) 2001 STN observations versus CMAQ predictions.

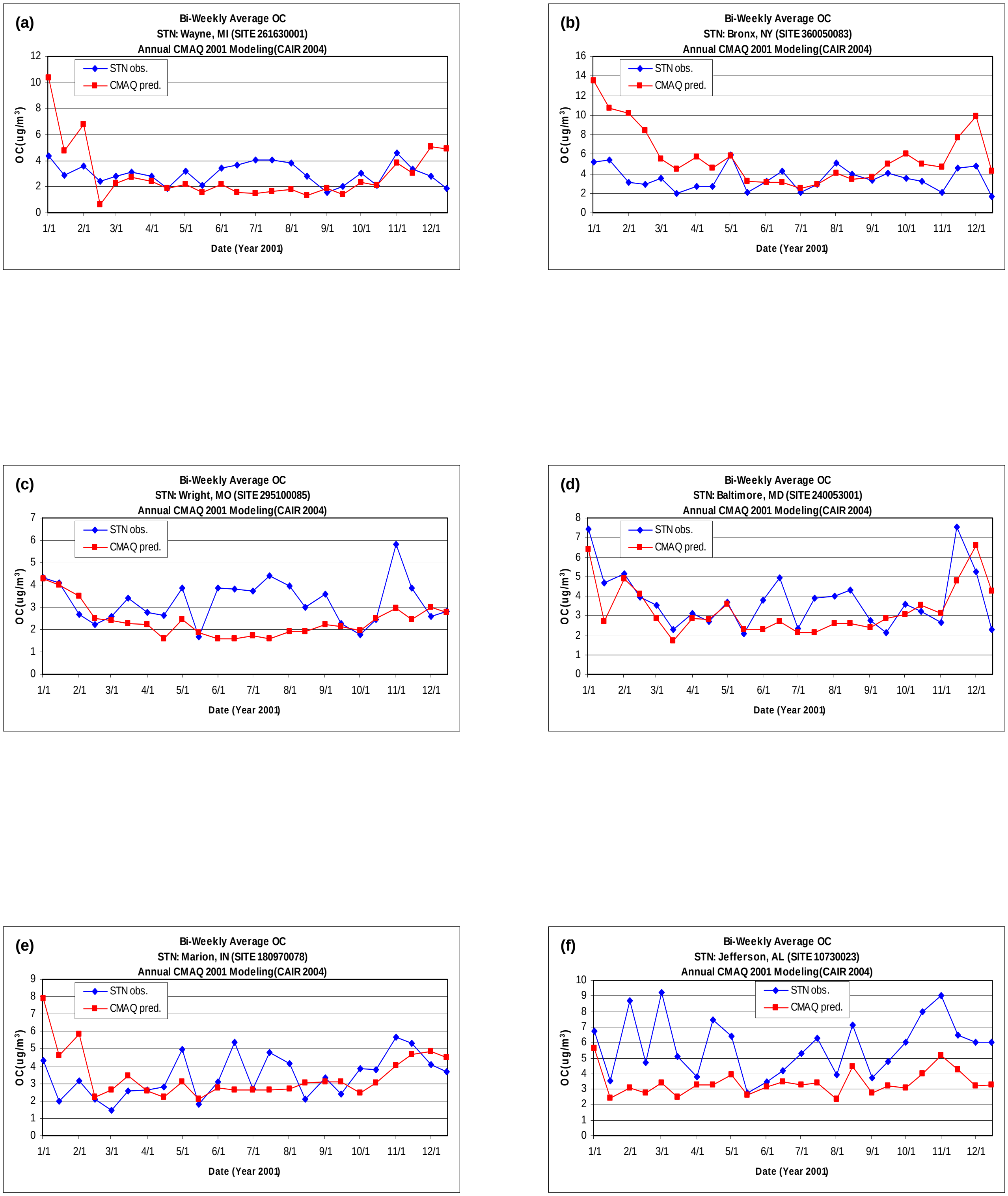
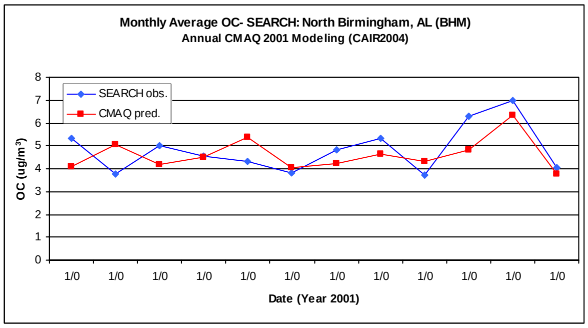
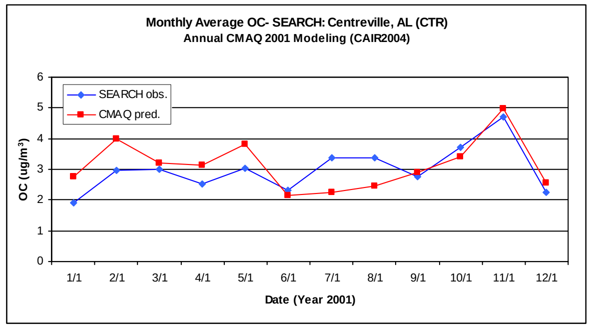
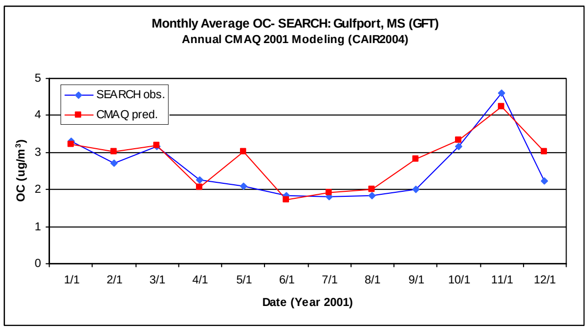
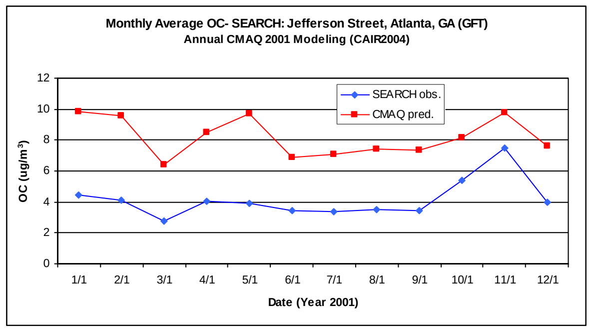


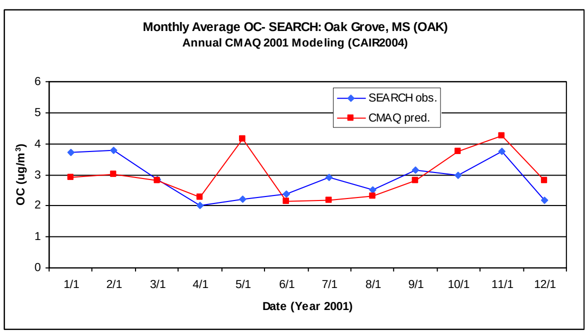
Figure D-25. Time-series analysis of annual organic carbon (OC) 2001 STN observations versus CMAQ predictions.











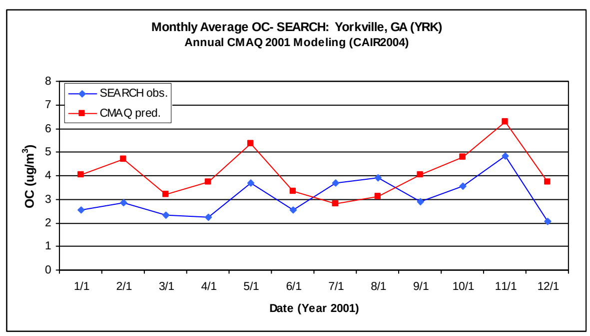


Figure D-26. Time-series analysis of annual nitrate (NO3) 2001 SEARCH observations versus CMAQ predictions.

