APPENDIX C

Model Performance Evaluation for the CMAQ 2002 Base F Base Case Simulation in the CENRAP Region

C.1 2002 Typical Base F Model Performance Evaluation Scenario

This Appendix presents the operational evaluation of the CMAQ model for the 2002 36 km Typical Base F emissions scenario. The final CENRAP 2002 and 2018 emissions scenarios used in the 2018 visibility projections was Base G. The main differences between Base G and Base F emissions inventories were updated Mexican emissions in the northern states, addition of Mexican emissions in the southern states that were not included in CENRAP's emission inventories prior to Base G and correction of a few point source stack parameters and emissions in the CENRAP states and Canada (see: http://pah.cert.ucr.edu/aqm/cenrap/QA_typ02g36.plots/log_inv_categ_Typ02g.doc). Figure C-1 displays the differences in annual average $PM_{2.5}$ and ozone concentrations between the 2002 Typical Base G and Base F simulations. Most of the differences in the two simulations are concentrations within Mexico where no monitoring data were available for the model evaluation. Thus, given the very small differences between the 2002 Typical Base F and G base case simulations, the model performance evaluation is presented for just the 2002 Typical Base F simulation (for additional comparisons of Base G and F see: http://pah.cert.ucr.edu/aqm/cenrap/cmaq.shtml#typ02gvstyp02f_mpe).

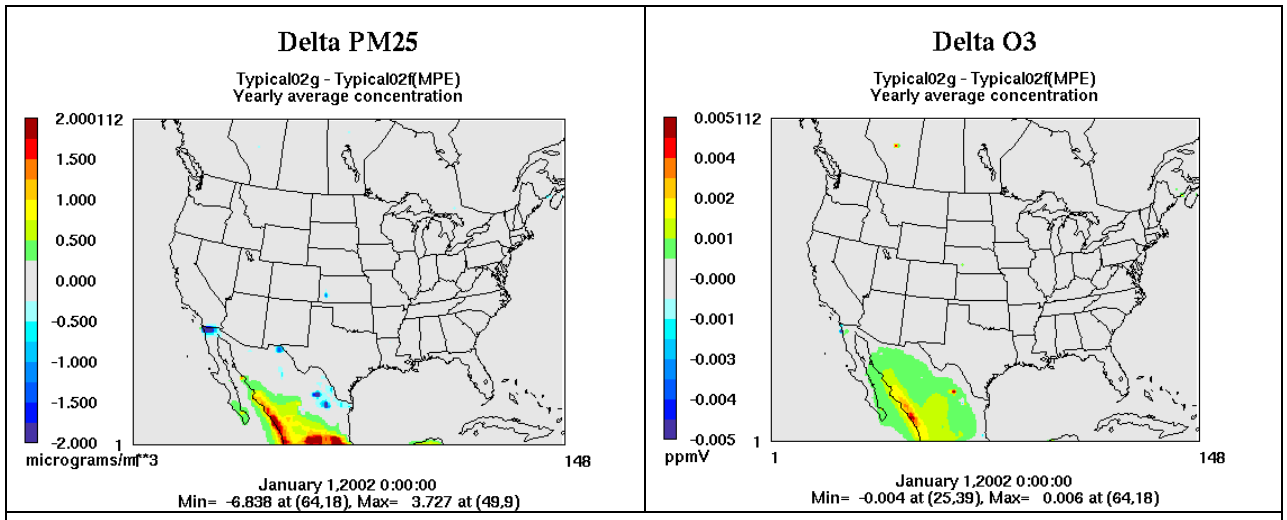


Figure C-1. Comparison of differences in annual average $PM_{2.5}$ (left) and ozone concentrations between 2002 Typical Base G and F (Base G – Base F).

The CENRAP emissions and air quality modeling initially conducted 2002 base case modeling for two 2002 base case emissions scenarios: a 2002 Actual emissions base case; and a 2002 Typical emissions base case. For the 2002 Actual base case, day-specific SO2 and NOx emissions for large stationary point sources were used based on measured continuous emissions monitoring (CEM) data along with actual 2002 fire emissions In the 2002 Typical base case, emissions for large stationary sources and fires were more representative of the 2000-2004 Baseline period. For large stationary sources' typical emissions, 5-years of CEM data were analyzed and typical seasonal and diurnally varying emissions were defined for when the sources where operating For the typical fire emissions, the locations of the 2002 Actual fire emissions were retained, but the intensity was reduced or increased to match the average conditions over the 5-year Baseline. The original intent of the CENRAP modeling of both a 2002 Actual and Typical base cases was to use the 2002 Actual base case for the model performance evaluation and the 2002 Typical base case with the 2018 emission scenario for the 2018 visibility projections.

The need to generate both the 2002 Typical and Actual base case inventories and perform CMAQ model simulations each time an emissions update or correction to the modeling occurred became burdensome and potentially could compromise the CENRAP schedule and available resources. For the Base F vintage emissions database, a model performance evaluation was conducted that compared the model performance of the 2002 Actual and Typical Base F CMAQ base case simulations to determine whether use of the Actual emissions substantially changed the interpretation of the model performance. The maximum change in model performance between the 2002 Actual and Typical base case was for sulfate and occurred during the summer months, when sulfate is the highest. Figure C-2 displays sulfate (SO4), nitrate (NO3), elemental carbon (EC) and organic matter carbon (OMC) performance for July 2002 across IMPROVE sites in the CENRAP region for the 2002 36 km Actual and Typical Base F CMAQ base case simulations. Although differences in predicted 24-hour SO4 concentrations are sometimes discernable in the scatter plot, the basic model performance conclusions remains the same and the difference in fractional bias (-48% vs. -49%) and fraction error (58% vs. 59%) are not significant. Similarly, the difference in NO3 model performance between the Actual and Typical Base F simulations are not significant. The performance of the CMAQ Actual and Typical simulation for EC and OMC is essentially identical. Given the similarity of the 2002 Base F Actual and Typical model performance evaluation, future CENRAP CMAQ model performance analysis were just performed on the Typical simulation.

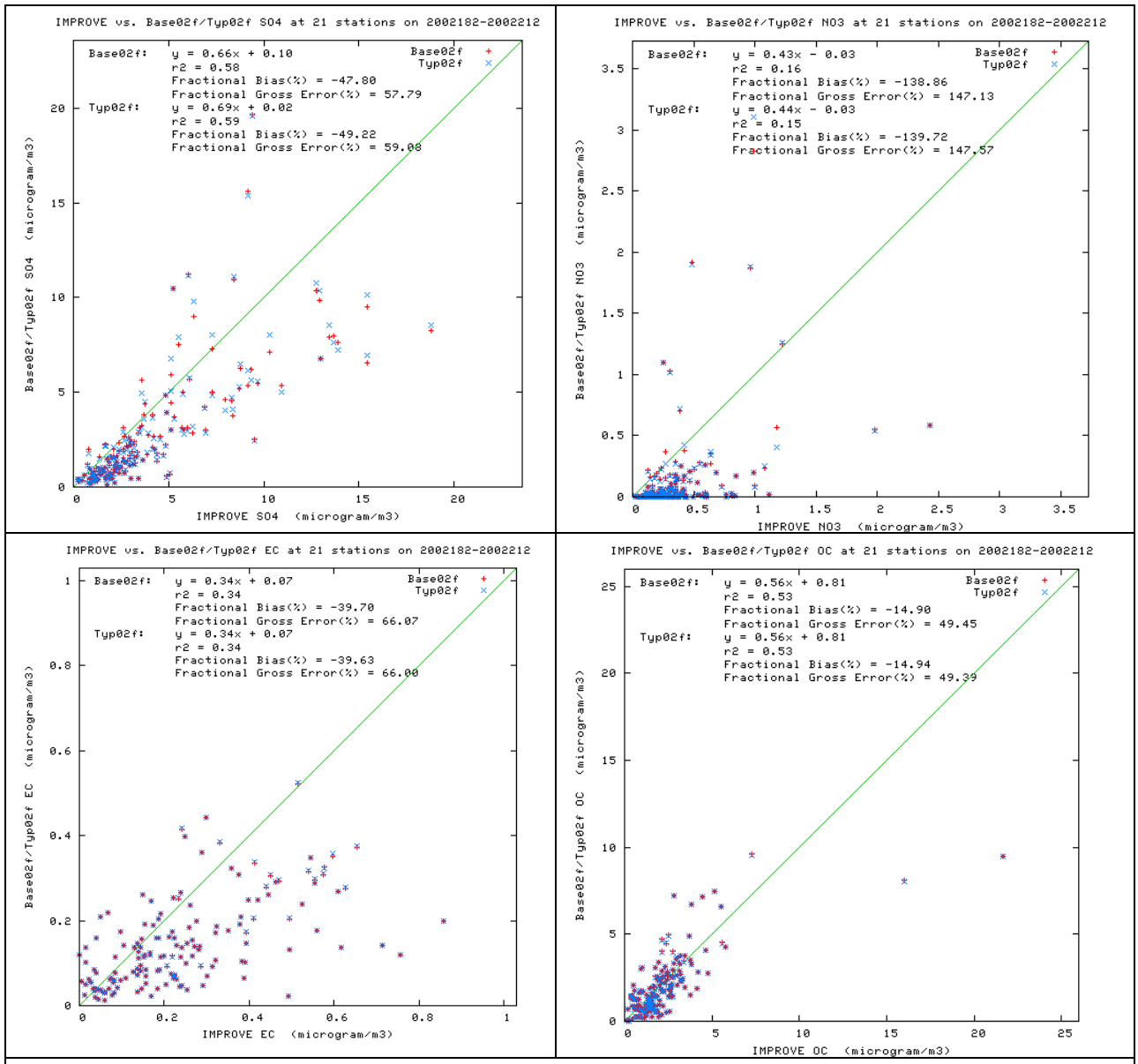


Figure C-2. Comparison of SO4 (top left), NO3 (top right), EC (bottom left) and OMC (bottom right) model performance for July 2002, the CENRAP region and the 2002 36 km Base F Actual (red) and Typical (blue) CMAQ base case simulation.

C.2 CMAQ Evaluation Methodology

EPA's integrated ozone, $PM_{2.5}$ and regional haze modeling guidance calls for a comprehensive, multi-layered approach to model performance testing, consisting of the four major components: operational, diagnostic, mechanistic (or scientific) and probabilistic (EPA, 2007). The CMAQ model performance evaluation effort focused on the first two components, namely:

- **Operational Evaluation**: Tests the ability of the model to estimate PM concentrations (both fine and coarse) and the components at PM_{10} and $PM_{2.5}$ including the quantities used to characterize visibility (i.e., sulfate, nitrate, ammonium, organic carbon, elemental carbon, other $PM_{2.5}$, and coarse matter ($PM_{2.5-10}$). This evaluation examines whether the measurements are properly represented by the model predictions but does not necessarily ensure that the model is getting "the right answer for the right reason"; and

- **Diagnostic Evaluation:** Tests the ability of the model to predict visibility and extinction, PM chemical composition including PM precursors (e.g., SOx, NOx, and NH_3) and associated oxidants (e.g., ozone and nitric acid); PM size distribution; temporal variation; spatial variation; mass fluxes; and components of light extinction (i.e., scattering and absorption).

The diagnostic evaluation also includes the performance of diagnostic tests to better understand model performance and identify potential flaws in the modeling system that can be corrected. The diagnostic evaluation may also includes the use of "probing tools" to understand why the model obtains a given prediction; probing tools include Process Analysis (PA), decoupled direct method (DDM) and source apportionment (SA).

In this final model performance evaluation for the 2002 Typical Base F CMAQ simulation, the operational evaluation has been given the greatest attention since this is the primarily thrust of EPA's modeling guidance. However, we have also examined certain diagnostic features dealing with the model's ability to simulate sub-regional and monthly/diurnal gas phase and aerosol concentration distributions. In the course of the CENRAP and other modeling process numerous diagnostic sensitivity tests were performed to investigate and improve model performance. Key diagnostic tests performed are discussed and the results for the rest are available on the CENRAP modeling website: http://pah.cert.ucr.edu/aqm/cenrap/index.shtml.

C.2.1 Ambient Air Quality Data for CENRAP Model Evaluation

The ground-level model evaluation database for 2002 was compiled by the modeling team using several routine and research-grade databases. The first is the routine gas-phase concentration measurements for ozone, NO, NO_2 and CO archived in EPA's Aerometric Information Retrieval System (AIRS) Air Quality System (AQS) database. Other sources of observed information come from the various PM monitoring networks in the U.S. These include the: (a) Interagency Monitoring of Protected Visual Environments (IMPROVE); (b) Clean Air Status and Trends Network (CASTNET); (c) Southeastern Aerosol Research and Characterization (SEARCH); (d) EPA Federal Reference Method $PM_{2.5}$ and PM_{10} Mass Networks (EPA-FRM); (e) EPA Speciation Trends Network (STN) of $PM_{2.5}$ species; and (f) National Acid Deposition Network (NADP). These PM

monitoring networks may also provide ozone and other gas phase precursors and product species, and visibility measurements at some sites. During the course of the CENRAP modeling, the numerous base case simulations were evaluated across the continental U.S. In this section we focus our evaluation on model performance within the CENRAP region. Table C-1 summarizes the observations collected at each monitoring network within the CENRAP region and their sampling frequency with Figure C-3 displaying the locations of the monitors for the various monitoring networks operating in the CENRAP region during 2002.

Table C-1. Ambient monitoring data available in the CENRAP region during 2002.

Monitoring Network	Chemical Species Measured	Sampling Frequency; Duration
IMPROVE	Speciated $PM_{2.5}$ and PM_{10}	1 in 3 days; 24 hr
CASTNET	Speciated $PM_{2.5}$, Ozone	Hourly, Weekly; 1 hr, Week
SEARCH	24-hr PM_{25} (FRM Mass, OC, BC, SO_4, NO_3, NH_4, Elem.); 24-hr PM coarse (SO_4, NO_3, NH_4, elements); Hourly $PM_{2.5}$ (Mass, SO_4, NO_3, NH_4, EC, TC); and Hourly gases (O_3, NO, NO_2, NO_y, HNO_3, SO_2, CO)	Daily, Hourly;
NADP	WSO_4, WNO_3, WNH_4	Weekly
EPA-FRM	Only total fine mass ($PM_{2.5}$)	1 in 3 days; 24 hr
EPA-STN	Speciated $PM_{2.5}$	Varies; Varies
AIRS/AQS	CO, NO, NO_2, NO_x, O_3	Hourly; Hourly

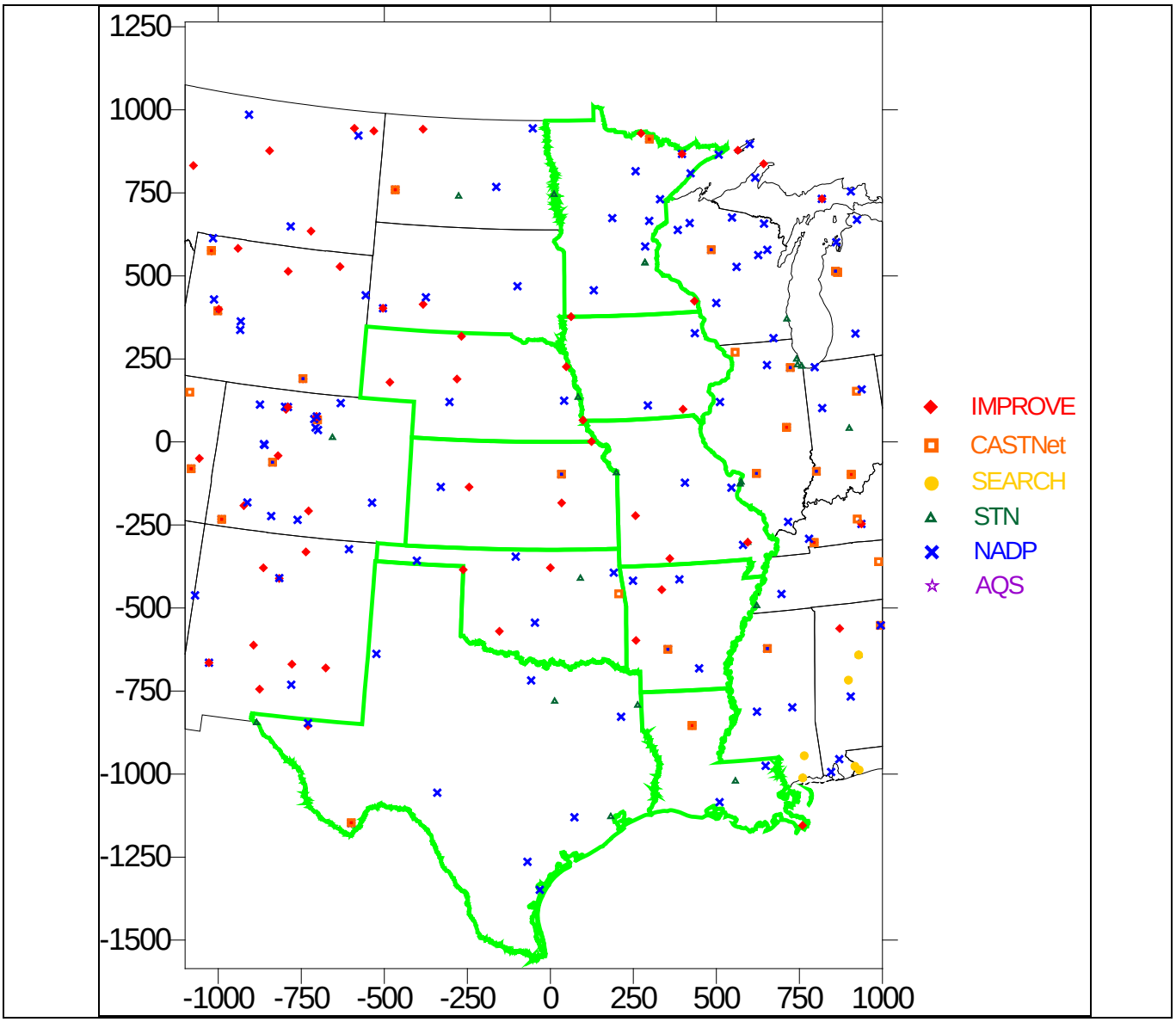


Figure C-3. Locations of surface monitors within the CENRAP states for sites operating during 2002.