CMAQ Model Performance Evaluation for 2001: Updated March 2005

Appendix E

Time Series Analysis of Gaseous Precursor Species :

CASTNet and SEARCH monitoring networks

conducted by

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Emissions Analysis and Monitoring Division
Air Quality Modeling Group
Research Triangle Park, NC 27711

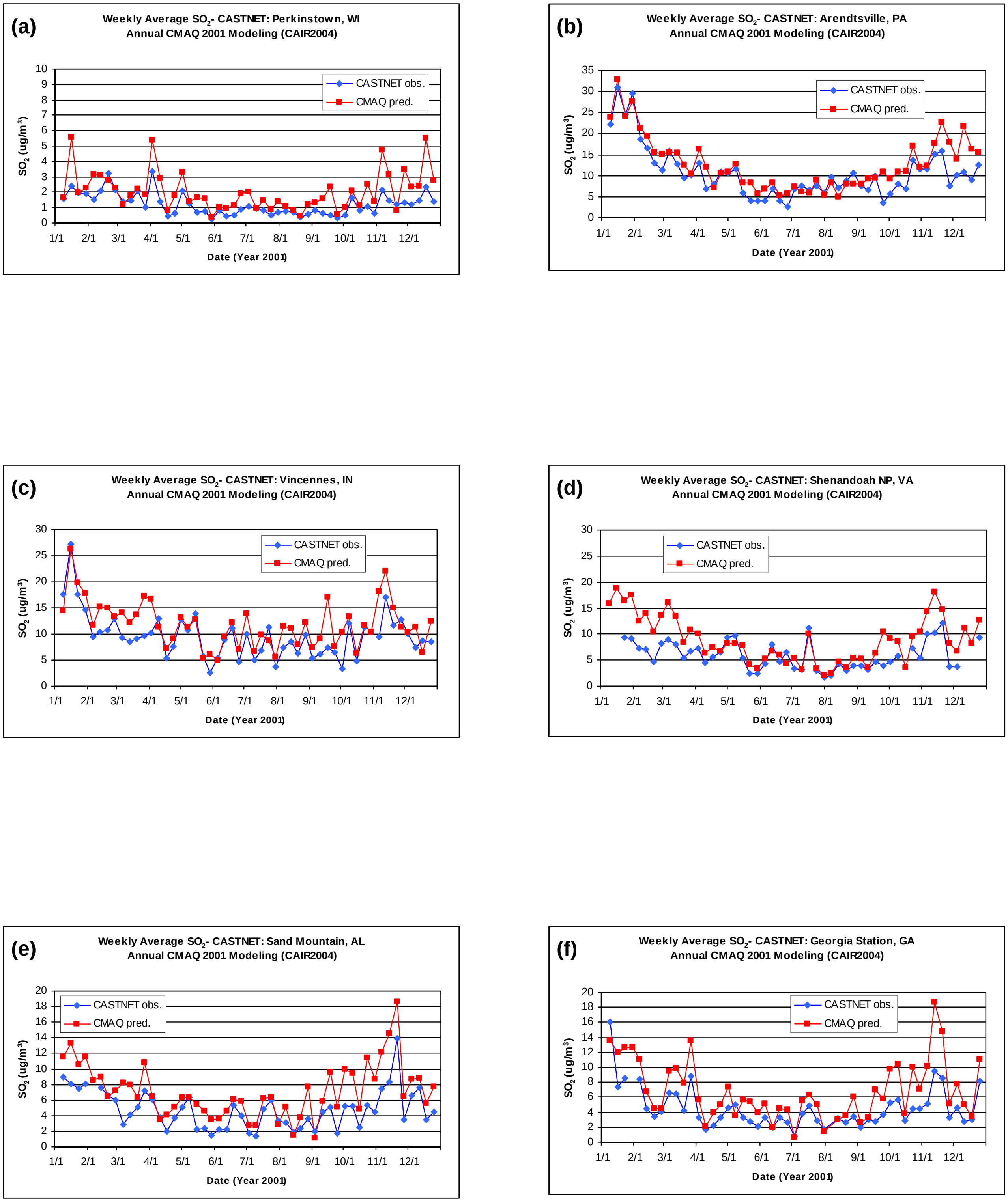


Figure E-1. Time-series analysis of annual sulfur dioxide (SO_2) 2001 CASTNet observations versus CMAQ predictions.

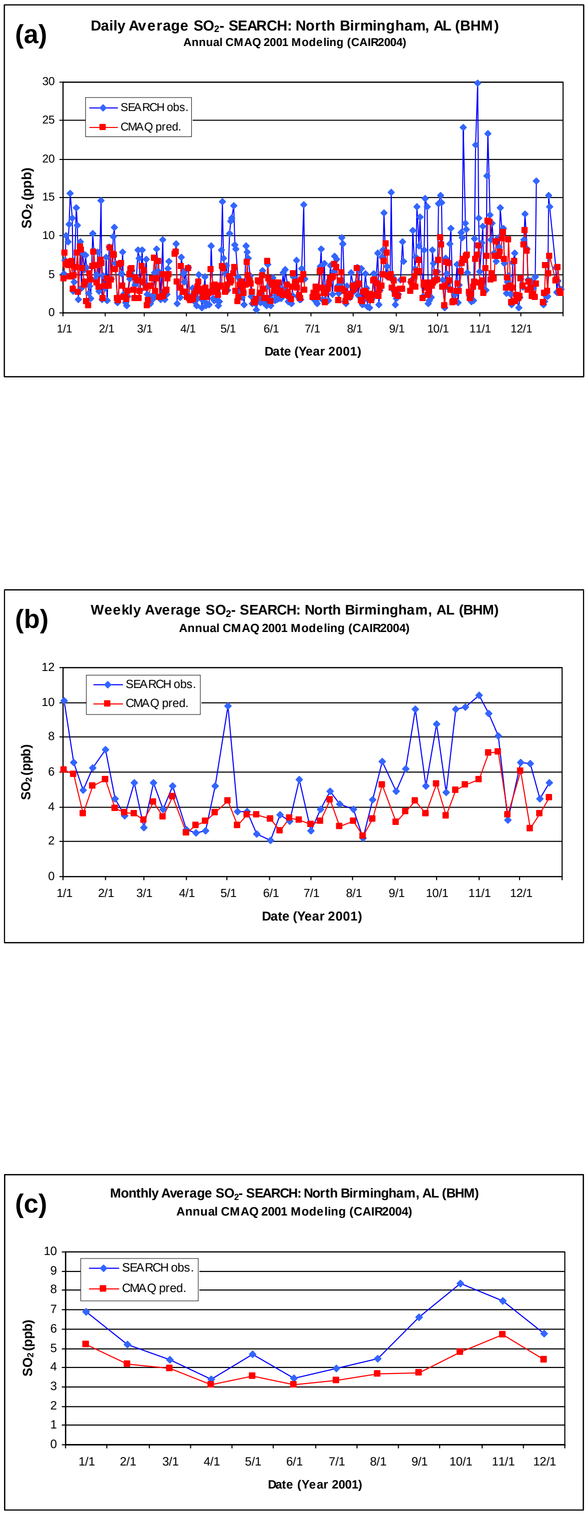


Figure E-2. Time-series analysis of annual sulfur dioxide (SO_2) 2001 SEARCH observations versus CMAQ predictions.

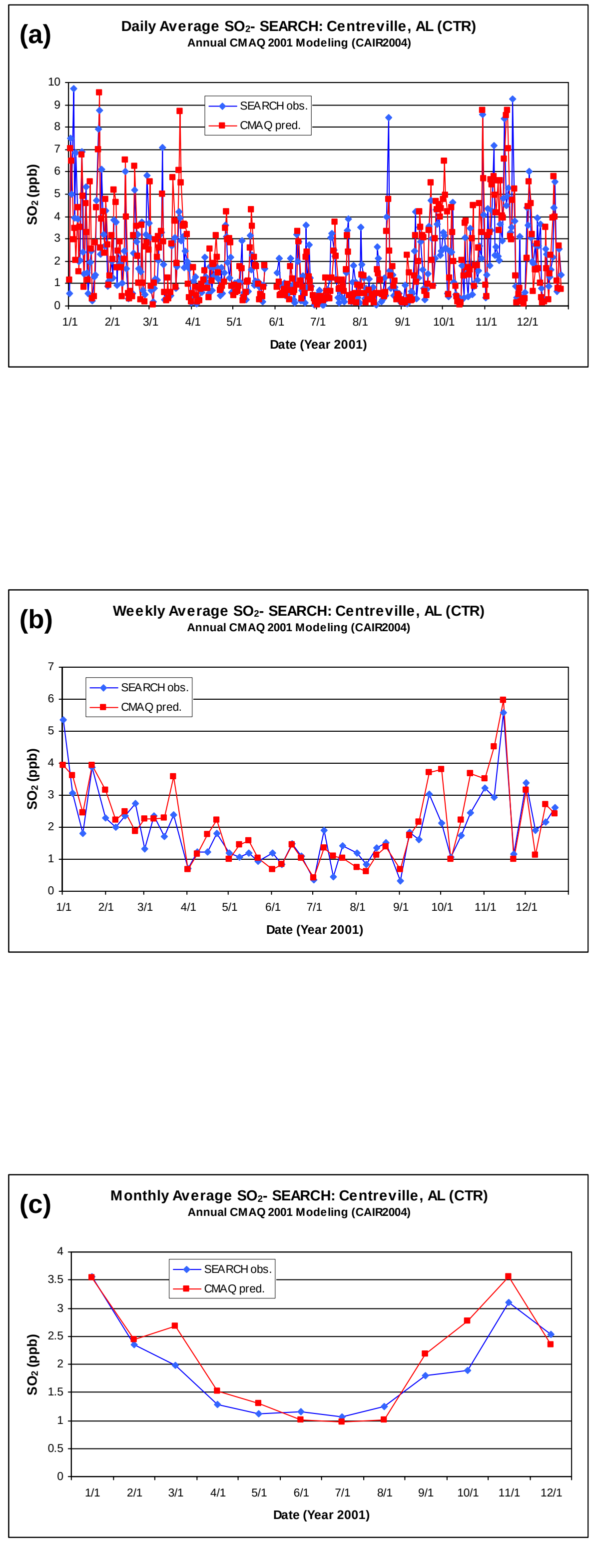


Figure E-3. Time-series analysis of annual sulfur dioxide (SO_2) 2001 SEARCH observations versus CMAQ predictions.