C.2.2 Scope of CMAQ Model Performance Evaluation

The primary focus of the CMAQ Base F evaluation is on how well the model is able to replicate observed concentrations gas-phase pollutants and precursors, the various components of $PM_{2.5}$, total observed mass of $PM_{2.5}$, and wet deposition amounts. The CMAQ operational evaluation, model outputs are compared statistically and graphically with observational data obtained from the IMPROVE, CASTNet, STN, NADP and AQS monitoring networks. Because the SEARCH network is located in the southeastern U.S. (VISTAS region) outside of the CENRAP region, it is not a major component of our evaluation. Also, since the EPA-FRM network focuses on just $PM_{2.5}$ mass measurements primarily in $PM_{2.5}$ nonattainment or near nonattainment areas it is not very relevant for simulating regional haze at mainly remote Class I areas so is also not used in our model performance evaluation. The primary focus of the operational evaluation of the CMAQ 2002 Base F simulation is the performance of PM components in the CENRAP region for predicting regional haze at Class I areas.

Many statistical performance measures have been calculated using the different monitoring networks and across the different model performance subdomains (e.g., RPO regions). Table C-2 lists the definitions of the model performance evaluation statistical metrics. These performance metrics are routinely generate by the UCR Analysis Tool and are available on the project website. Many of them are measures of bias and error that are somewhat redundant.

Table C-2. Statistical Measures Used in the CENRAP CMAQ Model Evaluation.

Statistical Measure	Shorthand Notation	Mathematical Expression	Notes
Accuracy of paired peak (***A_p***)	**Paired_Peak**	$\frac{P - O_{peak}}{O_{peak}}$	P_{peak} = paired (in both time and space) peak prediction
Coefficient of determination (***r^2***)	**Coef_Determ**	$\frac{\left[\sum_{i=1}^{N}(P_i - \overline{P})(O_i - \overline{O})\right]^2}{\sum_{i=1}^{N}(P_i - \overline{P})^2 \sum_{i=1}^{N}(O_i - \overline{O})^2}$	P_i = prediction at time and location *i*; O_i = observation at time and location *i*; $\overline{P}$ = arithmetic average of P_i, i=1,2,…, N; $\overline{O}$ = arithmetic average of O_i, i=1,2,…,N
Normalized Mean Error (***NME***)	**Norm_Mean_Err**	$\frac{\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\sum_{i=1}^{N} O_i}$	Reported as %
Root Mean Square Error (***RMSE***)	**Rt_Mean_Sqr_Err**	$\left[\frac{1}{N}\sum_{i=1}^{N}\left(P_i - O_i\right)^2\right]^{1/2}$	Reported as %
Fractional Gross Error (***F_E***)	**Frac_Gross_Err**	$\frac{2}{N}\sum_{i=1}^{N}\left\lvert\frac{P_i - O_i}{P_i + O_i}\right\rvert$	Reported as %
Mean Absolute Gross Error (***MAGE***)	**Mean_Abs_G_Err**	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert$	
Mean Normalized Gross Error (***MNGE***)	**Mean_Norm_G_Err**	$\frac{1}{N}\sum_{i=1}^{N}\frac{\lvert P_i - O_i\rvert}{O_i}$	Reported as %
Mean Bias (***MB***)	**Mean_Bias**	$\frac{1}{N}\sum_{i=1}^{N}\left(P_i - O_i\right)$	Reported as concentration (e.g., µg/m^3)

Statistical Measure	Shorthand Notation	Mathematical Expression	Notes
Mean Normalized Bias (***MNB***)	**Mean_Norm_Bias**	$\frac{1}{N}\sum_{i=1}^{N}\frac{(P_i - O_i)}{O_i}$	Reported as %
Mean Fractionalized Bias (Fractional Bias, ***MFB***)	**Mean_Fract_Bias**	$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$	Reported as %
Normalized Mean Bias (***NMB***)	**Norm_Mean_Bias**	$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N}O_i}$	Reported as %
Bias Factor (***BF***)	**Bias Factor**	$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{P_i}{O_i}\right)$	Reported as BF:1 or 1: BF or in fractional notation (BF/1 or 1/BF).

C.2.3 Operational Model Evaluation Approach

The CENRAP modeling databases will be used to develop the visibility State Implementation Plan (SIP) due in December 2007 as required by the Regional Haze Rule (RHR). Accordingly, the primary focus of the operational evaluation is on the six components of fine particulate ($PM_{2.5}$) and Coarse Matter ($PM_{2.5\text{-}10}$) within the CENRAP region that are used to characterize visibility at Class I areas:

- Sulfate (SO4);
- Particulate Nitrate (NO3);
- Elemental Carbon (EC);
- Organic Mass Carbon (OMC);
- Other inorganic fine particulate (IP or Soil); and
- Coarse Matter (CM).

The model performance for ozone and precursor and product species (e.g., SO_2 and HNO_3) is also evaluated to build confidence that the modeling system is sufficiently reliable to project future-year visibility.

C.2.5 Performance Evaluation Tools

One of the many challenges in evaluating an annual PM/ozone model simulation is how to synthesize model performance given the shear volume of output from an annual simulation. The model is run on a 148 x 112 x 19 grid with approximately 30 species producing hourly outputs for each day of the year. This results in approximately 90 trillion concentration estimates that are produced for an annual simulation. Thus, the synthesis and interpretation of numerous graphical and tabular displays of model performance into a few concise and descriptive displays that identify the most salient features of model performance is necessary. As part of the CENRAP modeling, as well as work performed by WRAP, VISTAS, MRPO and MANE-VU, several analysis tools and summary displays have been developed and are used:

UCR Analysis Tools: The University of California at Riverside (UCR) Analysis Tools have been used extensively to evaluate the CMAQ and CAMx models for CENRAP (e.g., Morris et al., 2005), WRAP (Tonnesen et al., 2004), VISTAS (Morris et al., 2004) as well as other studies and are run on a Linux platform separately for each network. Numerous graphical displays of model performance are automatically generated using gnuplot. The software generates the following summary and graphical displays of model performance:

- Tabular statistical measures (see Table C-2);
- Time Series Plots for each site and species; and
- Scatter Plots for each species by allsite_allday, allday_onesite and allsite_oneday.

The UCR Analysis Tool is run for a specific subregion (e.g., by RPO region) and for selected monitoring networks. Because each monitoring network has its own measurement artifacts, the model is evaluated separately for each monitoring network.

Summary Bias/Error Plots: The modeling team has developed additional displays of model performance statistics that elucidate model performance in a concise manner: (1) monthly time series plots of average bias and error; (2) soccer plots that display bias versus error and compares them to model performance goals and criteria; and (3) tools to analyze visibility model performance for the worst and best 20 percent visibility days that are used in visibility projections.

GA DNR Analysis Plots: Dr. James Boylan of the Georgia Department of Natural Resources has extended the concept in EPA's draft PM fine particulate and regional haze modeling guidance that model performance for species that make up a major contribution to visibility impairment be subjected to more stringent goals than species that are minor contributors by developing concentration-dependent performance goals and "Bugle Plots" to display them (Boylan, 2004).

The evaluation of the CENRAP 2002 36 km Base F CMAQ simulation used each of the analysis tools listed above taking advantage of their different descriptive and complimentary nature. The use of these analysis tools generated thousands of statistical measures and graphical displays of model performance that cannot all be displayed in this report. The modeling team has gone through the plots and measures using slide shows to identify those displays that are most descriptive in conveying model performance so should be included in this TSD. The complete set of model performance statistics and graphical performance displays can be found on the CENRAP modeling Website at:

http://pah.cert.ucr.edu/aqm/cenrap/cmaq.shtml#cmaq_typ02f_mpe

Note that model performance statistics are calculated separately for each of the monitoring networks. Different PM measurement technology can produce different measurement values even when measuring the same air parcel. Thus, when calculating model performance metrics, measurements in different networks are not mixed.

C.2.4 Subdomains Analyzed

CENRAP has been analyzing model performance in five subdomains corresponding to the states contained in the five RPOs (see Figure 1-1):

- CENRAP
- MRPO
- VISTAS
- MANE-VU
- WRAP

As CENRAP has refined its emissions inventory, the changes in model performance from one 2002 base case to another has diminished to the point where little has changed in the last few iterations. Thus, the CMAQ 2002 36 km Base F evaluation presented in this section was just performed for the CENRAP region and the reader is referred to the modeling Website (http://pah.cert.ucr.edu/aqm/cenrap/cmaq.shtml) and Morris and co-workers (2005) for the evaluation outside of the CENRAP region and the diagnostic model evaluation.

C.2.5 Model Performance Goals and Criteria

The issue of model performance goals for PM species is an area of ongoing research and debate. For ozone modeling, EPA has established performance goals for 1-hour ozone normalized mean bias and gross error of #±15% and #35%, respectively (EPA, 1991). EPA's draft fine particulate modeling guidance notes that performance goals for ozone should be viewed as upper bounds of model performance that PM models may not be able to always achieve and we should demand better model performance for PM components that make up a larger fraction of the PM mass than those that are minor contributors (EPA, 2001). EPA's final modeling guidance does not list any specific model performance goals for PM and visibility modeling and instead provides a summary of PM model performance across several historical applications that can be used for comparisons if desired. Measuring PM species is not as precise as ozone monitoring. In fact, the differences in measurement techniques for some species likely exceed the more stringent performance goals, such as those for ozone. For example, recent comparisons of the PM species measurements using the IMPROVE and STN measurement technologies found differences of approximately ∀20% (SO4) to ∀50% (EC) (Solomon et al., 2004).

For the CENRAP, VISTAS and WRAP modeling we have adopted three levels of model performance goals and criteria for bias and gross error as listed in Table C-3. Note that we are not suggesting that these performance goals be adopted as guidance or that they are the most appropriate goals to use. Rather, we are just using them to frame and put the PM model performance into

context and to facilitate model performance intercomparison across episodes, species, models and sensitivity tests.

Table C-3. Model performance goals and criteria used to assist in interpreting modeling results.

Fractional Bias	Fractional Error	Comment
#∀15%	#35%	Ozone model performance goal for which PM model performance would be considered good – note that for many PM species measurement uncertainties may exceed this goal.
#∀30%	#50%	Proposed PM model performance goal that we would hope each PM species could meet
#∀60%	#75%	Proposed PM criteria above which indicates potential fundamental problems with the modeling system.

As noted in EPA's PM modeling guidance, less abundant PM species should have less stringent performance goals (EPA, 2001; 2007). Accordingly, we are also using performance goals that are a continuous function of average concentrations, as proposed by Dr. James Boylan at the Georgia Department of Natural Resources (GA DNR), that have the following features (Boylan, 2004):

- Asymptotically approaching proposed performance goals or criteria (i.e., the ∀30%/50% and ∀60%/75% bias/error levels listed in Table C-1) when the mean of the observed concentrations are greater than 2.5 ug/m^3.
- Approaching 200% error and ∀200% bias when the mean of the observed concentrations are extremely small.

Bias and error are plotted as a function of average concentrations. As the mean concentration approach zero, the bias performance goal and criteria flare out to ∀200% creating a horn shape, hence the name "Bugle Plots". Dr. Boylan has defined three Zones of model performance: Zone 1 meets the ∀30%/50% bias/error performance goal and is considered "good" model performance; Zone 2 lies between the ∀30%/50% performance goal and ∀60%/75% performance criteria and is an area where concern for model performance is raised; and Zone 3 lies above the ∀60%/75% performance criteria and is an area of questionable model performance.

C.2.6 Performance Time Periods

The CMAQ 2002 36 km Base F evaluation, model performance statistics and graphical displays are generated monthly using the native averaging times of each monitoring network (i.e., 24-hour for IMPROVE and STN; weekly for CASTNet and NADP; and hourly for AQS). As the focus of the RHR is on daily average visibility that is calculated from daily average PM species concentrations then the evaluation of the model for 24-hour concentrations is particularly relevant. The RHR places particular emphasis on the Worst 20% (W20%) and Best 20% (B20%) days at Class I areas. Thus, we also place particular emphasis on the model performance for PM species on the W20% and B20% days during 2002 at Class I areas.

C.2.7 Key Measures of Model Performance

Although we have generated numerous statistical performance measures (see Table C-2) that are available on the CENRAP modeling website, when comparing model performance across months, subdomains, networks, grid resolution, models, studies, etc. it is useful to have a few key measurement statistics to be used to facilitate the comparisons. It is also useful to have a subset of the 2002 year that can represent the entire year so that a more focused evaluation can be conducted. We have found that the Mean Fractional Bias and Mean Fractional Gross Error appear to be the most consistent descriptive measure of model performance (Morris et al., 2004b; 2005). The Fractional Bias and Error normalize by the average of the observed and predicted value (see Table C-2) because it provides descriptive power across different magnitudes of the model and observed concentrations and is bounded by -200% to +200%. This is in contrast to the normalized bias and error (as recommended for ozone performance goals, EPA, 1991) that is normalized by just the observed value so can "blow up" to infinity as the observed value approaches zero. Below we perform a focused evaluation of model performance for four months of the 2002 year that are used to represent the seasonal variation in performance:

- January
- April
- July
- October

We also present fractional bias and error for all months of 2002 using time series and bugle plots.

C.3 Operational Model Performance Evaluation in the CENRAP Region

In the following discussions we use selected monthly scatter plots, time series plots and model performance statistical measures from the UCR Analysis Tools application to the 2002 CMAQ Base F base case simulation in an operational evaluation of the model for PM species. We focus on the six main components of PM that are used to project visibility.

C.3.1 Sulfate (SO4) Monthly Model Performance

C.3.1.1 SO4 in January 2002

Figure C-4a displays scatter plots of predicted and observed SO4 concentrations or wet depositions for sites in the CENRAP regions using observations from the IMPROVE, STN, CASTNet and NADP monitoring networks; the IMPROVE and STN SO4 concentrations are 24-hour averages whereas the CASTNet SO4 concentrations and NADP SO4 wet deposition are weekly averages. The January SO4 performance at the IMPROVE and STN networks in the CENRAP region is quite good with low fractional bias (-12% to -13%) and some scatter (fractional error of 42% and 34%) but centered in the 1:1 line of perfect agreement. There is a net SO4 underestimation bias in January across the CASTNet network (fractional bias of -34%) with wet SO4 deposition overstated on average across the NADP sites in the CENRAP region (+40% fractional bias). Whether the overstated SO4 wet deposition is a contributor to the SO4 concentration underestimation bias is unclear, but it is in the correct direction to account for it.

The time series comparisons of predicted and observed 24-hour SO4 concentrations at CENRAP Class I area IMPROVE sites during January 2002 shown in Figure C-4b are quite encouraging. Although there are some days and sites with mismatches (e.g., January 26 at BOWA and VOYA) and sites with systematic performance problems (SO4 underestimated at BIBE), the time series in generally are quite good with the model tracking the observed temp[oral variation in daily sulfate in January and some sites exhibiting remarkable agreement (e.g., MING).

Figure C-4c displays the spatial variations in the predicted and IMPROVE observed SO4 concentrations for January 20, 23, 26 and 29, 2002, which are four consecutive days of IMPROVE monitoring using its 1:3 day monitoring frequency. On January 20 both the model and observations agree on that an elevated sulfate clouds is entering the CENRAP region across southern Illinois and Missouri. There is a sharp SO4 concentration gradient going east to west with both the model and observations estimating relatively clean SO4 values over Colorado. By January 23 the model and observations agree that elevated SO4 exists along a diagonal orientation from Chicago to East Texas. Although there are some SO4 model/observed spatial mismatches on this day (e.g., northern Louisiana and western Arkansas) the model generally reproduces the areas of elevated and low observed SO4. By January 29 the model and observations agree that SO4 has cleaned out of the CENRAP region. Although there are elevated SO4 observations in western North Dakota and northern Minnesota not reflected in the model. On January 29 there is an elevated tongue of SO3 entering the CENRAP region through southern Illinois stretching to the southwest almost to Big Bend in western Texas. Observed SO4 is measured at Big Bend but the modeled high SO4 is slightly east of there. There is very good agreement on this day between the predicted and observed spatial distribution of SO4.