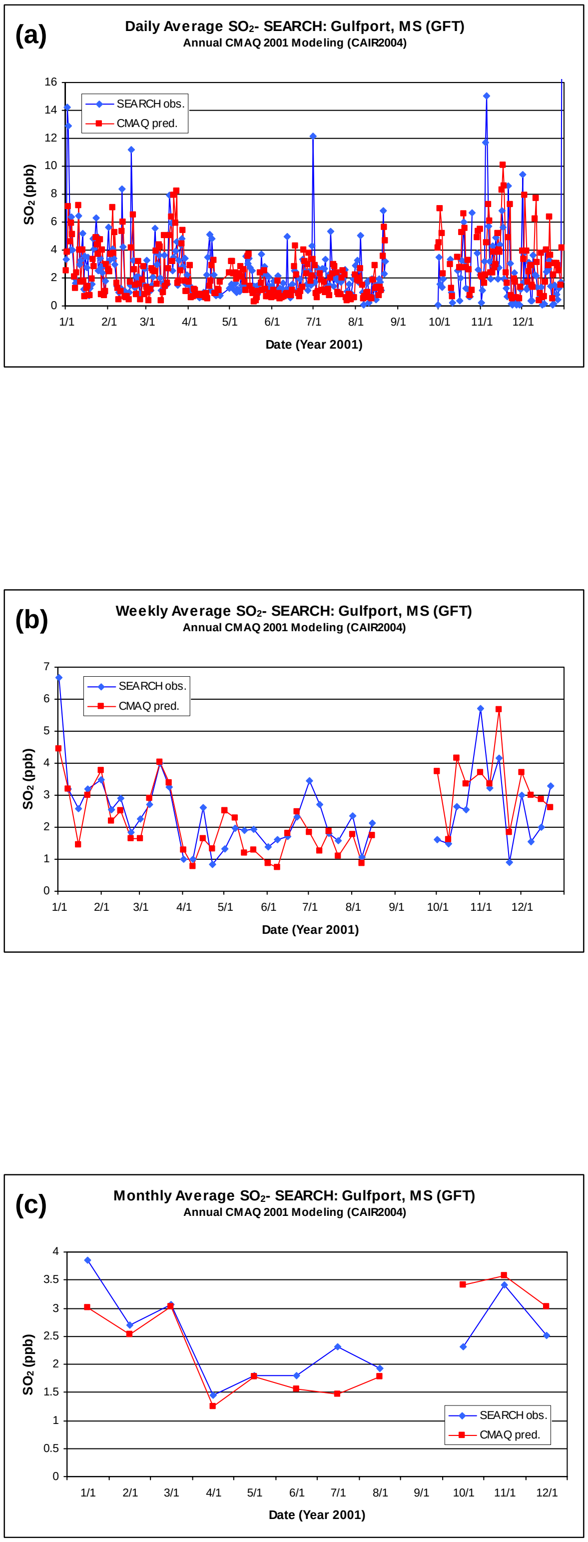


Figure E-4. Time-series analysis of annual sulfur dioxide (SO_2) 2001 SEARCH observations versus CMAQ predictions.

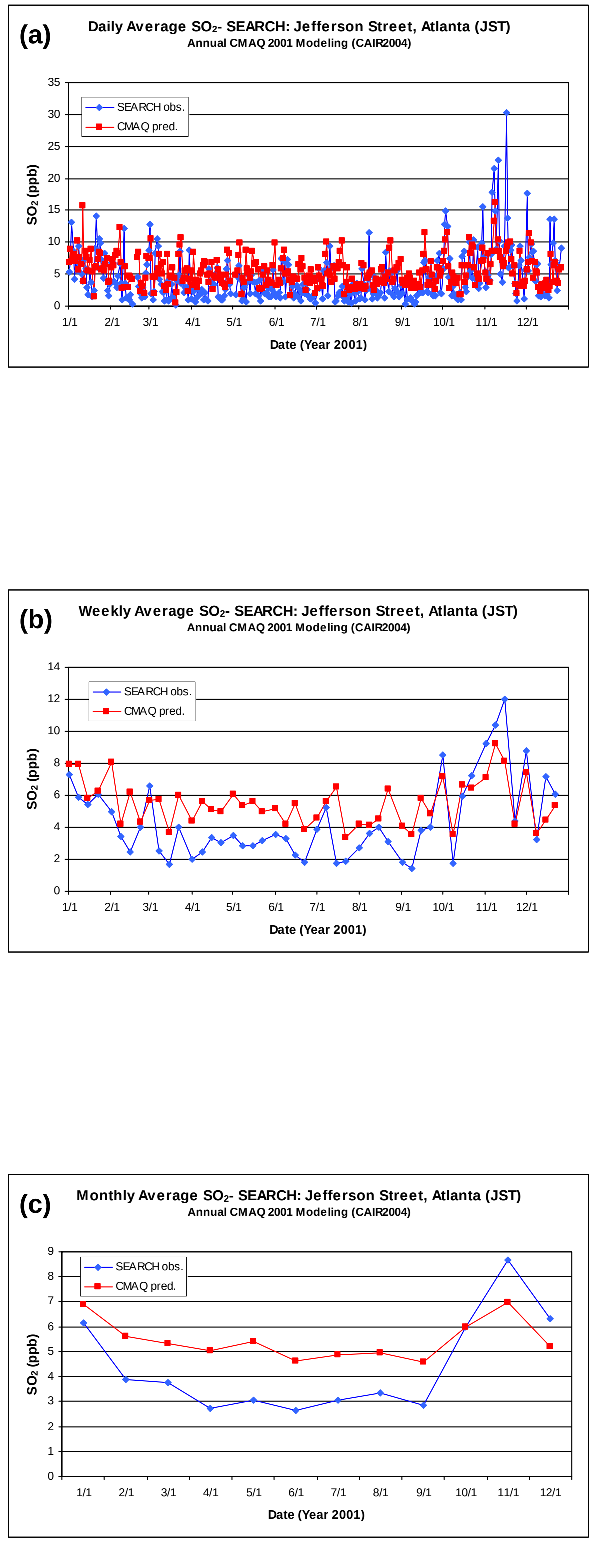


Figure E-5. Time-series analysis of annual sulfur dioxide (SO_2) 2001 SEARCH observations versus CMAQ predictions.

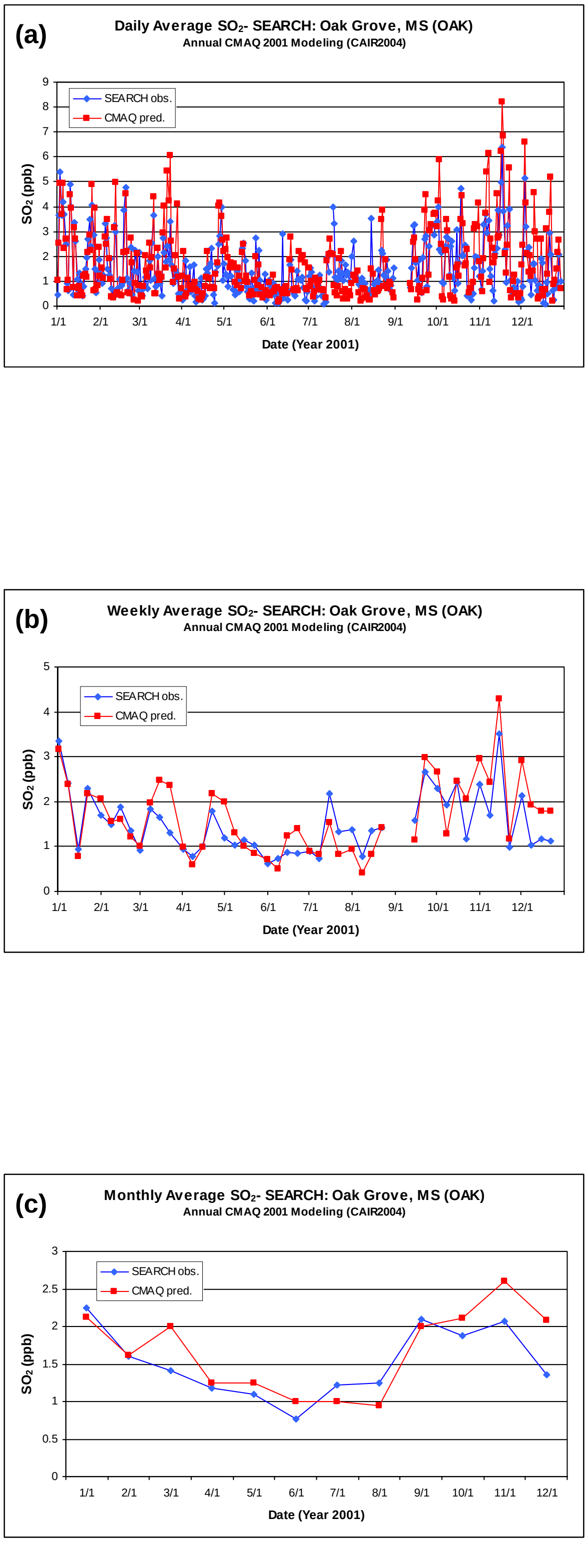


Figure E-6. Time-series analysis of annual sulfur dioxide (SO_2) 2001 SEARCH observations versus CMAQ predictions.