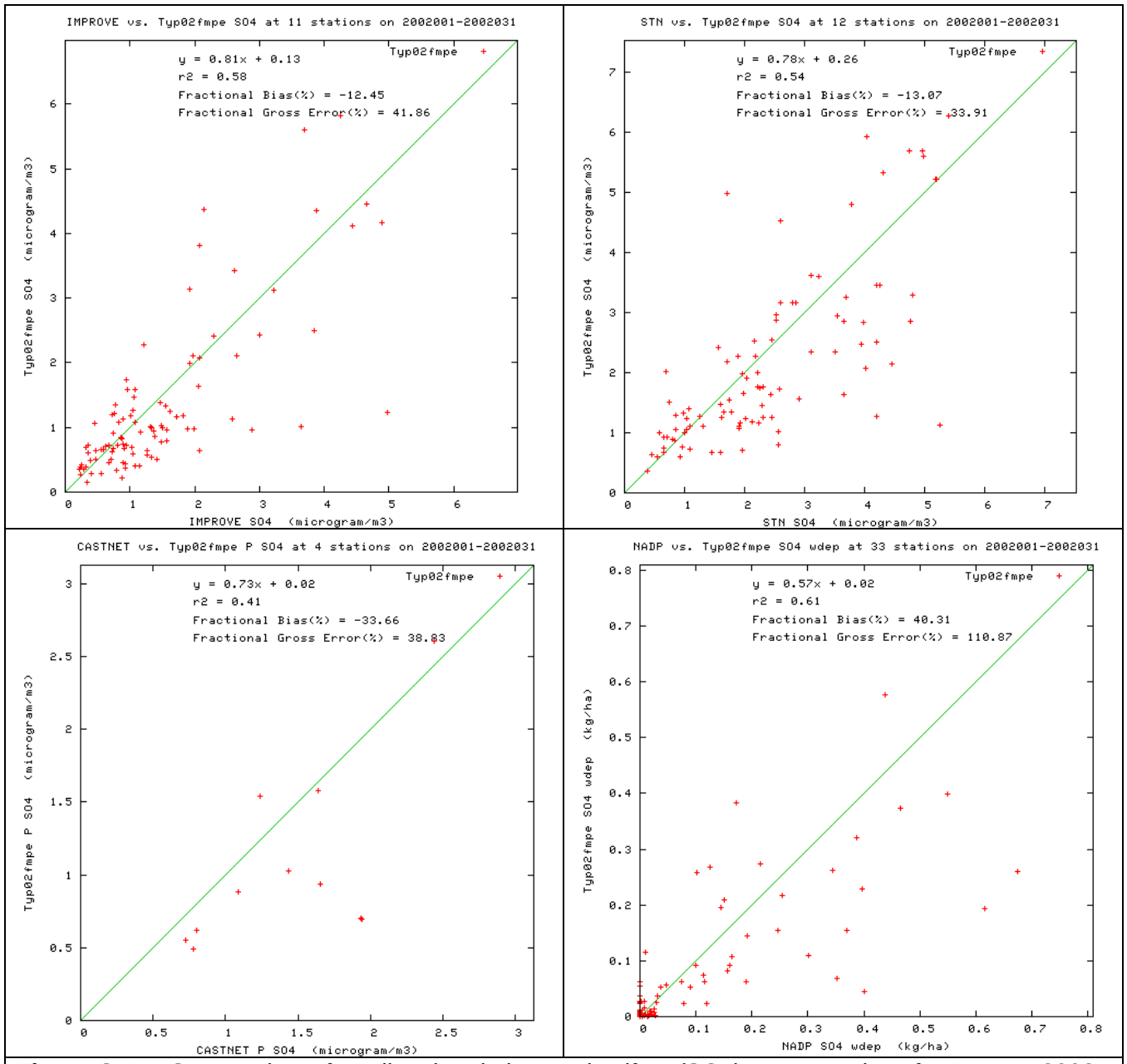
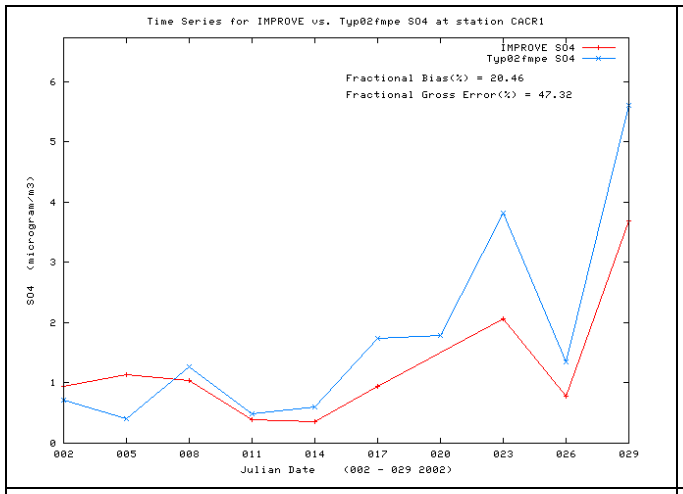
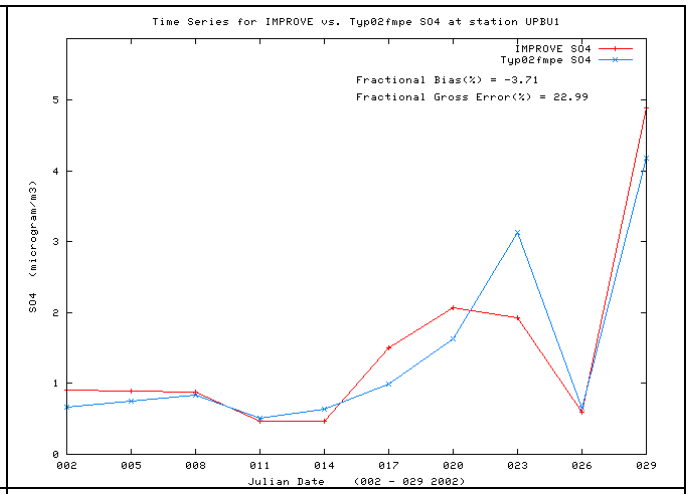
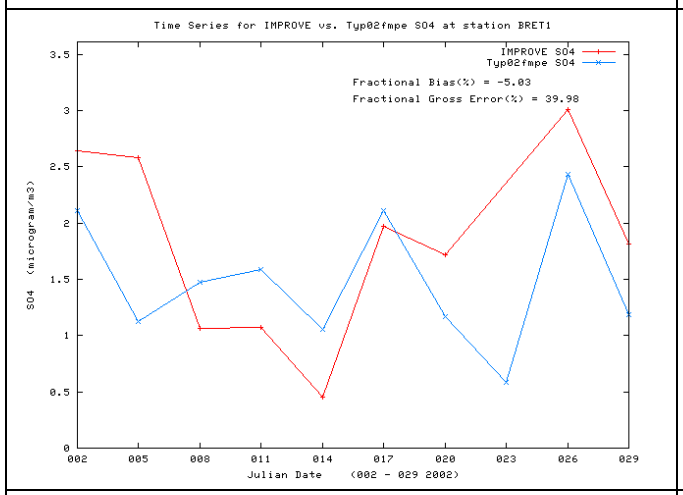
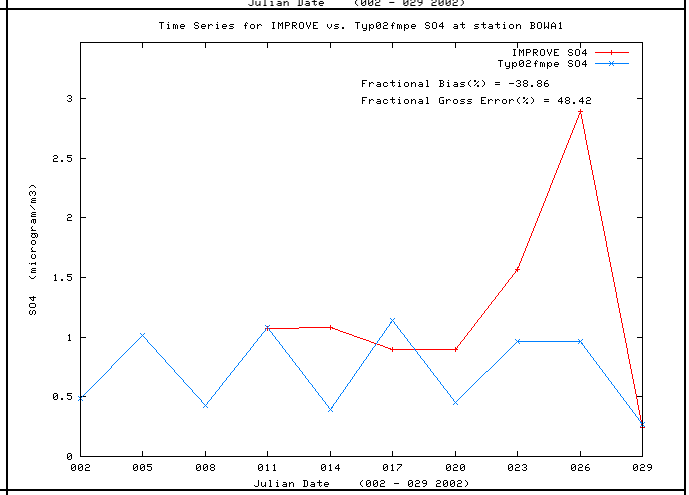


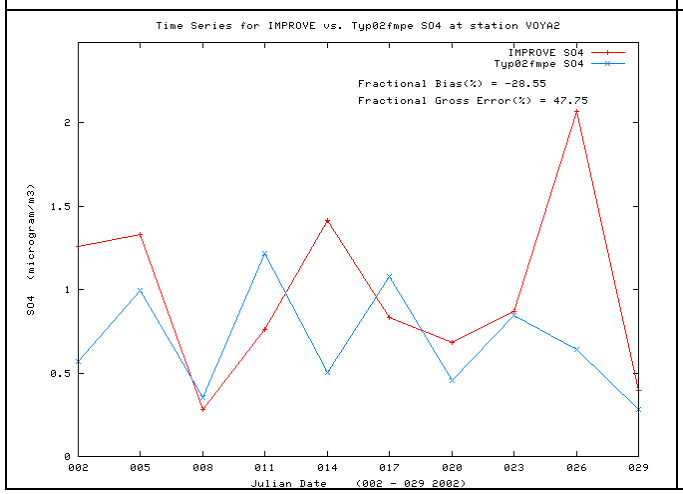
Figure C-4a. Scatter plots of predicted and observed sulfate (SO4) concentrations for January 2002 and sites in the CENRAP region using IMPROVE (top left), STN (top right), CASTNet (bottom left) and NADP monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

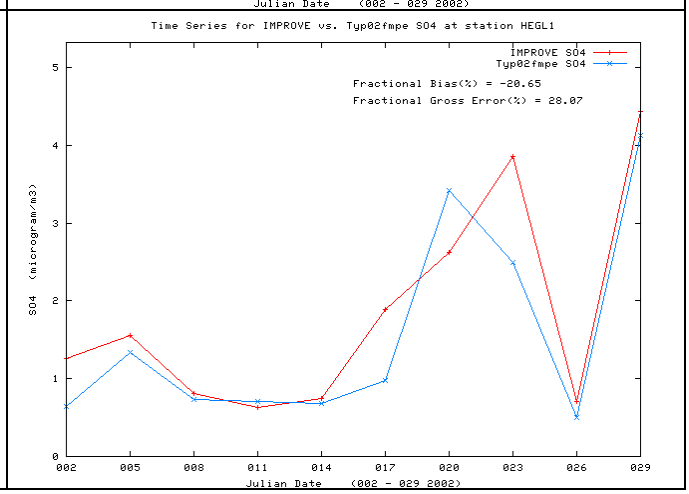

Time Series for IMPROVE vs. Typ02fmpe SO4 at station CACR1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = 20.46
Fractional Gross Error(%) = 47.32
SO4 (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station UPBU1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -3.71
Fractional Gross Error(%) = 22.99
SO4 (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station BRET1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -5.03
Fractional Gross Error(%) = 39.98
SO4 (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station BOWA1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -38.86
Fractional Gross Error(%) = 48.42
SO4 (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station VOYA2
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -28.55
Fractional Gross Error(%) = 47.75
SO4 (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station HEGL1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -20.65
Fractional Gross Error(%) = 28.07
SO4 (microgram/m3)
Julian Date (002 - 029 2002)

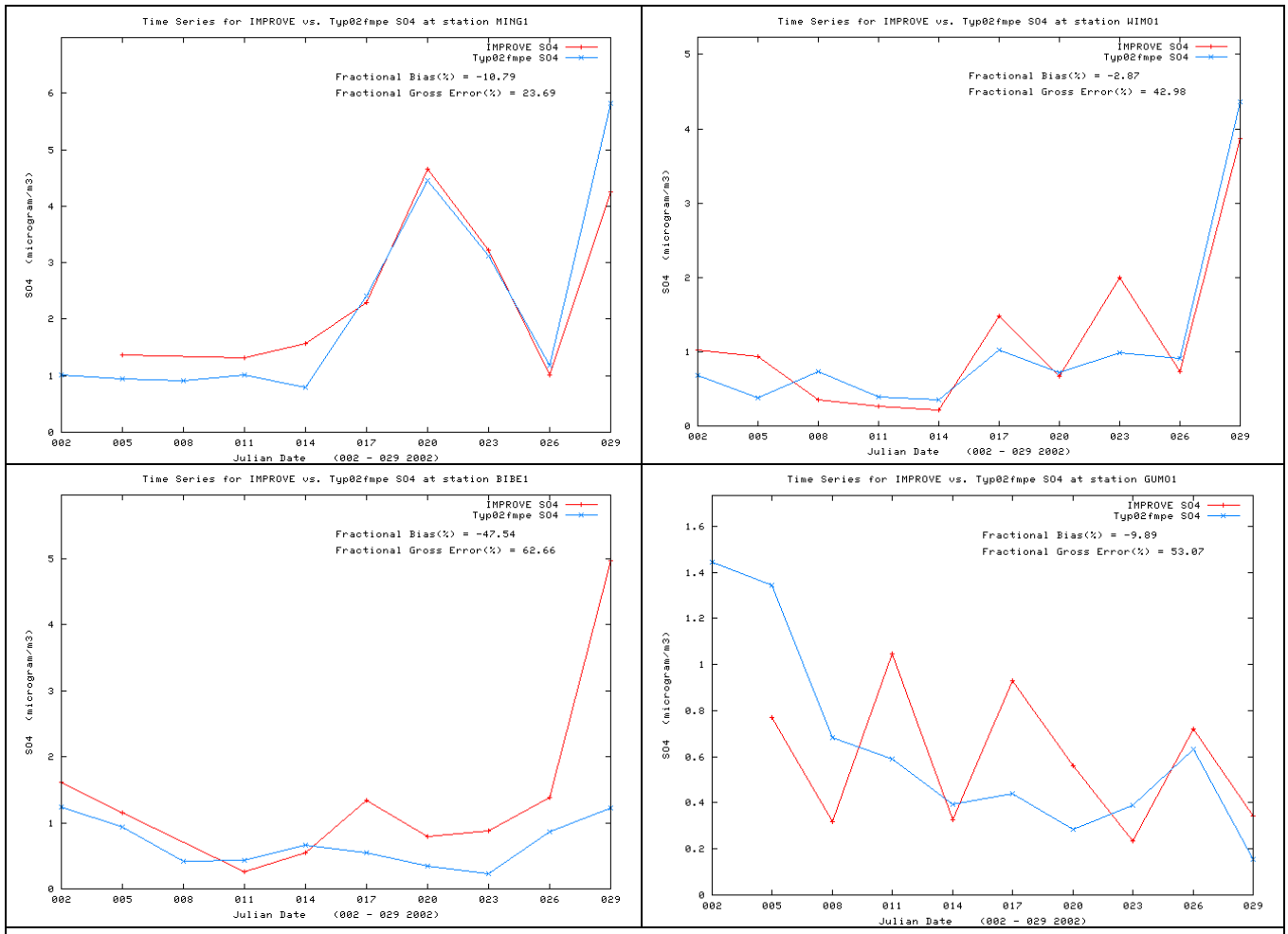


Figure C-4b. Time series of predicted and observed 24-hour sulfate (SO4) concentrations at CENRAP IMPROVE CLASS I AREA sites in January 2002 for CMAQ 2002 36 km Base F base case simulation.