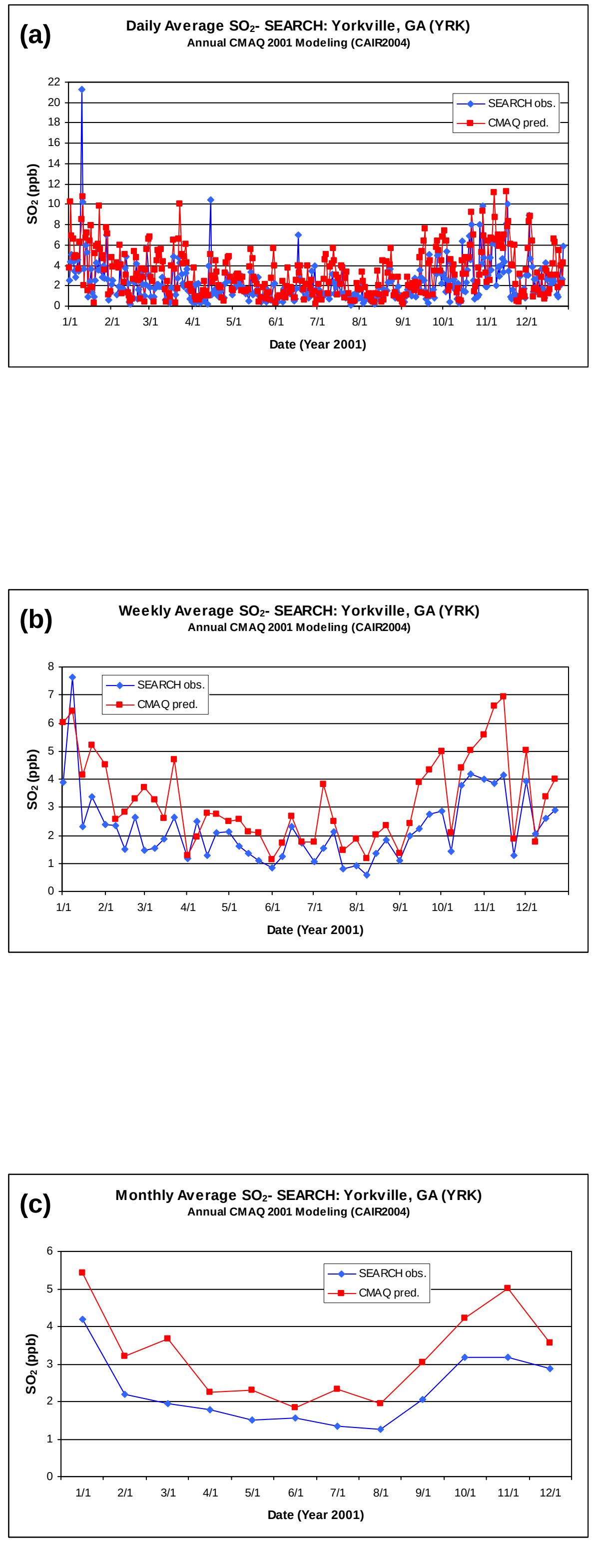


Figure E-7. Time-series analysis of annual sulfur dioxide (SO_2) 2001 SEARCH observations versus CMAQ predictions.

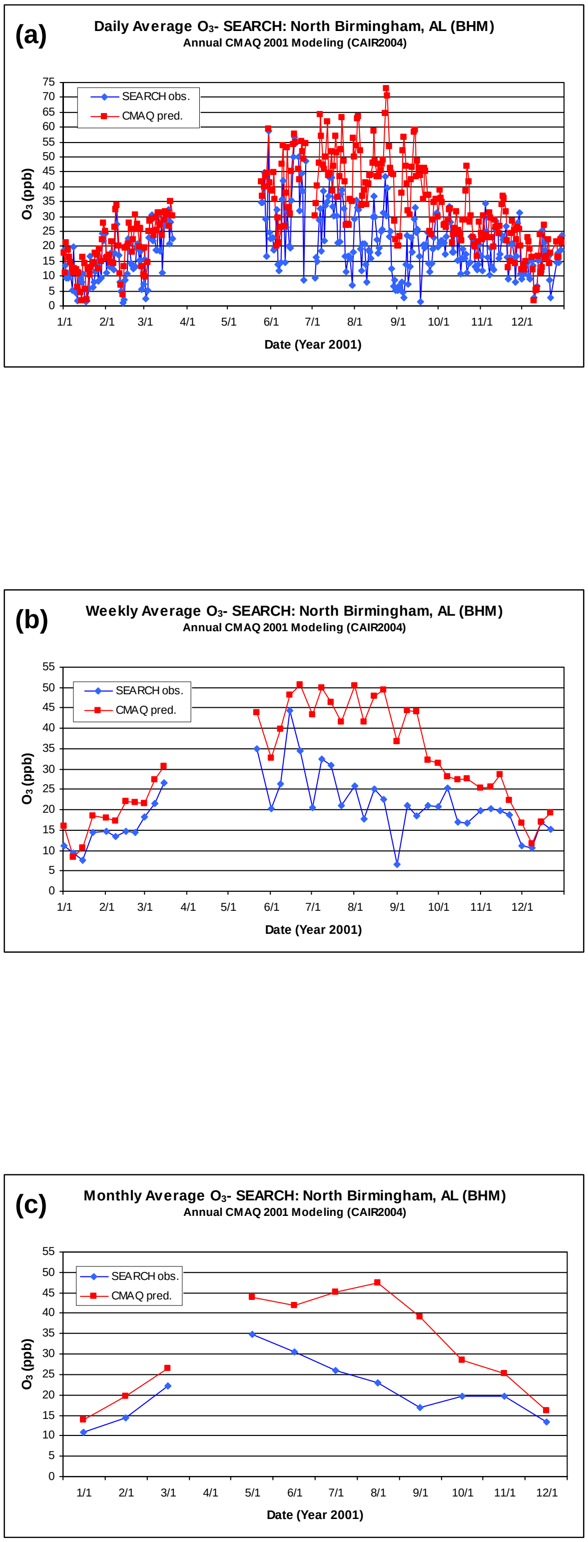


Figure E-8. Time-series analysis of annual ozone (O_3) 2001 SEARCH observations versus CMAQ predictions.

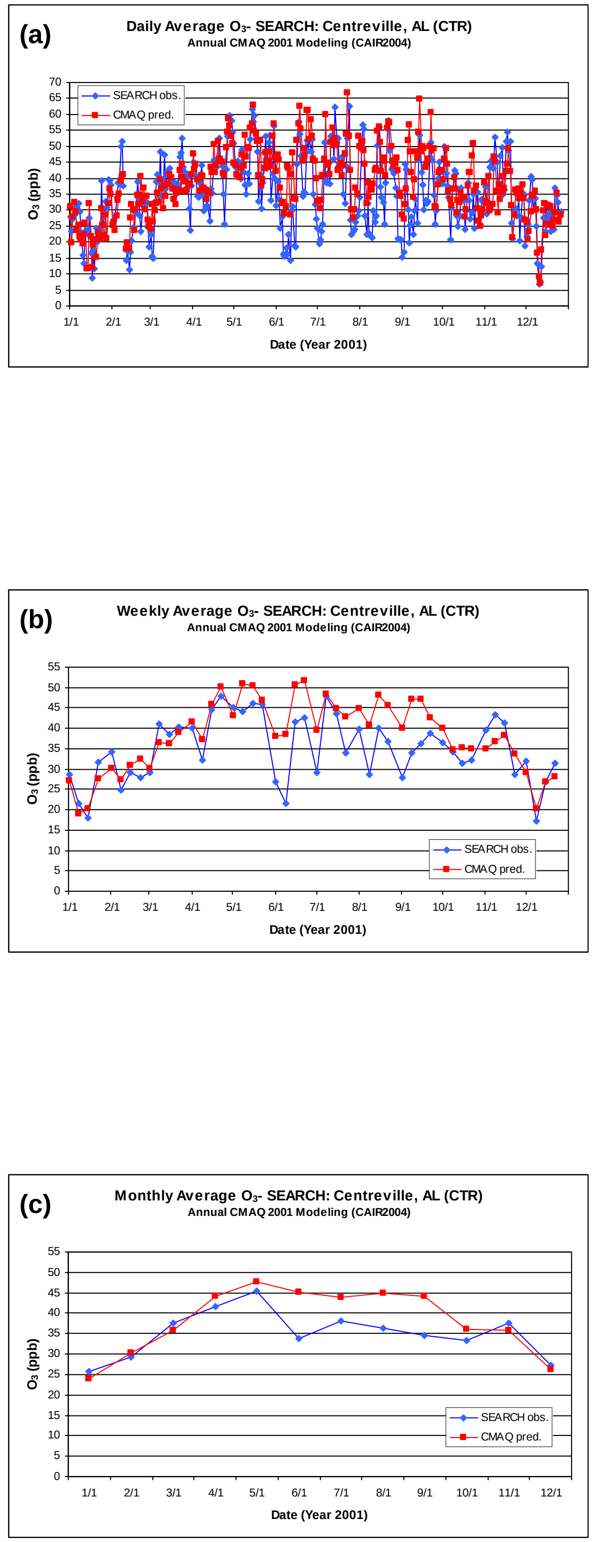


Figure E-9. Time-series analysis of annual ozone (O_3) 2001 SEARCH observations versus CMAQ predictions.

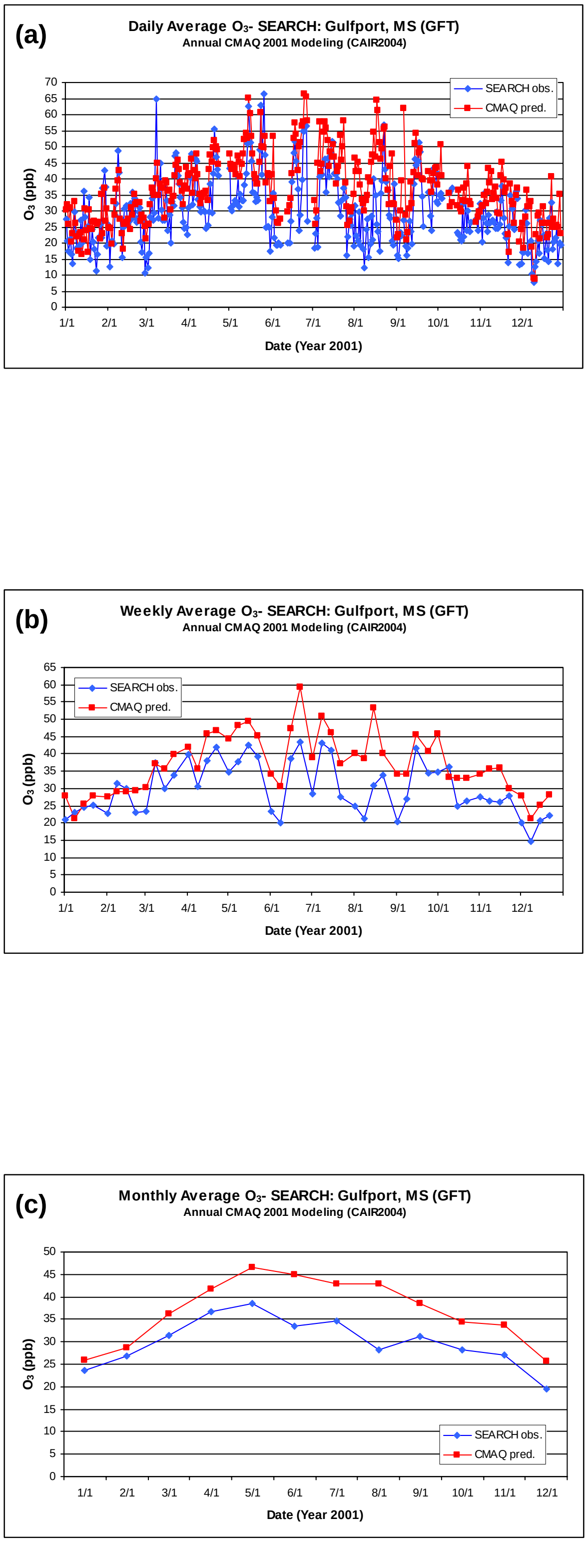


Figure E-10. Time-series analysis of annual ozone (O_3) 2001 SEARCH observations versus CMAQ predictions.

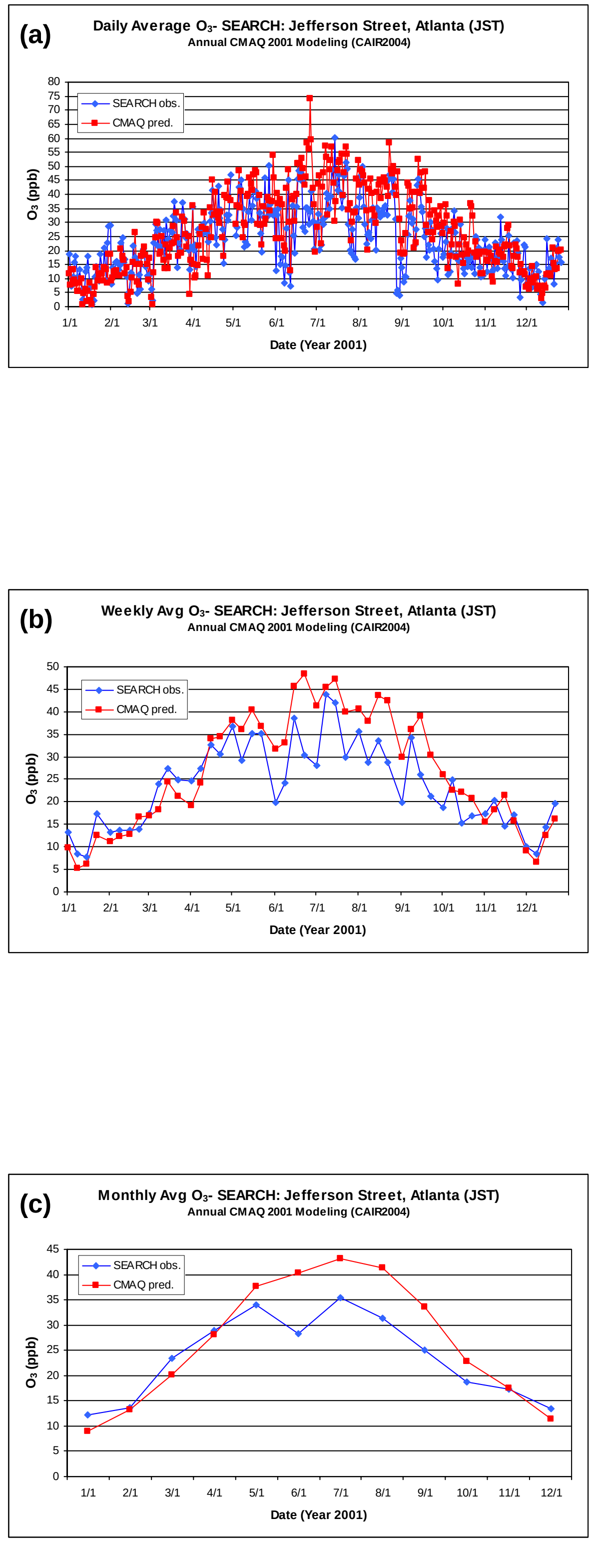


Figure E-11. Time-series analysis of annual ozone (O_3) 2001 SEARCH observations versus CMAQ predictions.

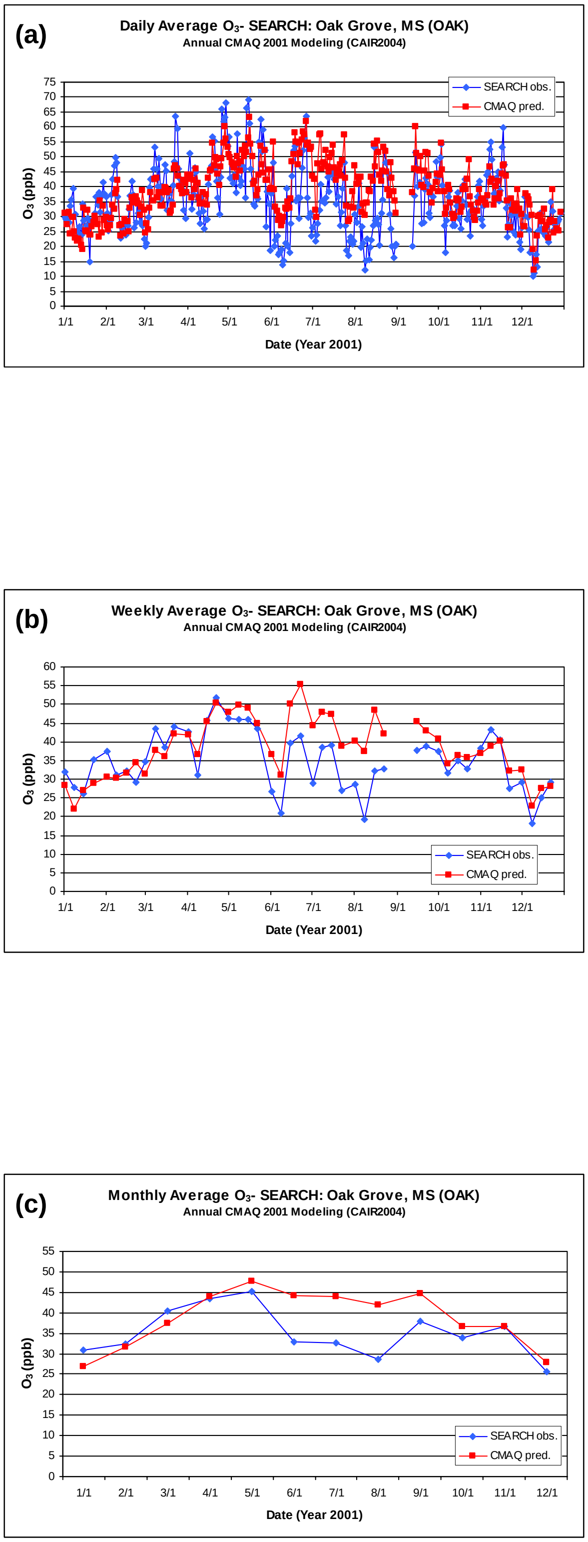


Figure E-12. Time-series analysis of annual ozone (O_3) 2001 SEARCH observations versus CMAQ predictions.