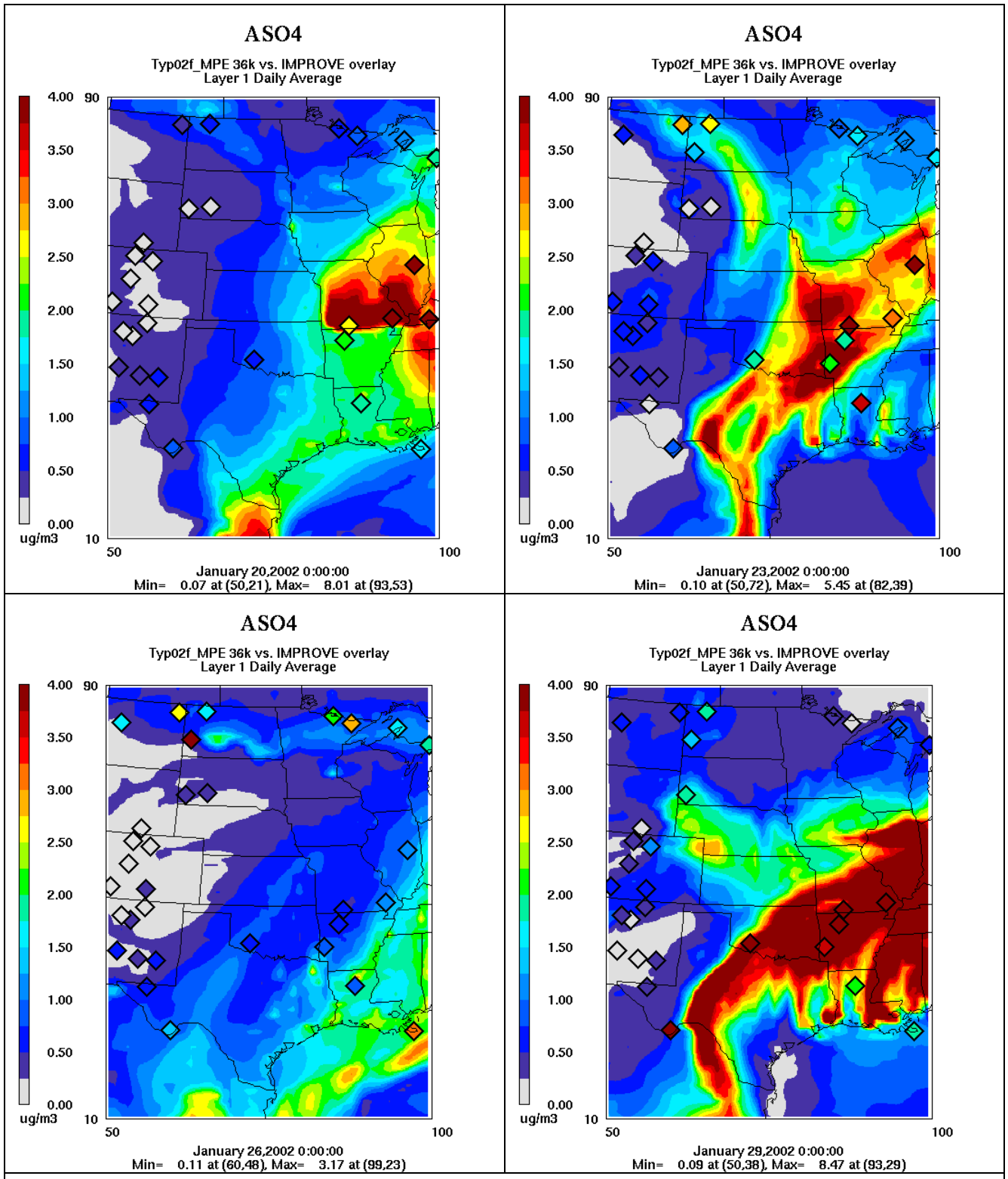


Figure C-4c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour SO4 concentrations for January 20, 23, 26 and 29, 2002.

C.3.1.2 SO4 in April 2002

In April CMAQ underestimates the observed SO4 in the CENRAP region with fractional bias values of -52%, -30% and -58% across the IMPROVE, STN and CASTNet networks (Figure C-5a). The fractional bias for wet SO4 deposition is quite low (3%) albeit with a lot of scatter which is reflected in high fractional error (78%). The ability of the model to reproduce the temporal variability of the April observed SO4 concentrations at the IMPROVE sites is quite variable. The SO4 under-prediction bias is clearly present at several sites (e.g., HEGL, BIBE and GUMO), whereas there is quite good agreement at others (UPBU, BRET and VOYA). Comparisons of the spatial distributions of the predicted and observed SO4 concentrations on April 5, 8, 11 and 14 are shown in Figure C-5c. On April 5 the model reproduces the half circle of elevated SO4 across Texas-Louisiana, but appears to not be as large an area as observed coming up short from some of the sites (e.g., BIBE and GUMO). Model and observations agree that April 8 is a relatively low SO4 day in the CENRAP region with just a small intrusion of elevated values across Mississippi. On April 14 the model has two separate clouds of elevated SO4, one over East Texas-Louisiana and one over northeastern Illinois and eastward with a clean area in between in southern Missouri. The observations agree except that it has these two elevated SO4 areas connected with the southern Missouri area not as clean as in the model.

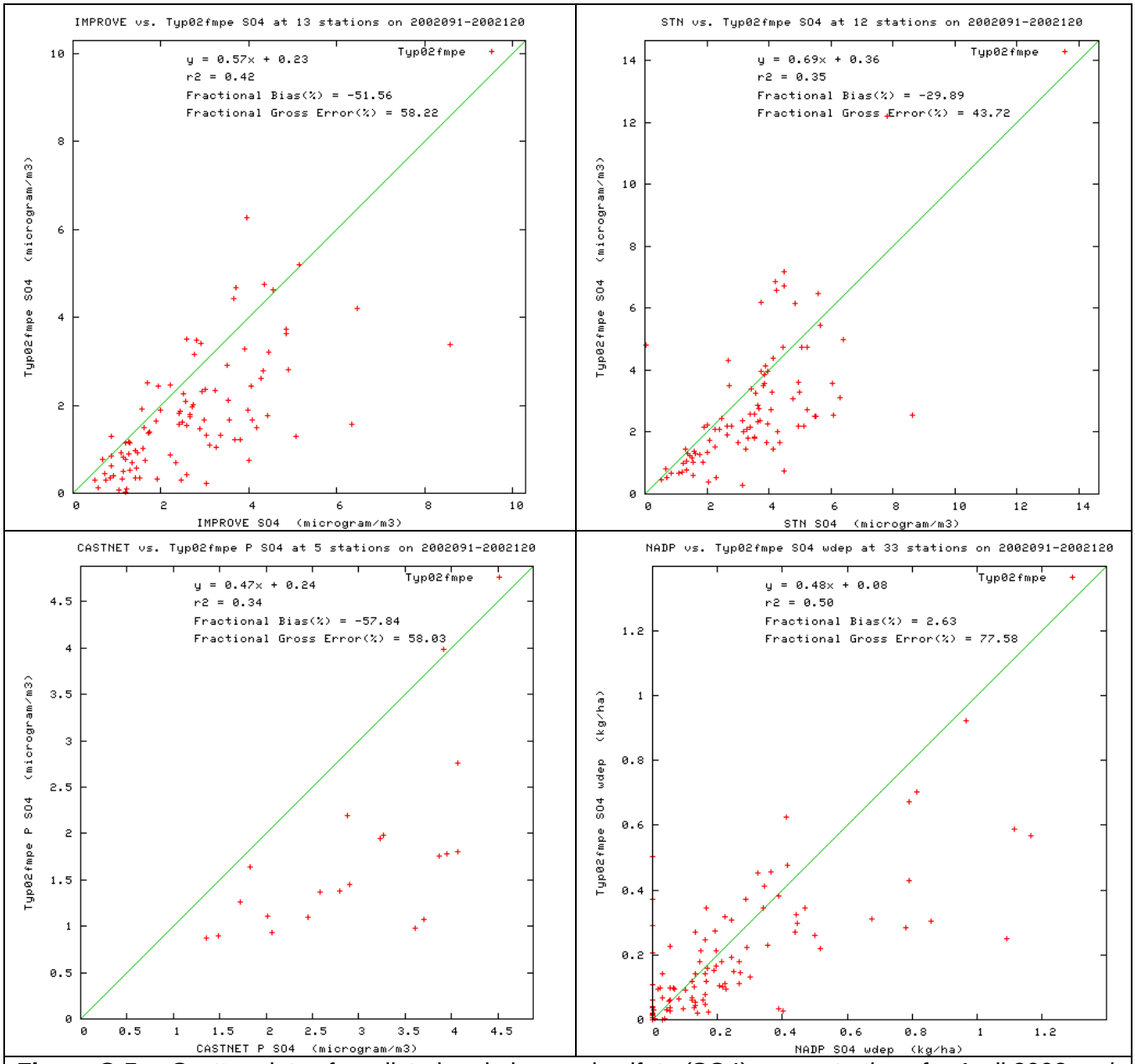
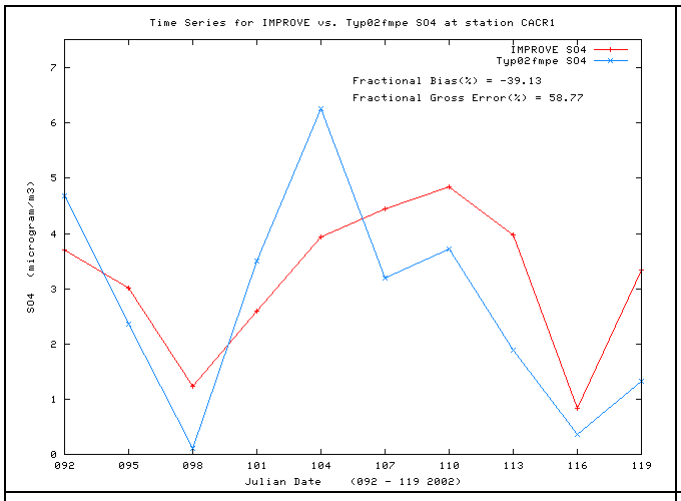
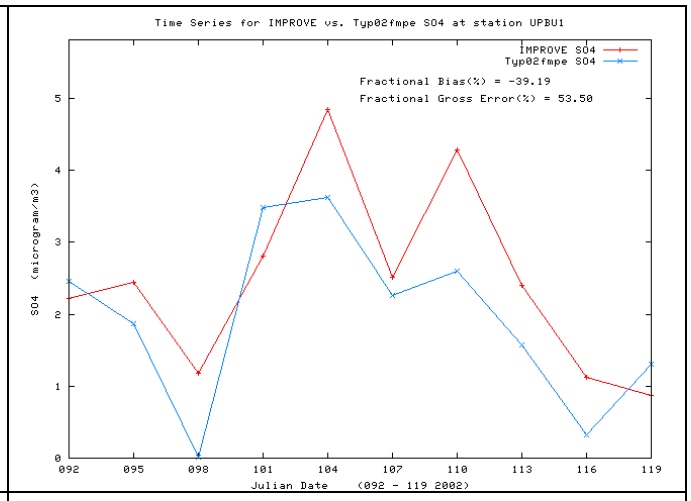
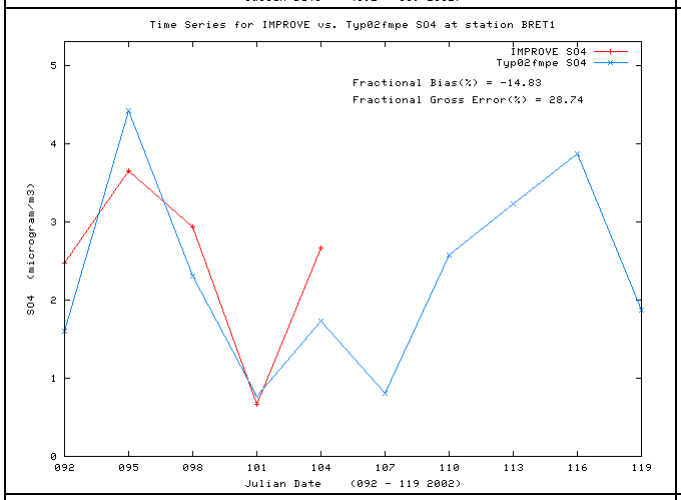
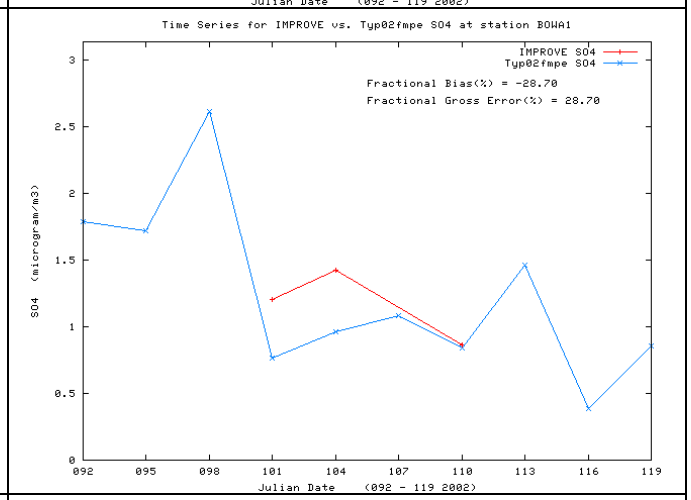


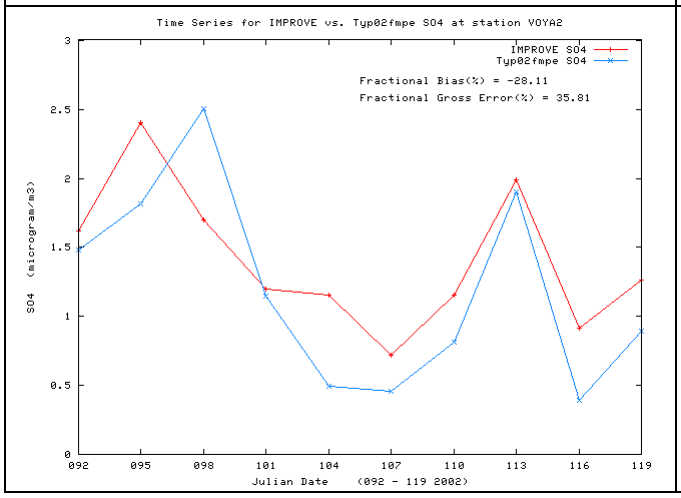
Figure C-5a. Scatter plots of predicted and observed sulfate (SO4) concentrations for April 2002 and sites in the CENRAP region using IMPROVE (top left), STN (top right), CASTNet (bottom left) and NADP monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

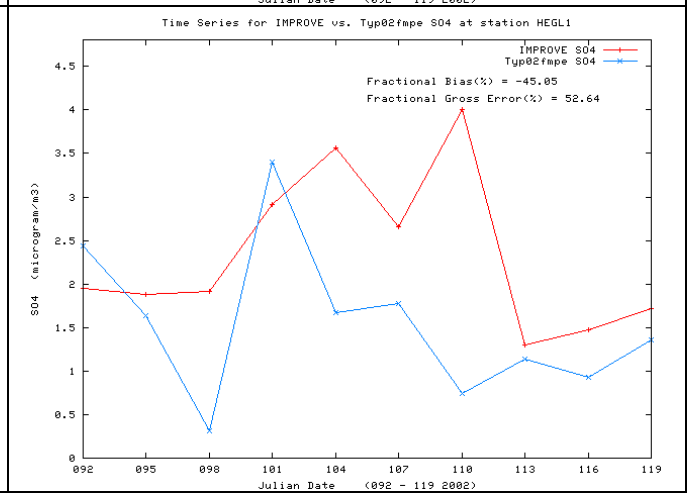

Time Series for IMPROVE vs. Typ02fmpe SO4 at station CACR1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -39.13
Fractional Gross Error(%) = 58.77
SO4 (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station UPBU1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -39.19
Fractional Gross Error(%) = 53.50
SO4 (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station BRET1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -14.83
Fractional Gross Error(%) = 28.74
SO4 (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station BOWA1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -28.70
Fractional Gross Error(%) = 28.70
SO4 (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station VOYA2
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -28.11
Fractional Gross Error(%) = 35.81
SO4 (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station HEGL1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -45.05
Fractional Gross Error(%) = 52.64
SO4 (microgram/m3)
Julian Date (092 - 119 2002)

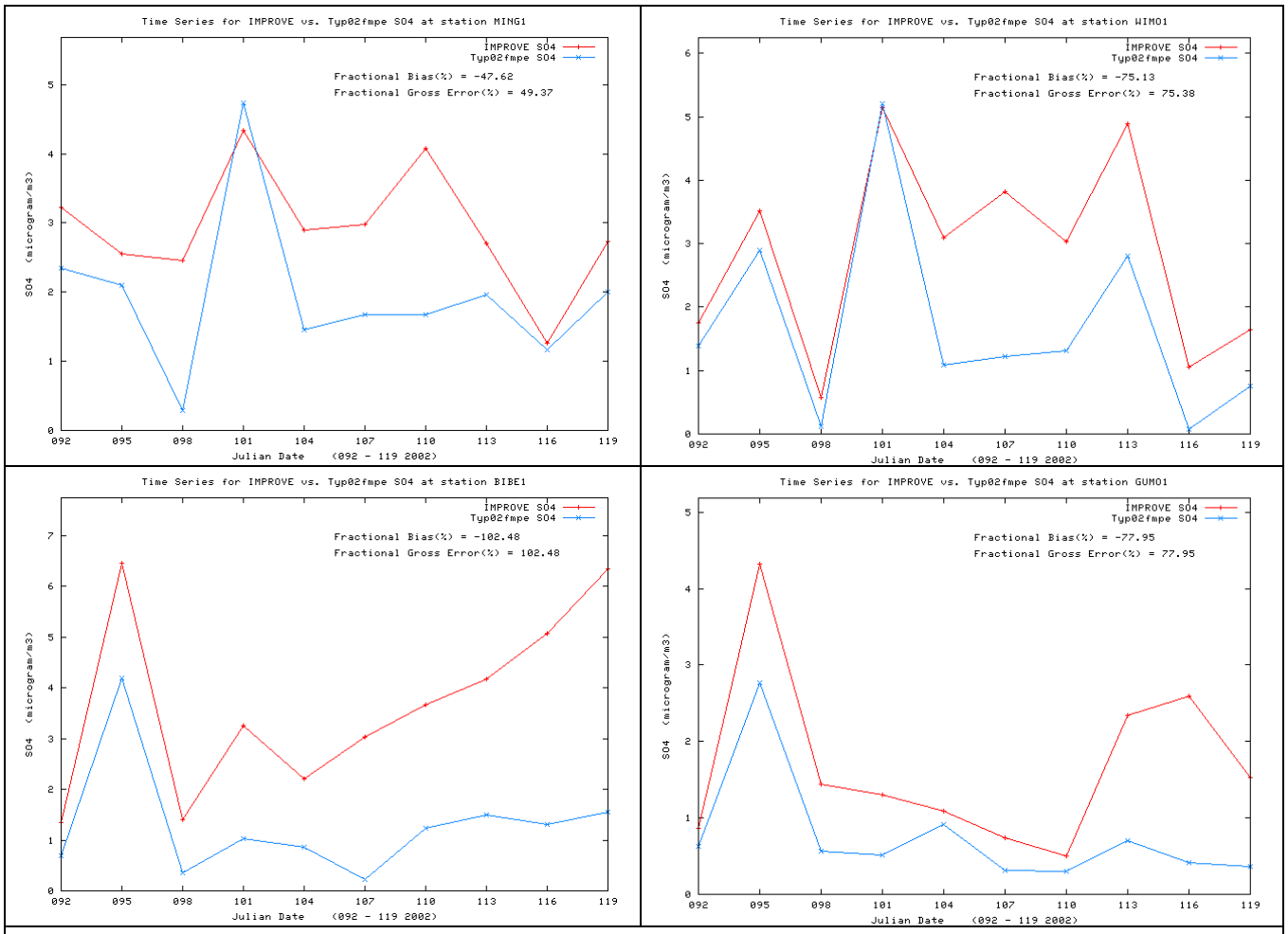


Figure C-5b. Time series of predicted and observed 24-hour sulfate (SO4) concentrations at CENRAP IMPROVE CLASS I AREA sites in April 2002 for CMAQ 2002 36 km Base F base case simulation.

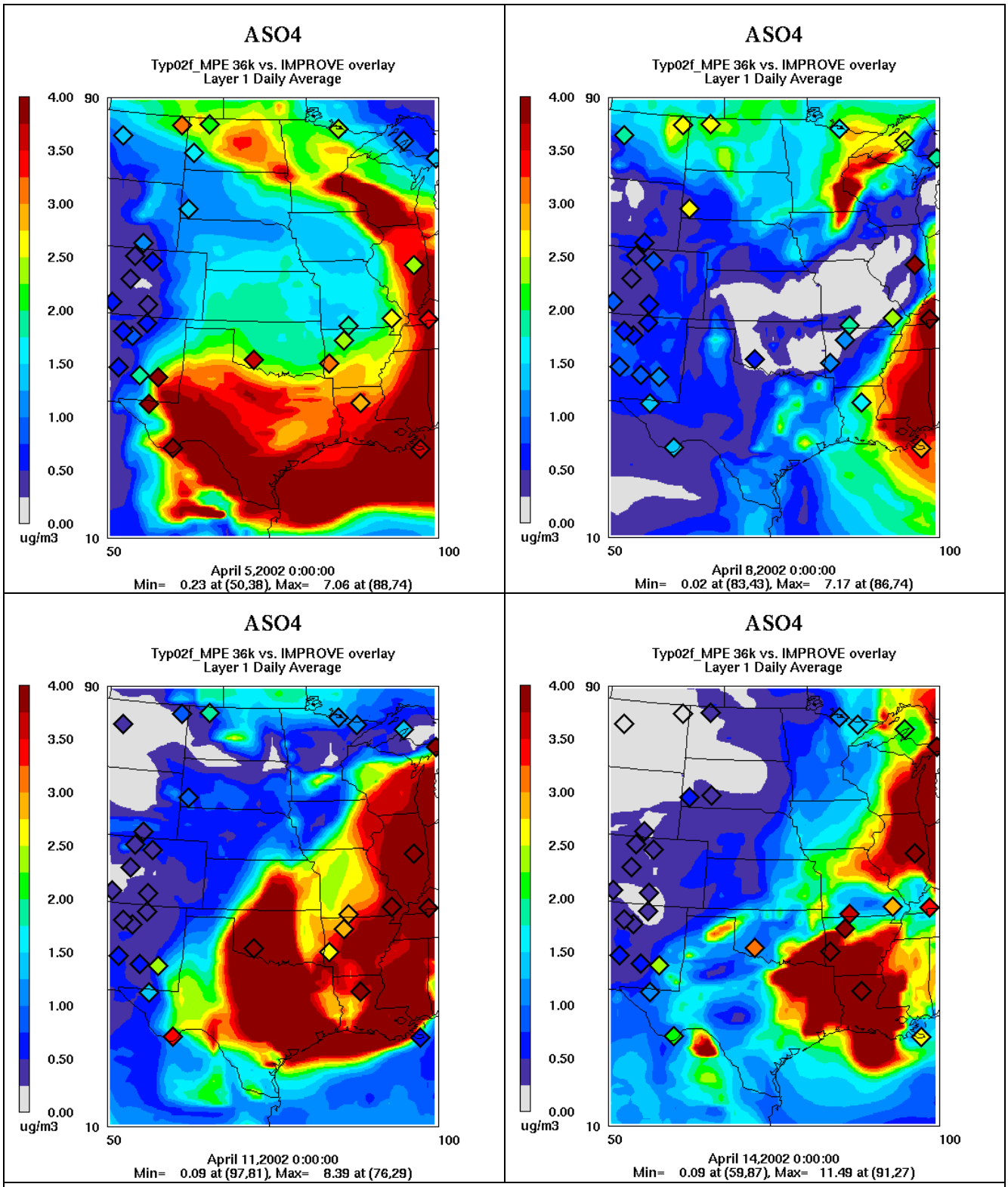


Figure C-5c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour SO4 concentrations for April 5, 8, 11 and 14, 2002.

C.3.1.3 SO4 in July 2002

SO4 concentrations are also underestimated by CMAQ in July (Figure C-6a) with fractional bias value ranging from -22 to -52%. Wet SO4 deposition is slightly overstated (22%) with a lot of scatter (83% error). The July SO4 under-prediction bias is also reflected in the time series plots (Figure C-6b). Comparisons of the predicted and observed spatial distribution of SO4 in the CENRAP region for July 7, 10, 13 and 16, 2002 are shown in Figure C-6c. In general the model and observations agree on the locations of the elevated SO4, except that the observed extent is somewhat larger so that the modeled elevated SO4 fails to impact some of the sites on the edge of the elevated cloud of SO4 (e.g., Big Bend, Guadalupe Mountains and northwestern Oklahoma).

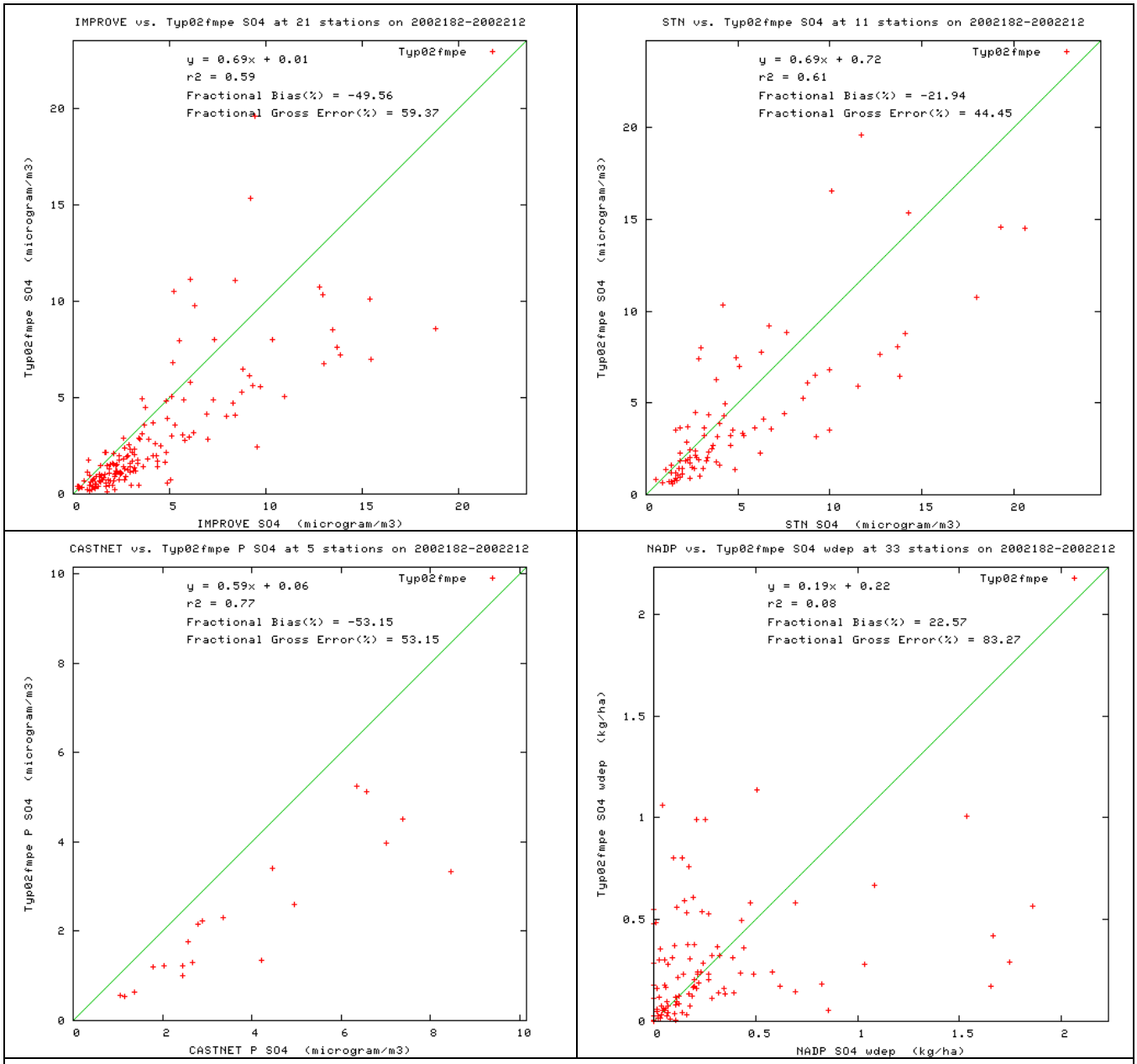
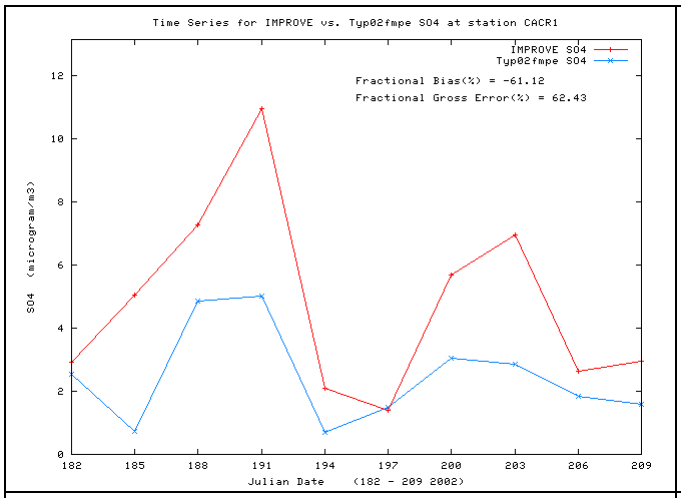
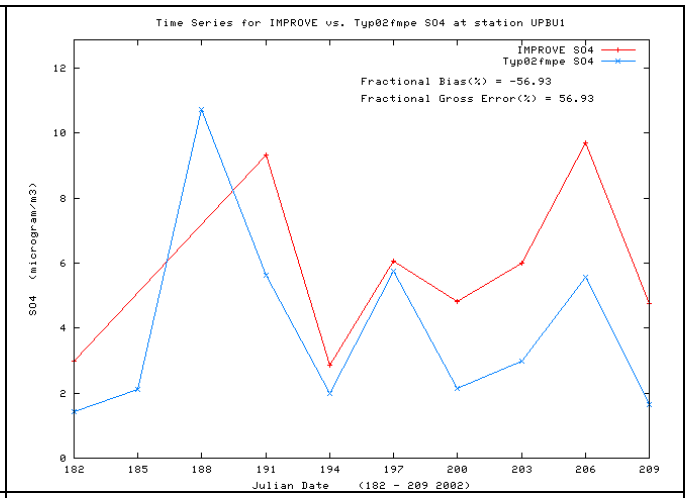
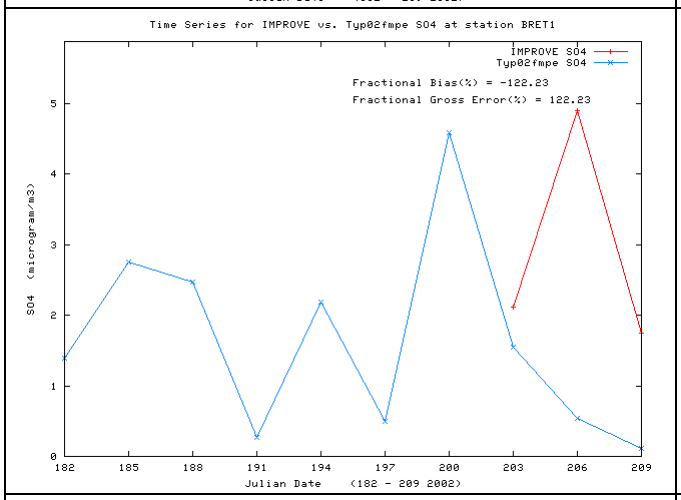
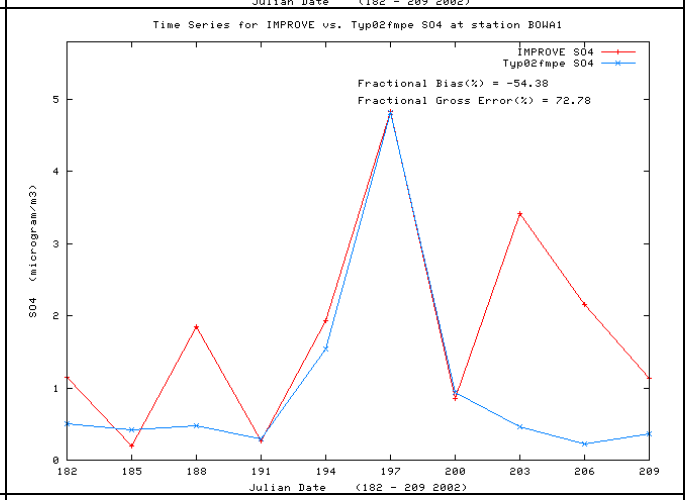


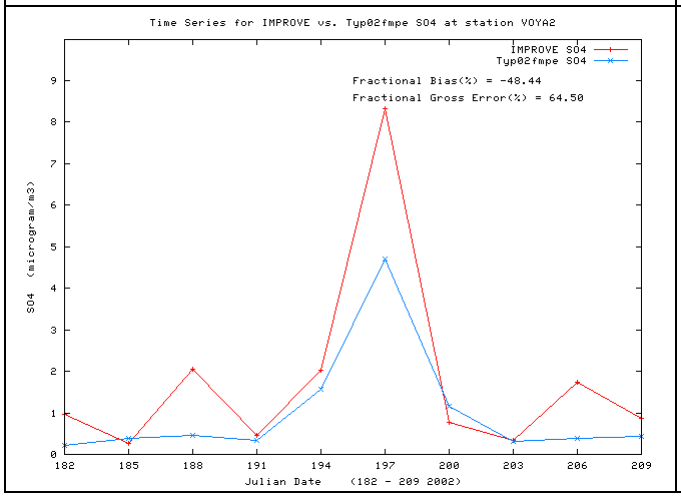
Figure C-6a. Scatter plots of predicted and observed sulfate (SO4) concentrations for July 2002 and sites in the CENRAP region using IMPROVE (top left), STN (top right), CASTNet (bottom left) and NADP monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