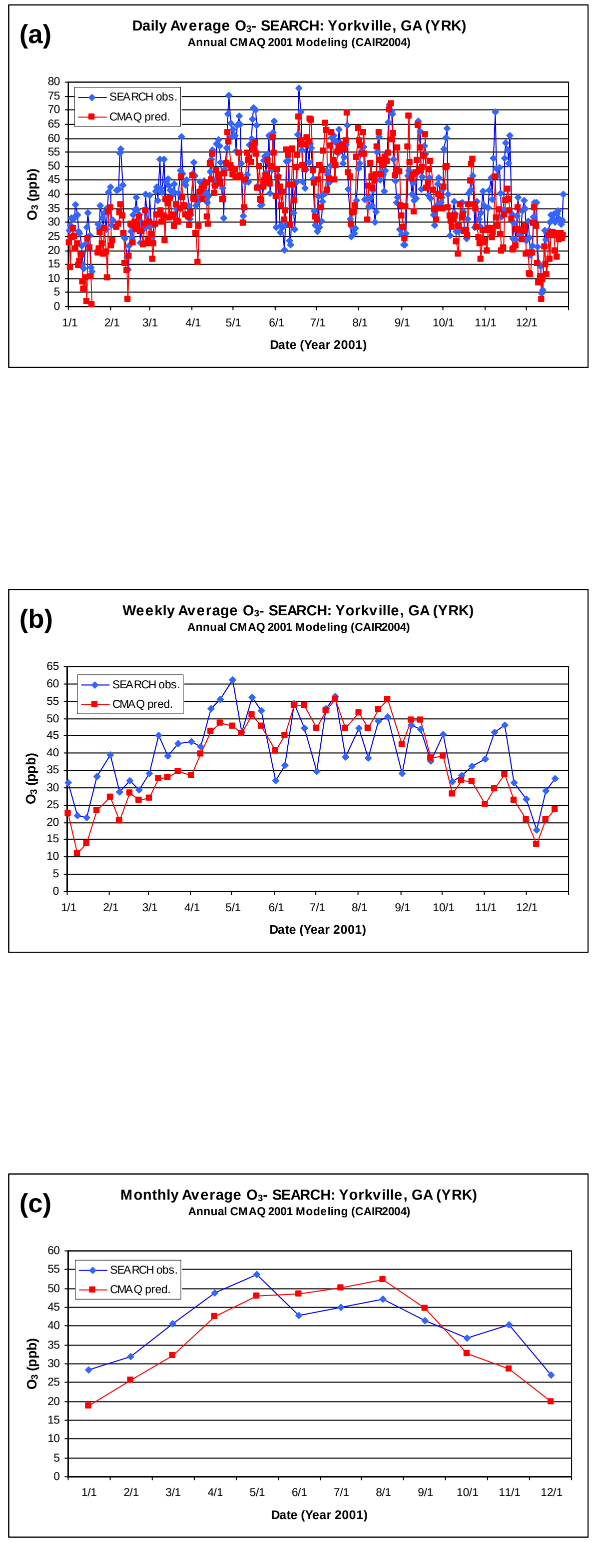


Figure E-13. Time-series analysis of annual ozone (O_3) 2001 SEARCH observations versus CMAQ predictions.

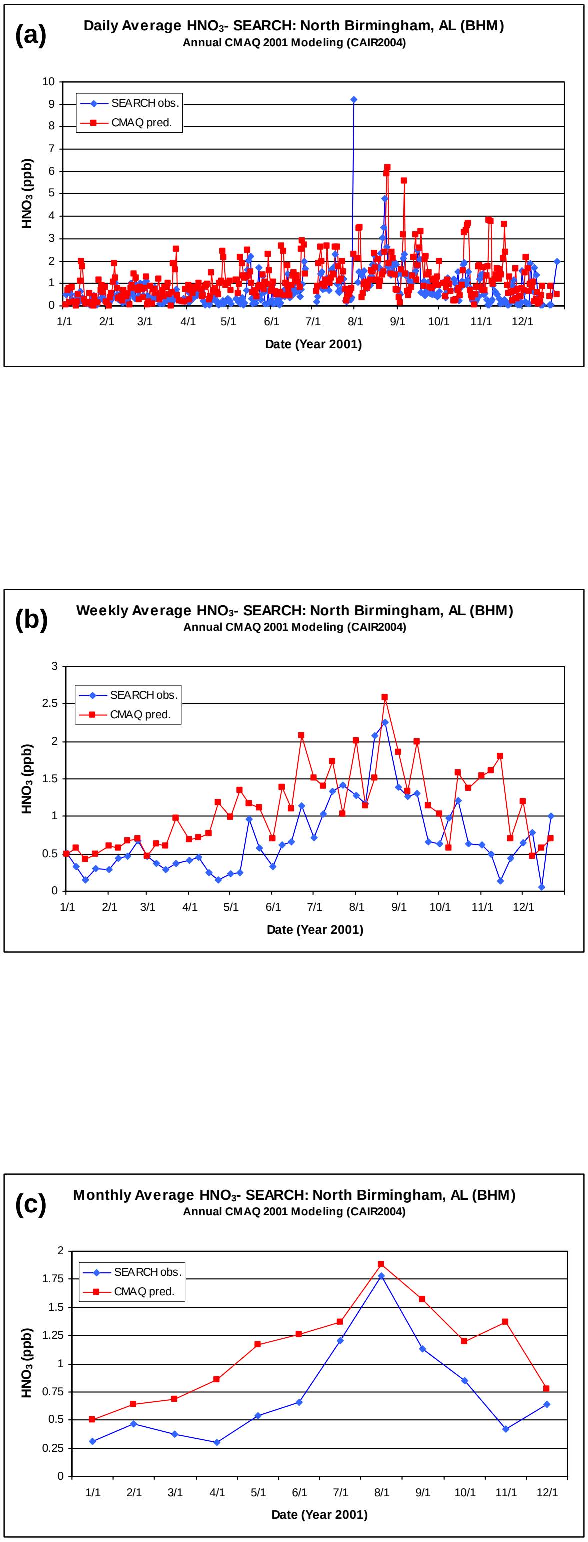


Figure E-14. Time-series analysis of annual nitric acid 2001 SEARCH observations versus CMAQ predictions.

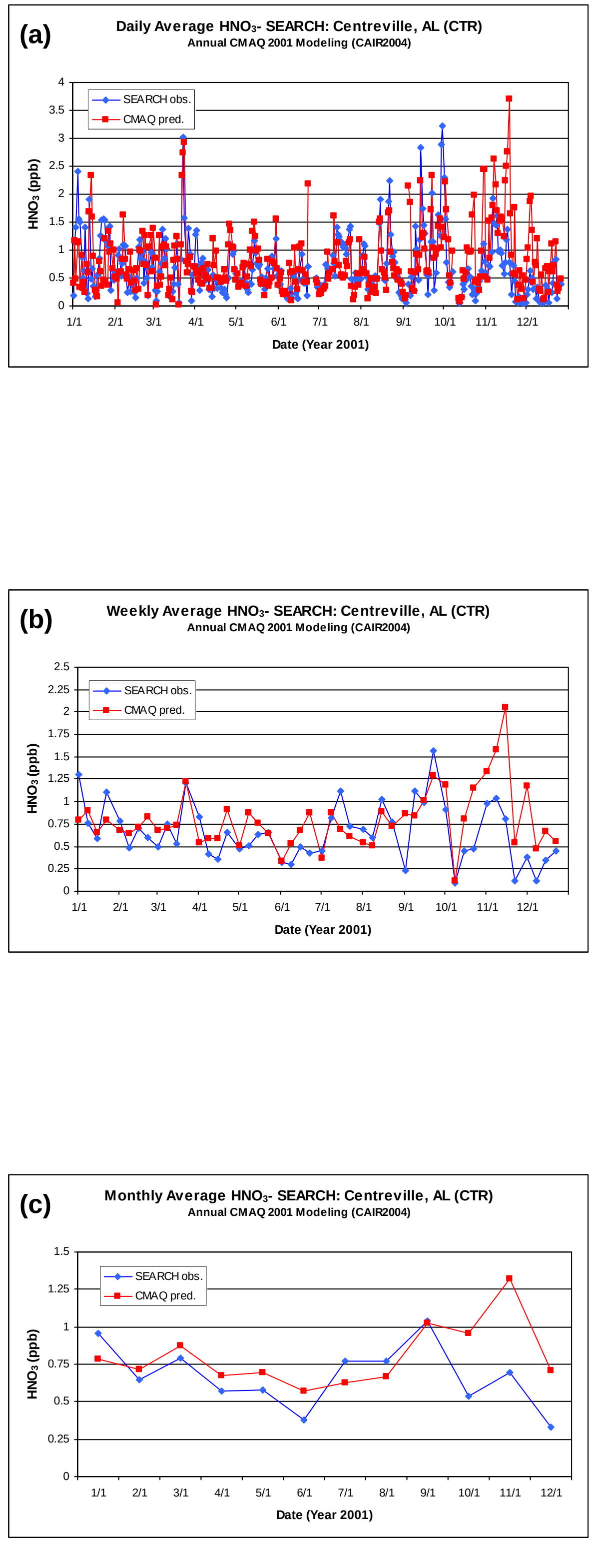


Figure E-15. Time-series analysis of annual nitric acid 2001 SEARCH observations versus CMAQ predictions.

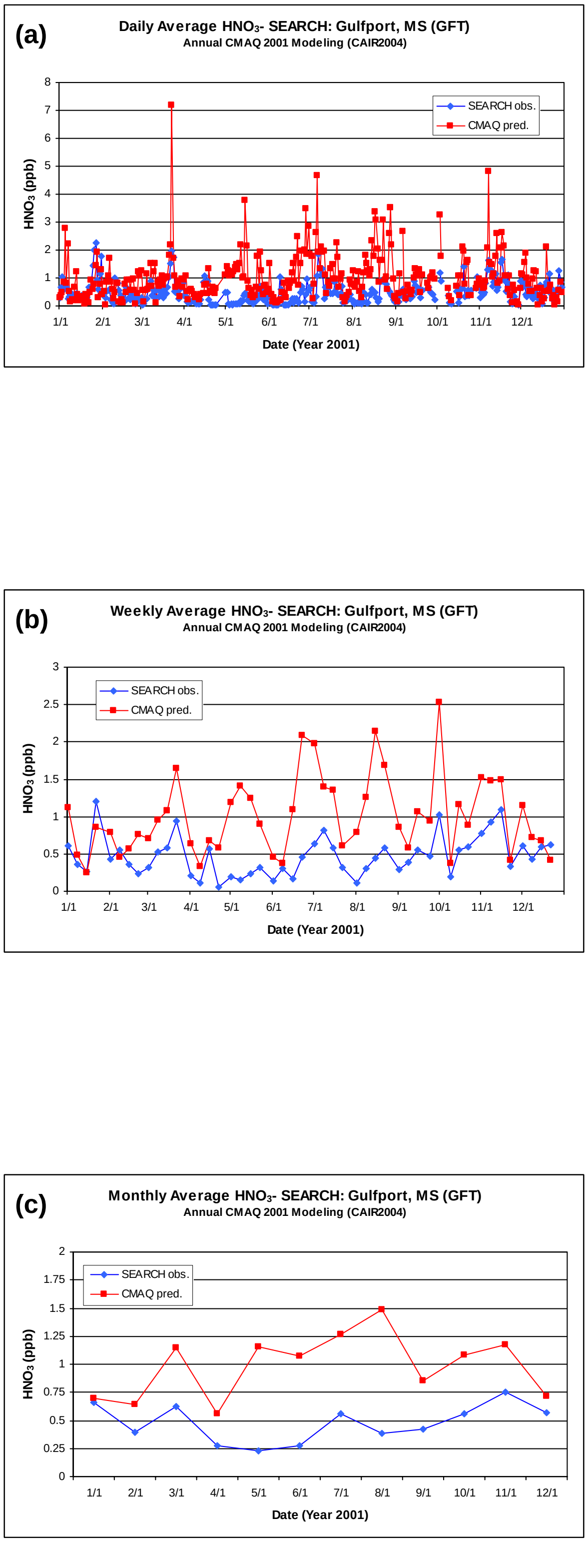


Figure E-16. Time-series analysis of annual nitric acid 2001 SEARCH observations versus CMAQ predictions.

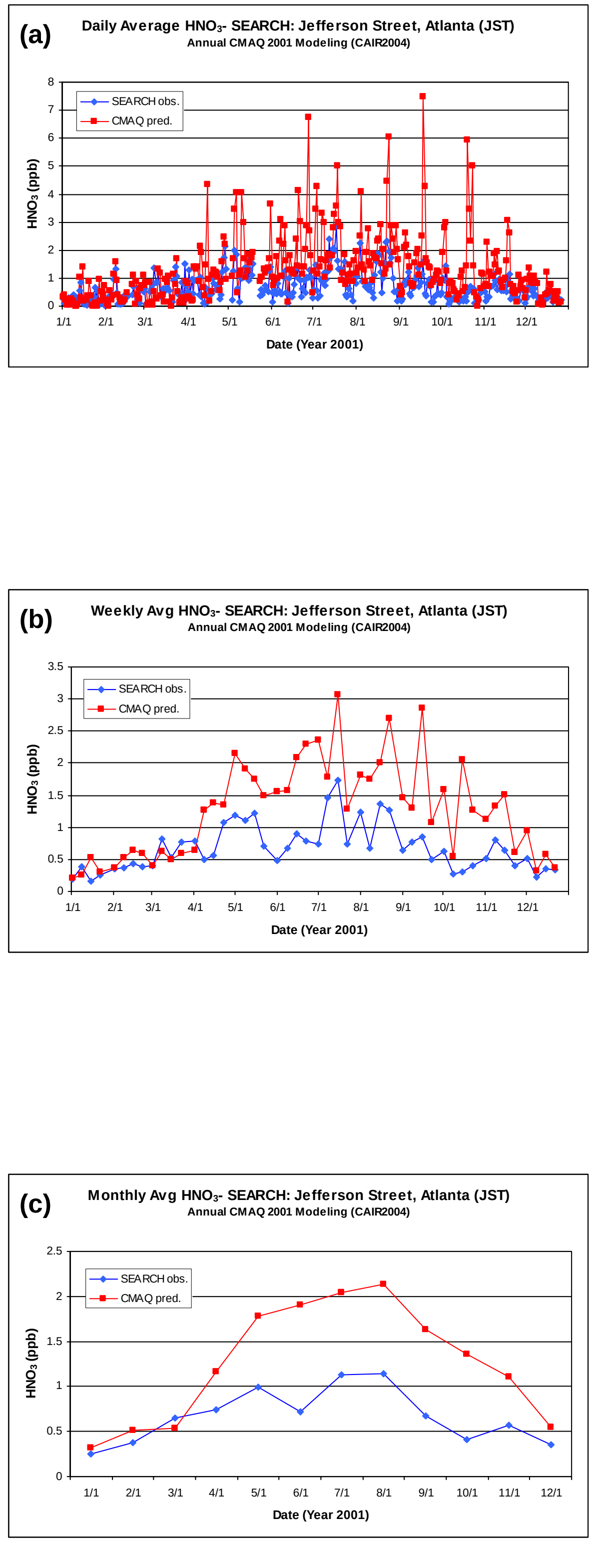
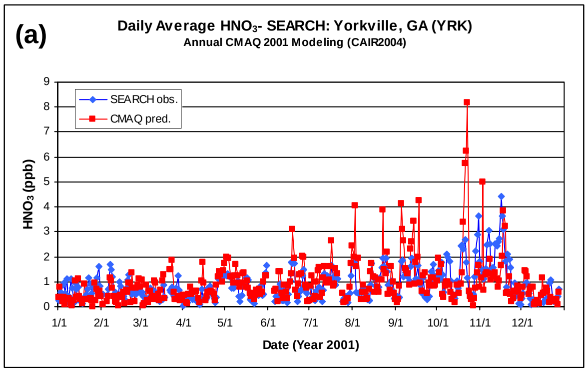
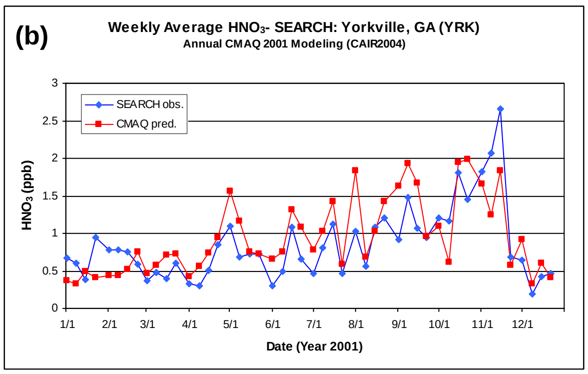


Figure E-17. Time-series analysis of annual nitric acid 2001 SEARCH observations versus CMAQ predictions.