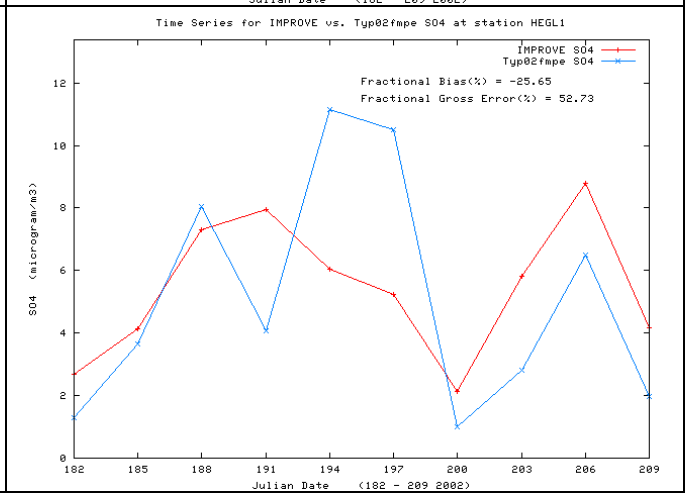

Time Series for IMPROVE vs. Typ02fmpe SO4 at station CACR1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -61.12
Fractional Gross Error(%) = 62.43
SO4 (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station UPBU1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -56.93
Fractional Gross Error(%) = 56.93
SO4 (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station BRET1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -122.23
Fractional Gross Error(%) = 122.23
SO4 (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station BOWA1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -54.38
Fractional Gross Error(%) = 72.78
SO4 (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station VOYA2
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -48.44
Fractional Gross Error(%) = 64.50
SO4 (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station HEGL1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -25.65
Fractional Gross Error(%) = 52.73
SO4 (microgram/m3)
Julian Date (182 - 209 2002)

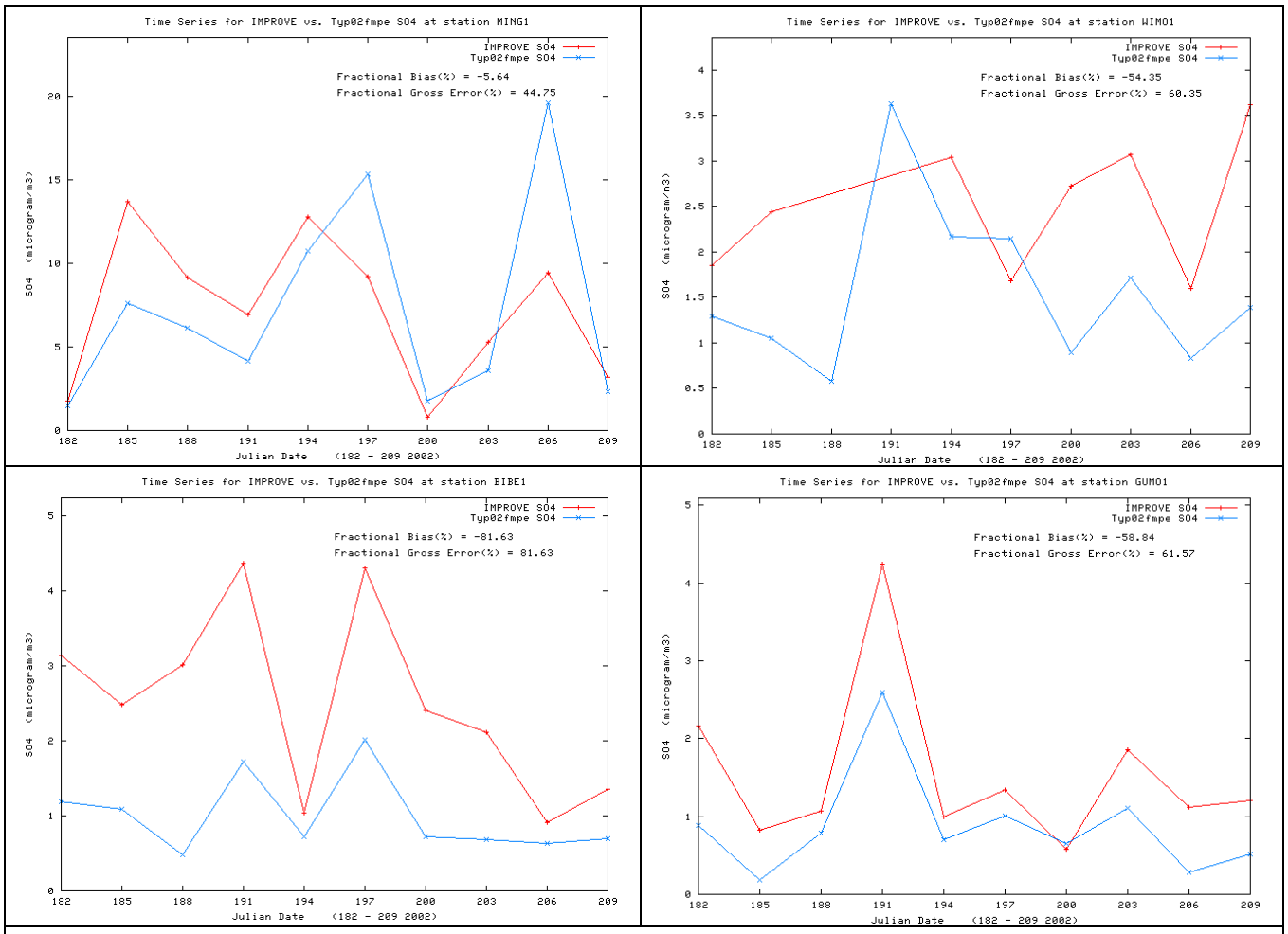


Figure C-6b. Time series of predicted and observed 24-hour sulfate (SO4) concentrations at CENRAP IMPROVE CLASS I AREA sites in July 2002 for CMAQ 2002 36 km Base F base case simulation.

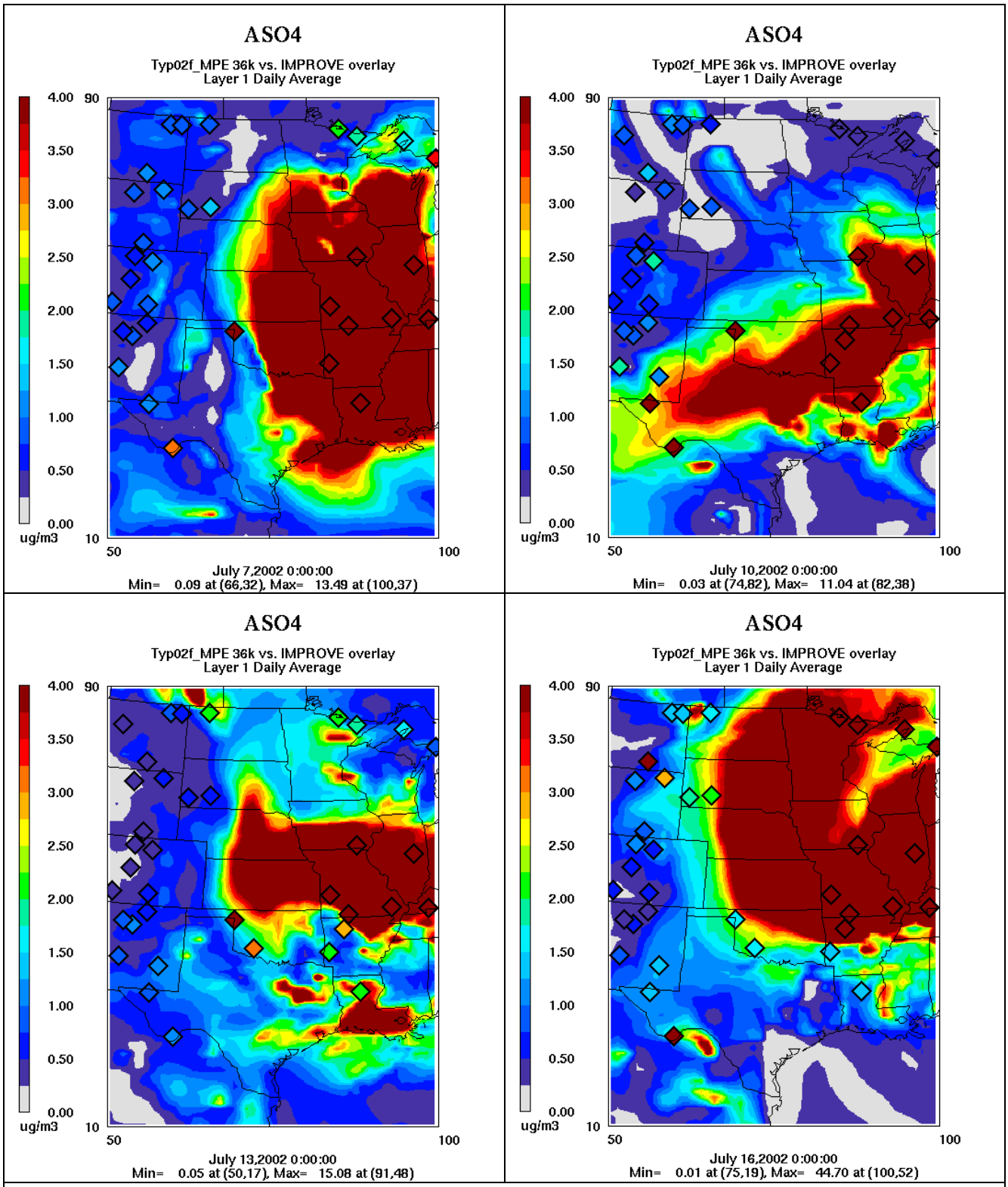


Figure C-6c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour SO4 concentrations for July 7, 10, 13 and 16, 2002.

C.3.1.4 SO4 in October 2002

In October 2002, CMAQ is doing a better job of reproducing the observed SO4 concentrations with much lower fractional bias values (-6%, 0% and -23%) and fractional errors < 40% (Figure C-7a). The observed SO4 time series are also reproduced well by the model, although an under-prediction bias is clearly evident at Big Bend, Guadalupe Mountains and Wichita Mountains. The model also reproduces the observed spatial distribution of SO4 well in October (Figure C-7c).

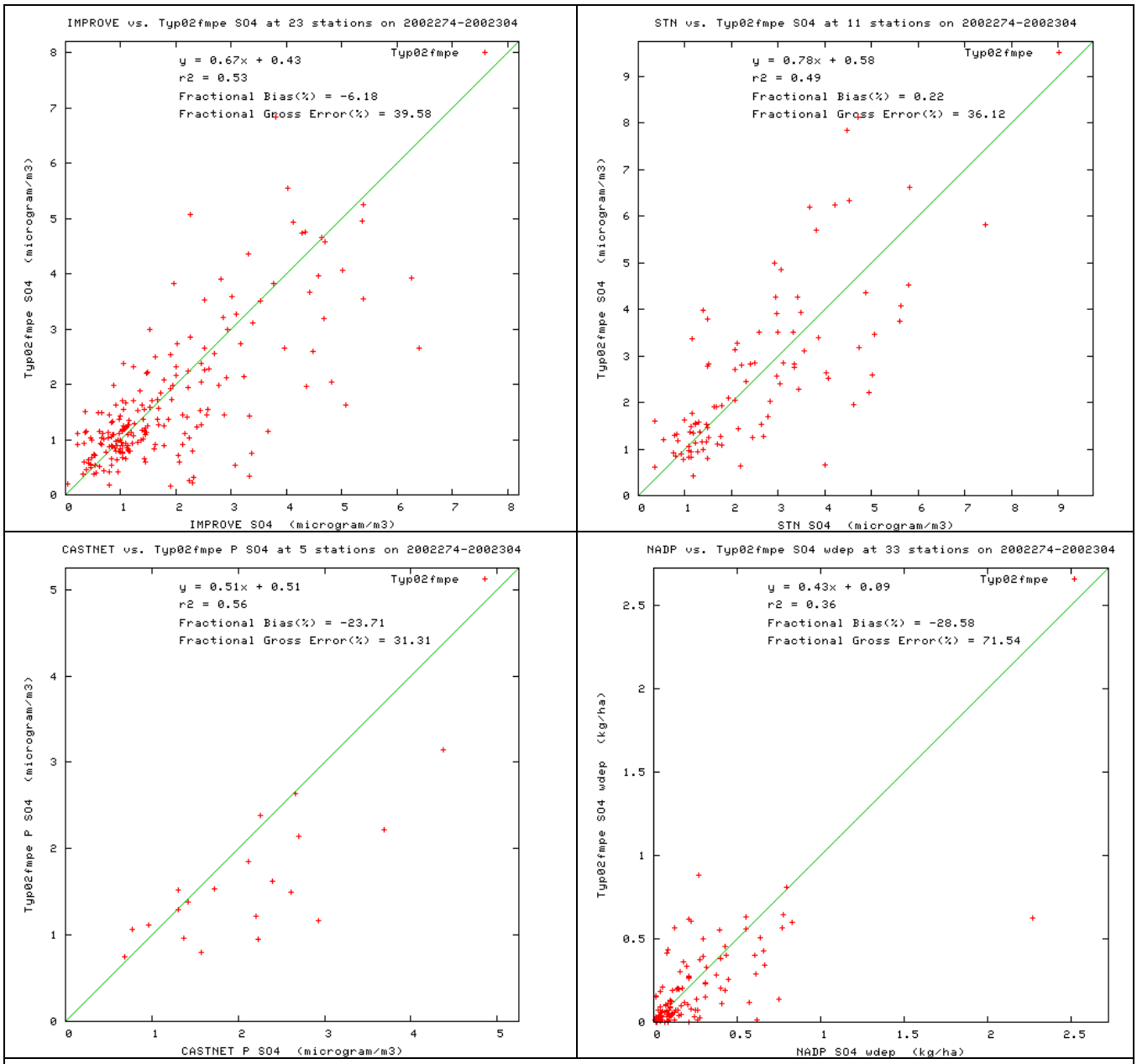
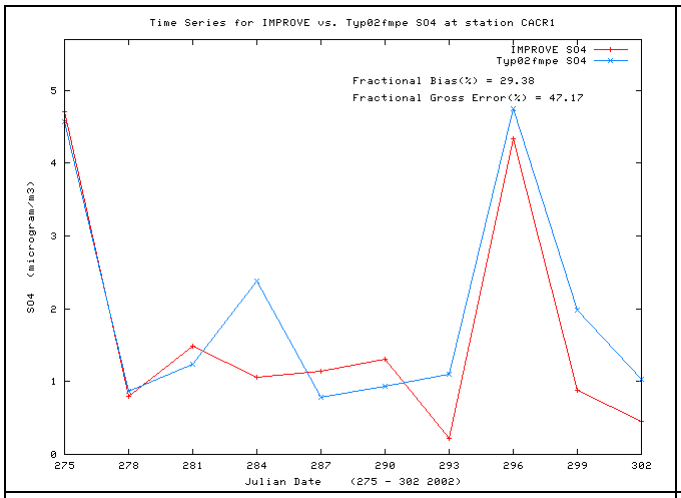
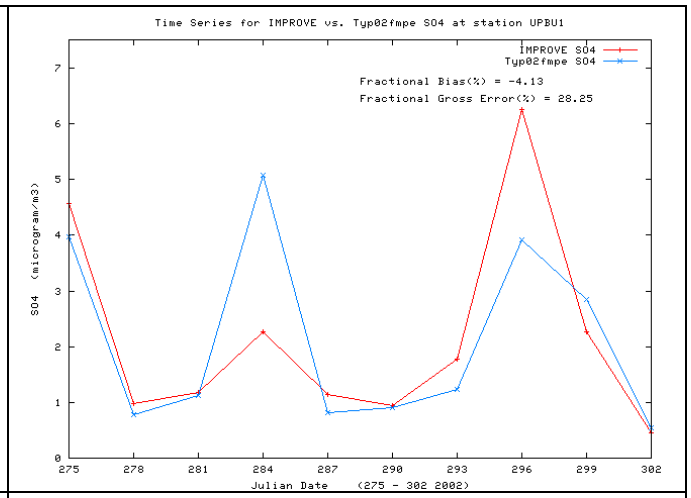
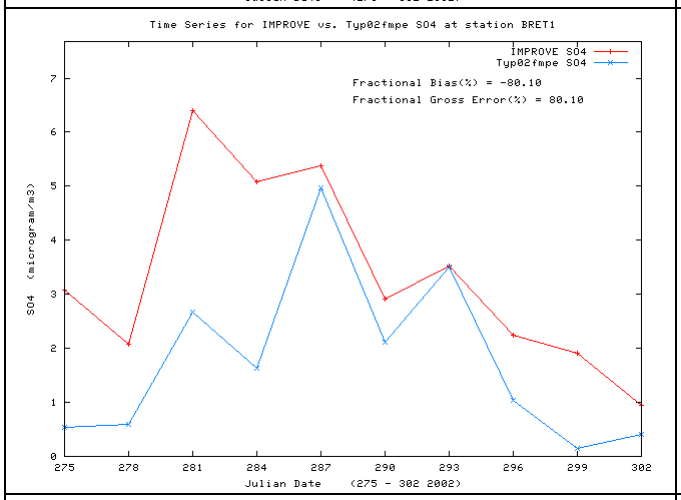
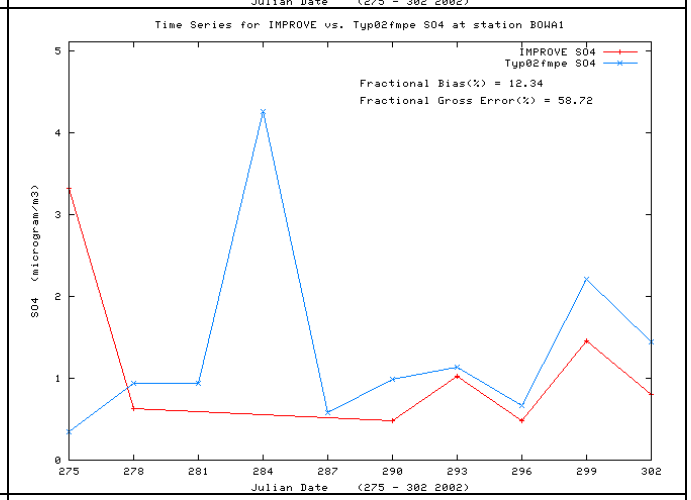


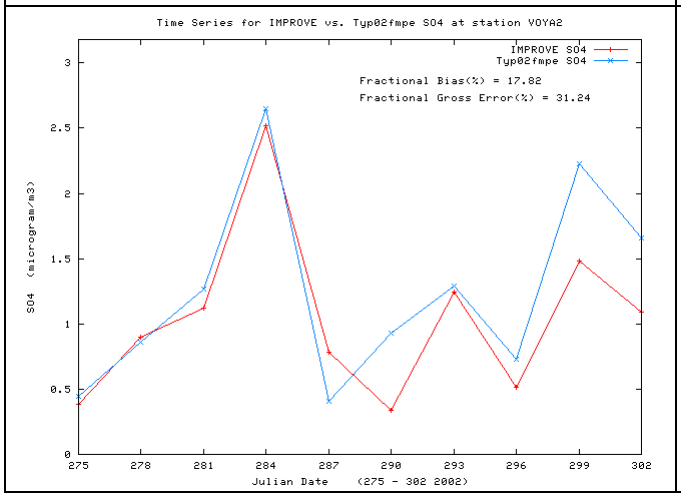
Figure C-7a. Scatter plots of predicted and observed sulfate (SO4) concentrations for October 2002 and sites in the CENRAP region using IMPROVE (top left), STN (top right), CASTNet (bottom left) and NADP monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

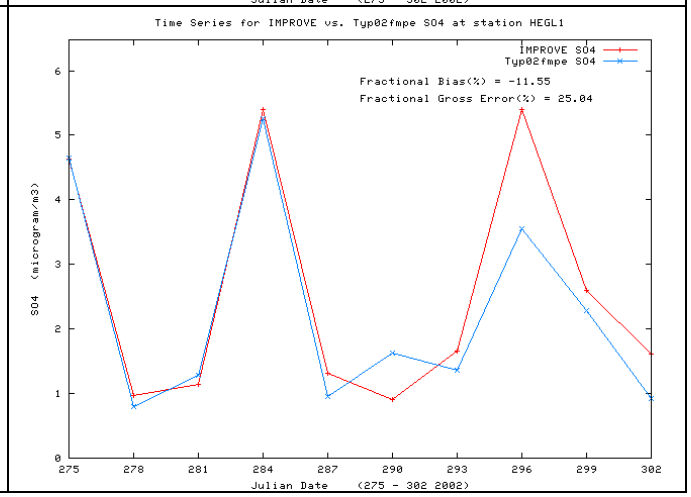

Time Series for IMPROVE vs. Typ02fmpe SO4 at station CACR1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = 29.38
Fractional Gross Error(%) = 47.17
SO4 (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station UPBU1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -4.13
Fractional Gross Error(%) = 28.25
SO4 (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station BRET1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -80.10
Fractional Gross Error(%) = 80.10
SO4 (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station BOWA1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = 12.34
Fractional Gross Error(%) = 58.72
SO4 (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station VOYA2
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = 17.82
Fractional Gross Error(%) = 31.24
SO4 (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe SO4 at station HEGL1
IMPROVE SO4
Typ02fmpe SO4
Fractional Bias(%) = -11.55
Fractional Gross Error(%) = 25.04
SO4 (microgram/m3)
Julian Date (275 - 302 2002)

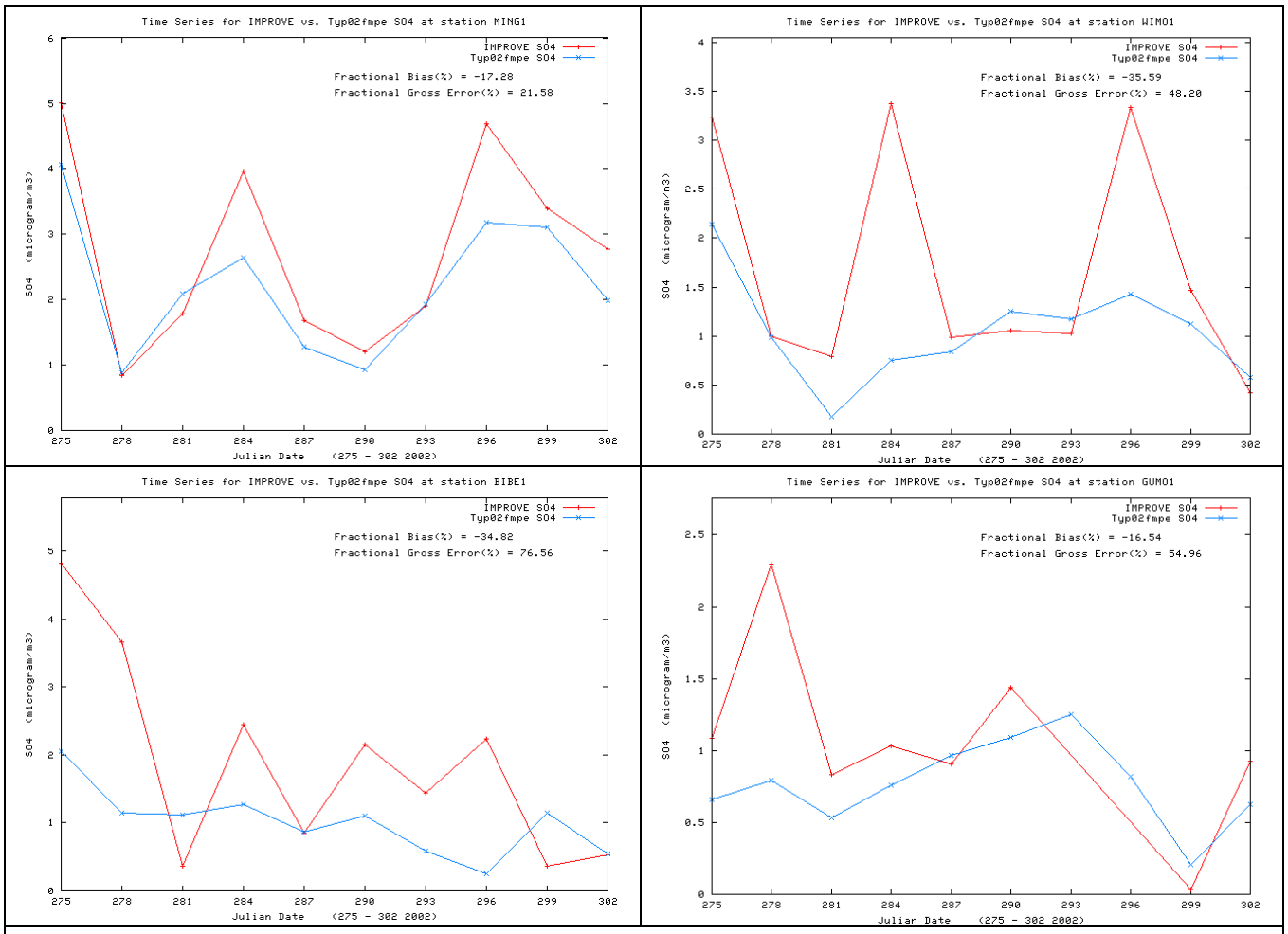


Figure C-7b. Time series of predicted and observed 24-hour sulfate (SO4) concentrations at CENRAP IMPROVE CLASS I AREA sites in October 2002 for CMAQ 2002 36 km Base F base case simulation.

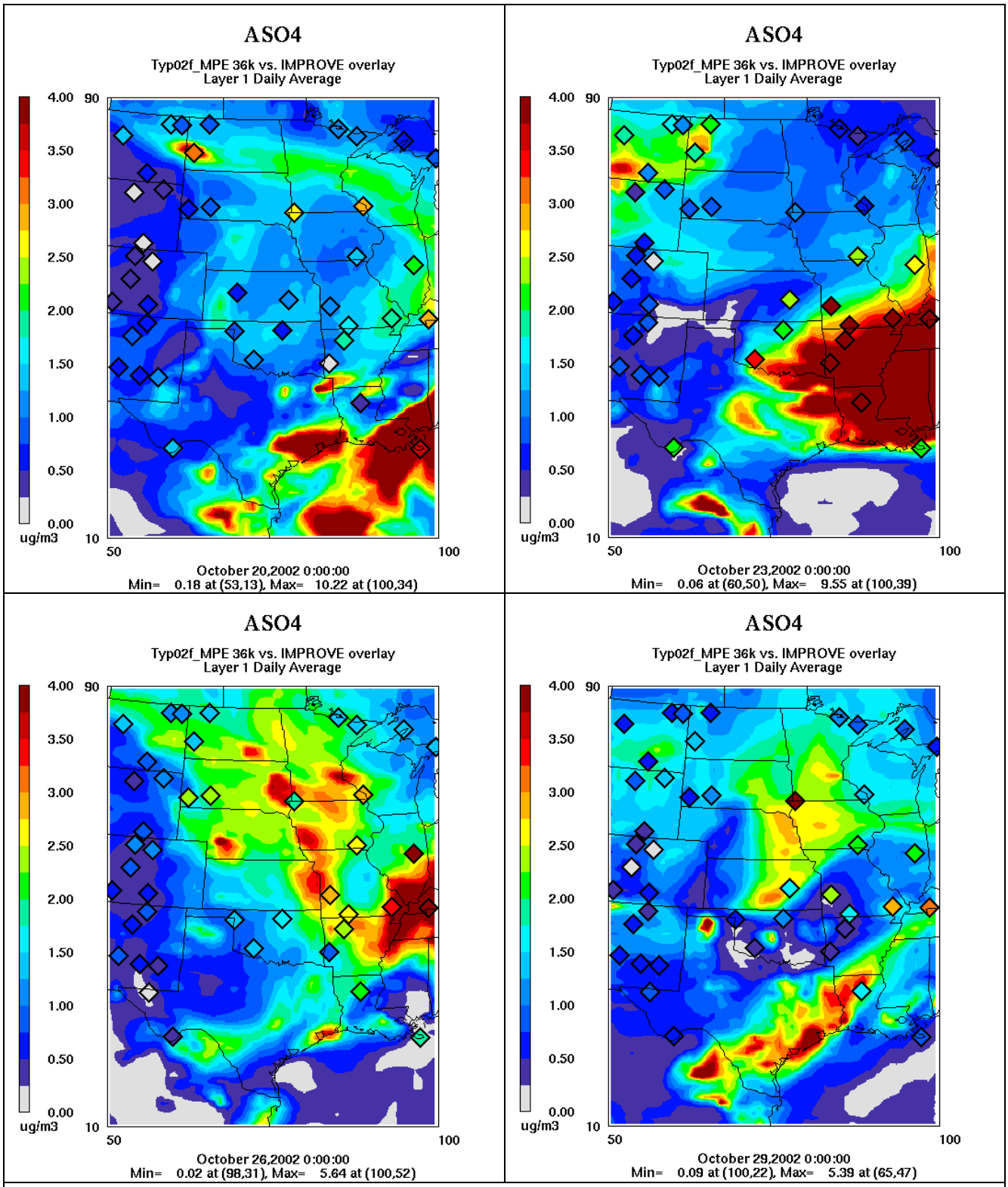


Figure C-7c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour SO4 concentrations for October 20, 23, 26 and 29, 2002.

C.3.1.5 SO4 Monthly Bias and Error

Figure C-8 compares the monthly SO4 fractional bias and error across the CENRAP region for the three monitoring networks. The under-prediction bias is clearly evident the first 8-10 months of the year. This underestimation bias is greatest across the CASTNet network which persists through out the year and is least for the STN network where it disappears by August-September. The monthly SO4 fractional errors are generally between 30% and 60% and are greatest in the summer when SO4 concentrations are the highest.

Figure C-9 presents a Bugle Plot of monthly So4 fractional bias and error statistics and compares them against the proposed PM model performance goal and criteria (see Table C-3). For the STN network, it appears that SO4 performance for all months achieves the proposed PM model performance goal. For the IMPROVE network, approximately half of the months achieve the proposed PM performance goal with the other half exceed the goal but within the performance criteria. Across the CASTNet network most months exceed the proposed goal and are within the criteria. Although the CASTNet fractional bias for some months is right at the criteria (≤±60%). With the exception of two IMPROVE months, all of the monthly SO4 fractional error performance statistics achieve the proposed PM model performance goal.

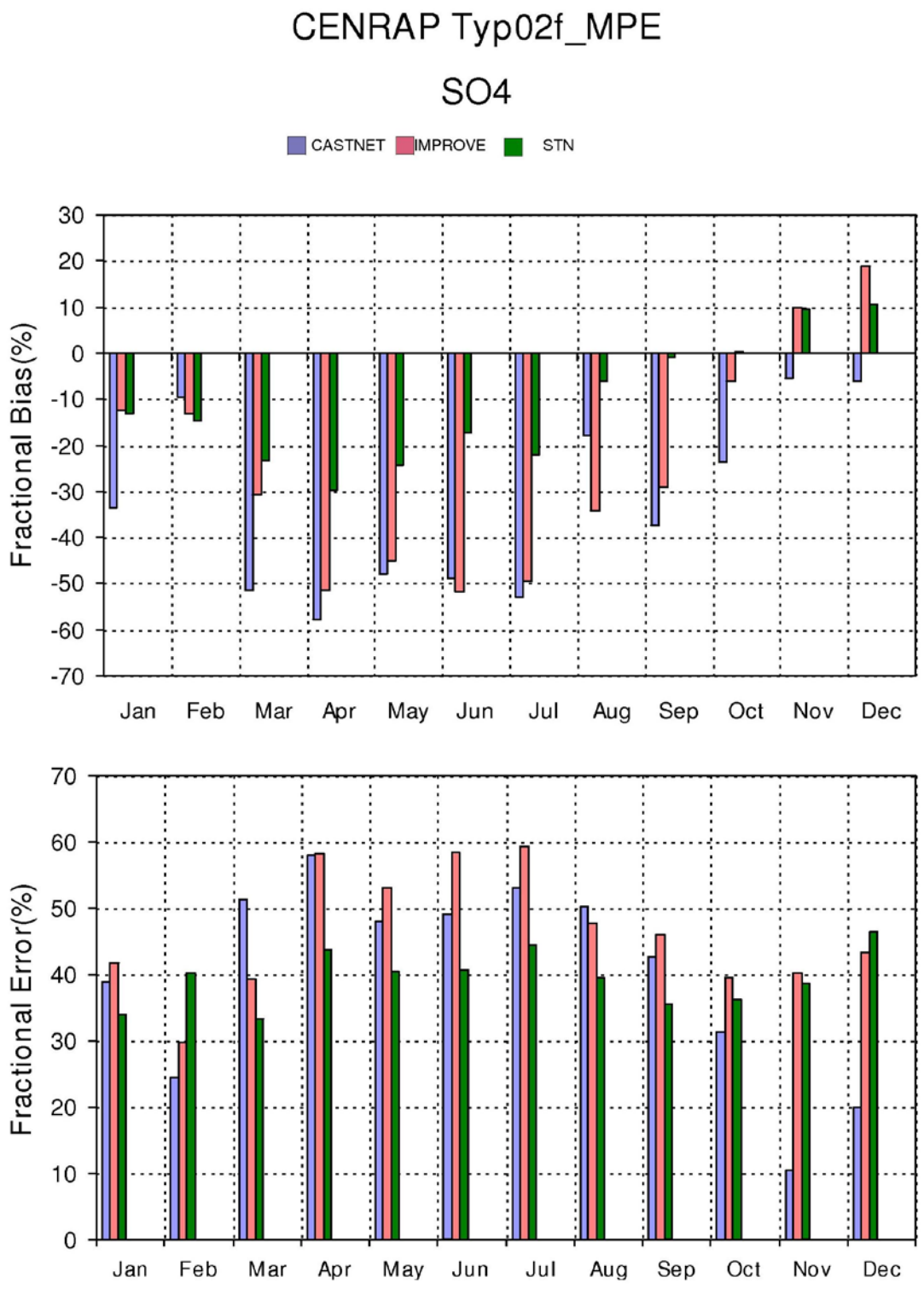


Figure C-8. Monthly SO4 fractional bias (top) and fractional gross error (bottom) statistical measures for IMPROVE, STN and CASTNet monitoring sites in the CENRAP region.