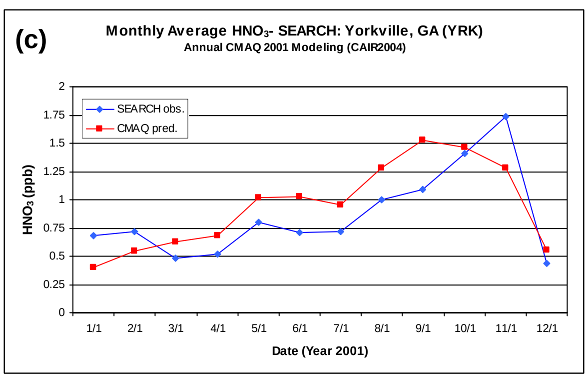


Figure E-18. Time-series analysis of annual nitric acid 2001 SEARCH observations versus CMAQ predictions.

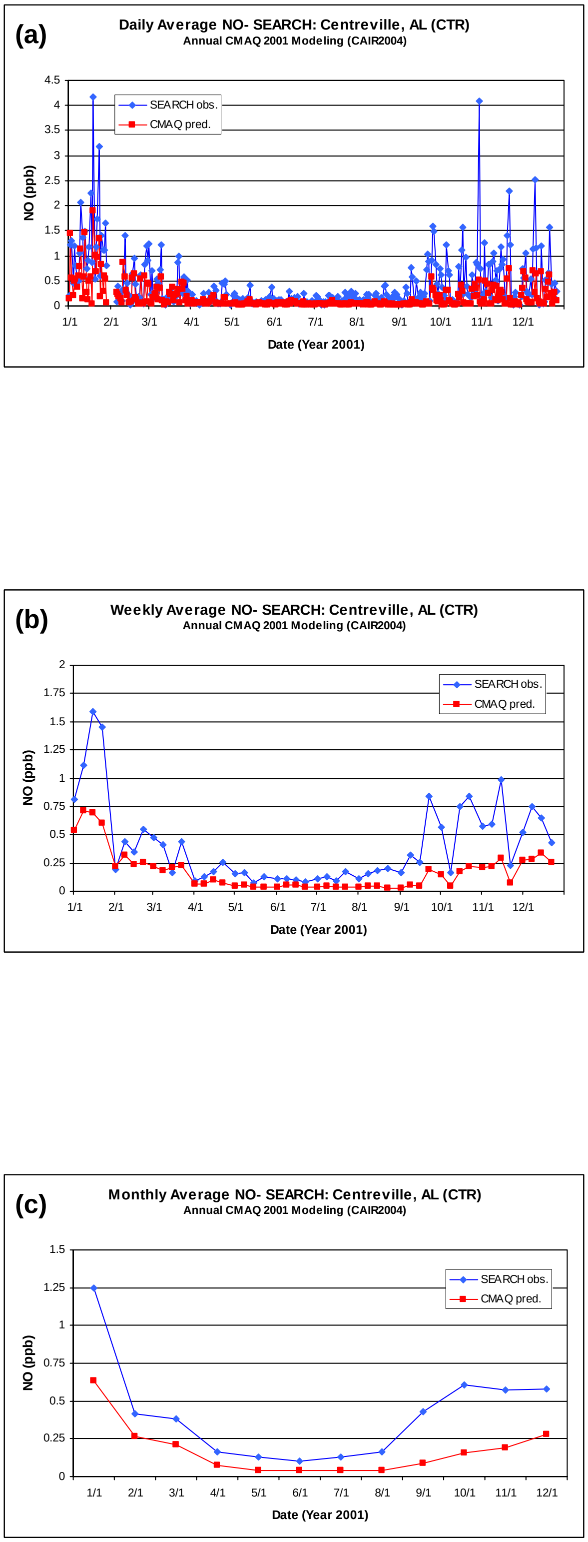


Figure E-19. Time-series analysis of annual nitric oxide (NO) 2001 SEARCH observations versus CMAQ predictions.

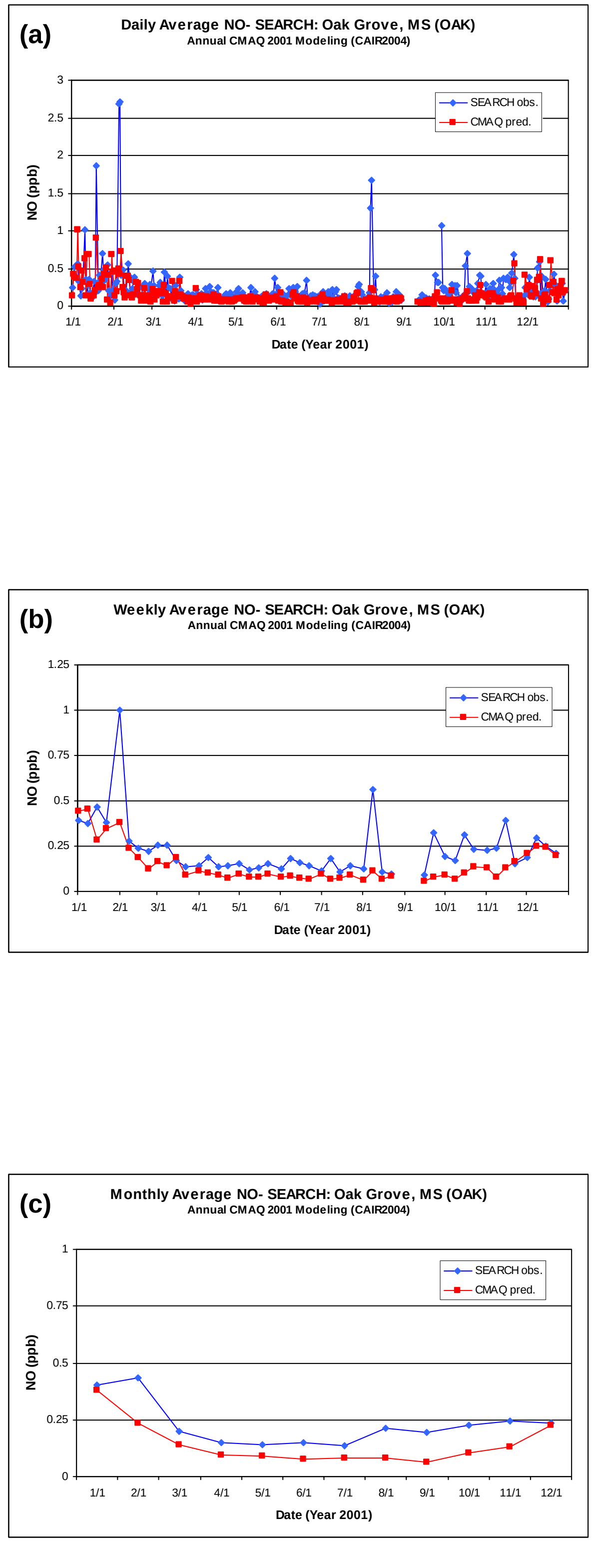
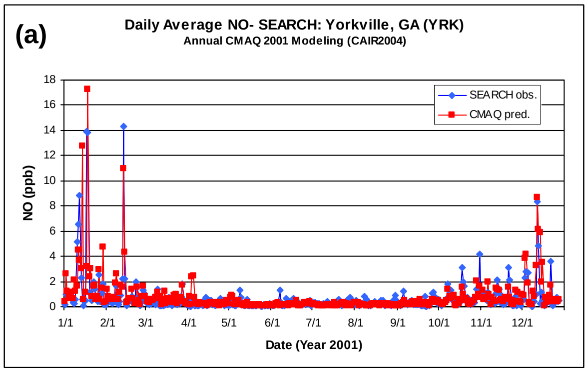
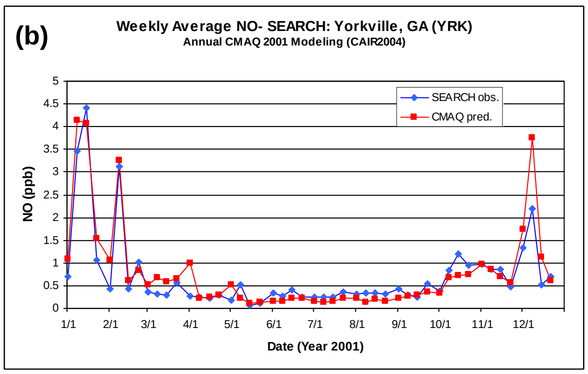


Figure E-20. Time-series analysis of annual nitric oxide (NO) 2001 SEARCH observations versus CMAQ predictions.





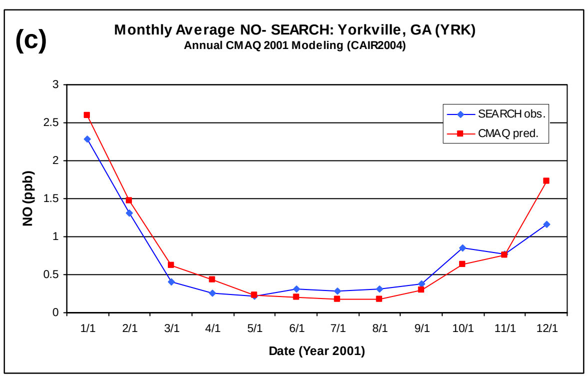


Figure E-21. Time-series analysis of annual nitric oxide (NO) 2001 SEARCH observations versus CMAQ predictions.