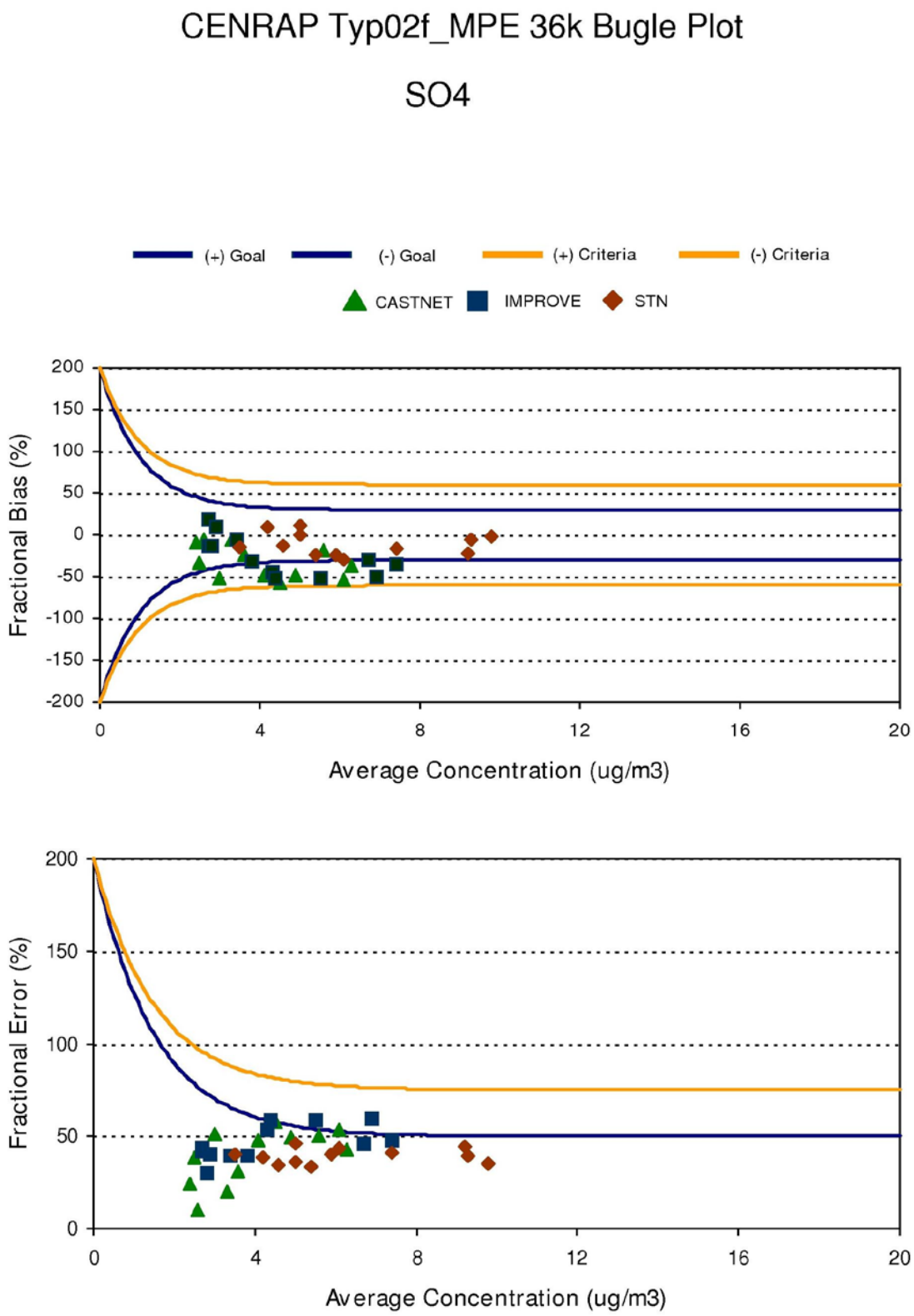


Figure C-9. Bugle Plots of monthly fractional bias (top) and fractional gross error (bottom) and comparisons with model performance goals and criteria for SO4 and IMPROVE, STN and CASTNet monitoring sites in the CENRAP region.

C.3.2 Nitrate (NO3) Monthly Model Performance

The following sections discuss the monthly NO3 model performance across the IMPROVE, STN and CASTNet monitoring networks in the CENRAP region.

C.3.2.1 NO3 in January 2002

January NO3 CMAQ model performance is characterized by an overestimation bias across the CENRAP region (Figure C-10a). The fractional bias values for the IMPROVE, STN and CASTNet networks are 38%, 29% and 61%. Unlike SO4, wet deposition of NO3 is also overstated in January (43%). Fractional errors range from 90%-100% for the IMPROVE and CASTNet networks and are lower (54%) for the STN network and higher (114%) for the NADP network.

With the exception of Breton Island and Big Bend, the model NO3 over-prediction bias occurs at the other 8 CENRAP Class I areas (Figure C-10b). The observed time series is reproduced reasonable well at a couple sites, such as Wichita Mountains and the first half of January for Voyageurs. However, for most sites the observed NO3 time series is not reproduced very well and is extremely poorly reproduced for Breton Island, Big Bend and Guadalupe Mountains.

The model typically estimates a larger area of elevated NO3 concentrations than is observed. This is shown for January 20, 23, 26 and 29 in Figure C-10c. Whereas the model exhibits large areas of brown indicated daily average NO3 concentrations of 4 $\mu g/m^3$ or higher, the observed values of this high rarely occur and are usually limited to the central Illinois site. On January 20 the model estimates the entire eastern half of the CENRAP region should be covered by elevated NO3 concentrations, whereas the observations indicate much lower values. On January 23 the modeled elevated NO3 concentrations lies between the IMPROVE monitoring sites, although the central Illinois site suggests high NO3 did occur in the region. The observations on January 26 also suggest lower NO3 than the model is predicting. On January 29 the model estimates elevated NO3 from the central Illinois site to Wichita Mountains, Oklahoma that is supported by these two observations. In general, the model is estimating more wide-spread elevated NO3 concentrations than observed, whereas the observations suggest that the elevated NO3 occurrences is less frequent and more spotty.

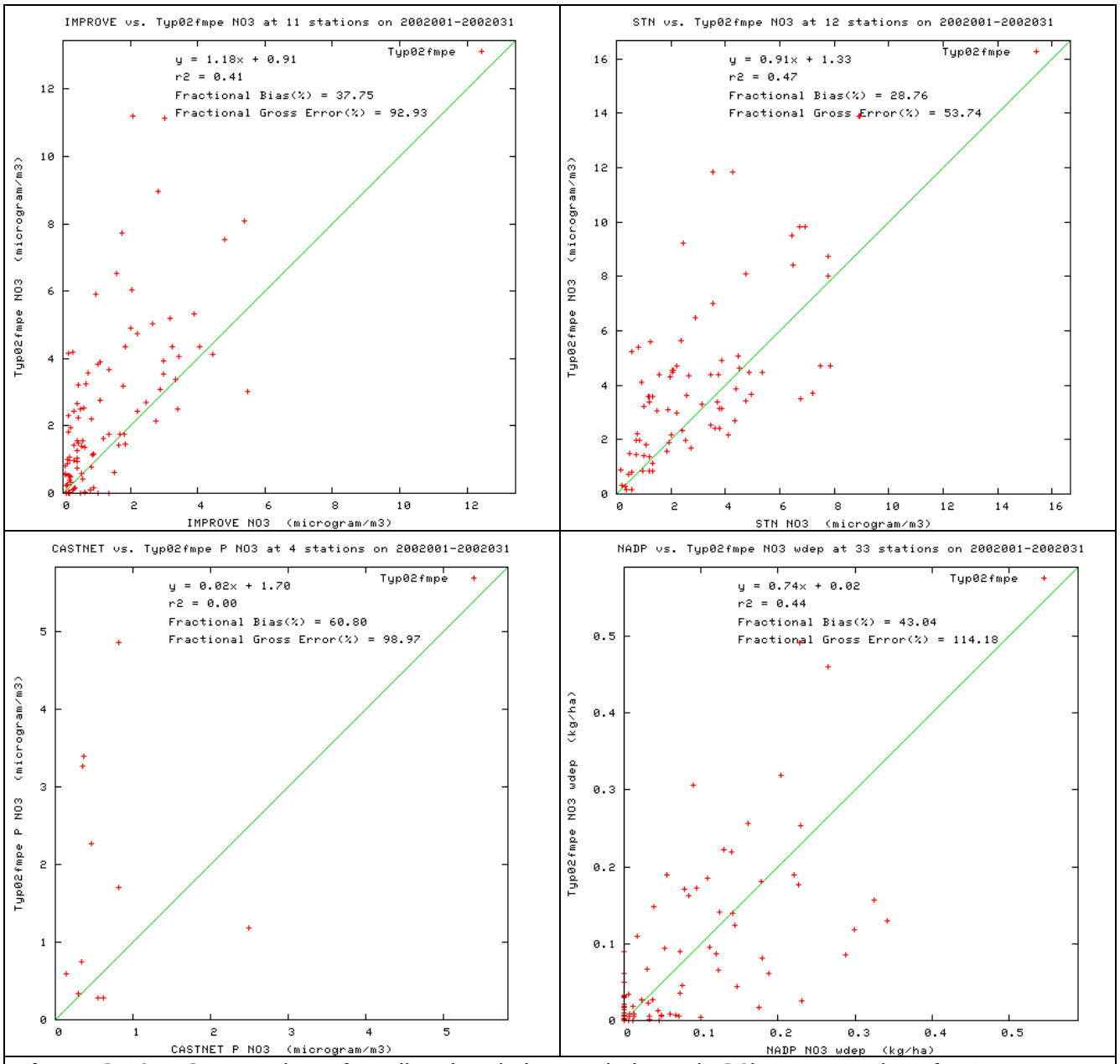
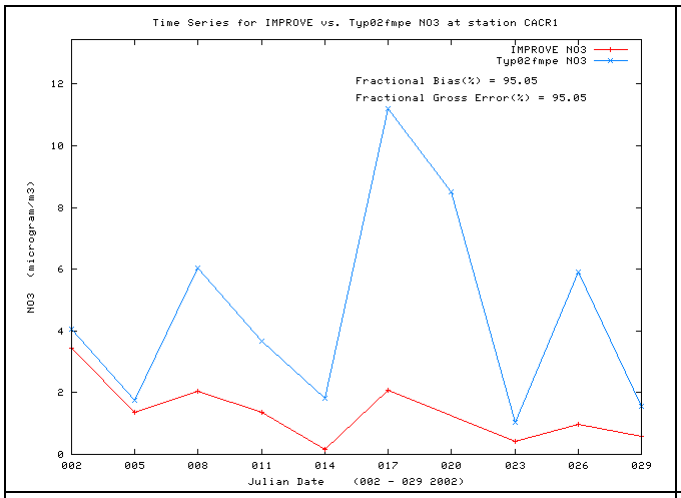
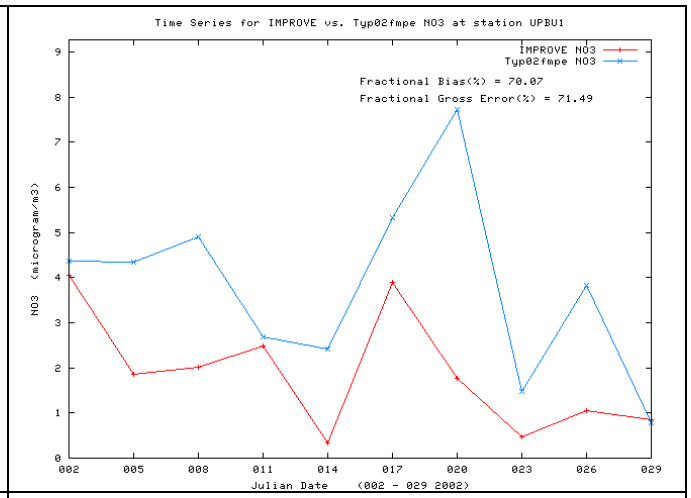
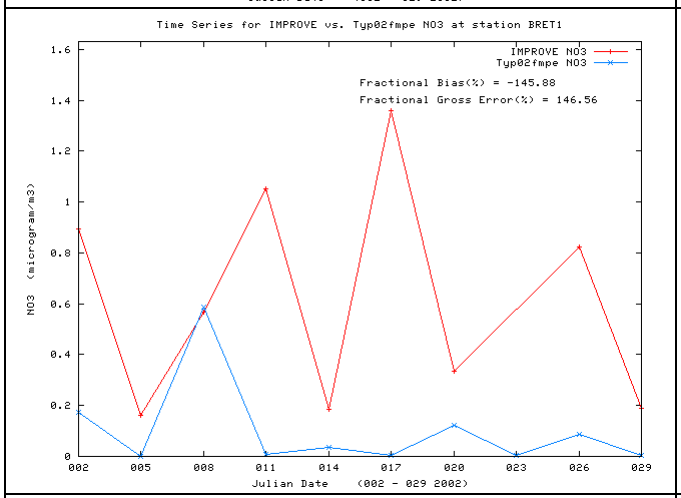
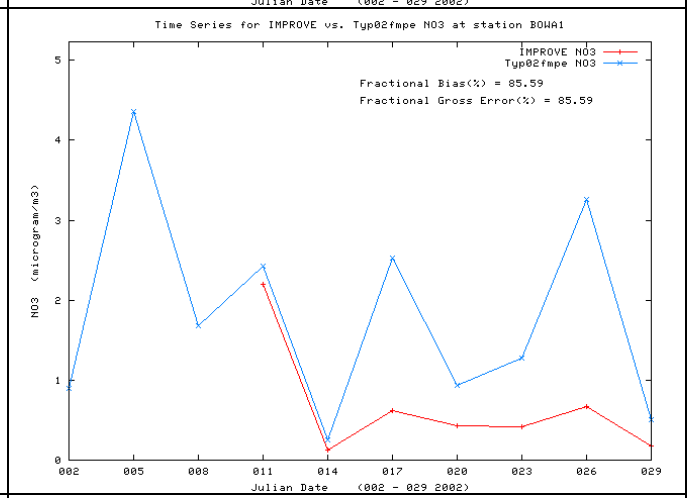


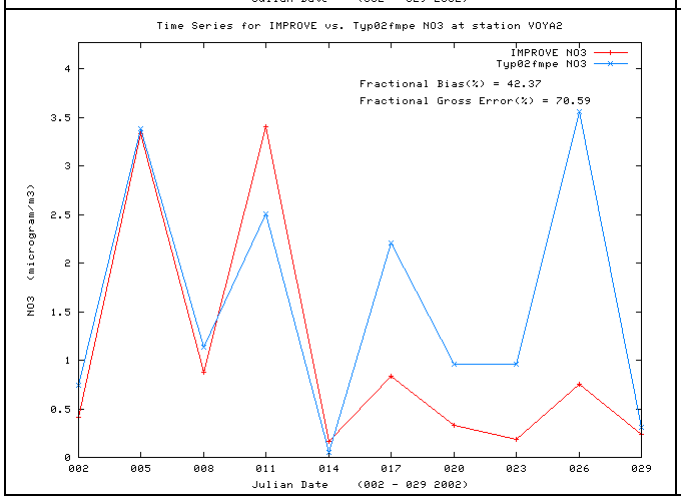
Figure C-10a. Scatter plots of predicted and observed nitrate (NO3) concentrations for January 2002 and sites in the CENRAP region using IMPROVE (top left), STN (top right), CASTNet (bottom left) and NADP monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

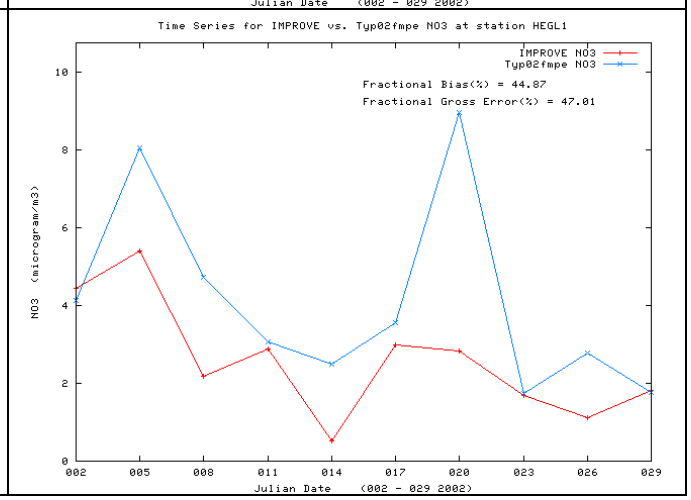

Time Series for IMPROVE vs. Typ02fmpe NO3 at station CACR1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 95.05
Fractional Gross Error(%) = 95.05
NO3 (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station UPBU1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 70.07
Fractional Gross Error(%) = 71.49
NO3 (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station BRET1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -145.88
Fractional Gross Error(%) = 146.56
NO3 (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station BOWA1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 85.59
Fractional Gross Error(%) = 85.59
NO3 (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station VOYA2
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 42.37
Fractional Gross Error(%) = 70.59
NO3 (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station HEGL1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 44.87
Fractional Gross Error(%) = 47.01
NO3 (microgram/m3)
Julian Date (002 - 029 2002)

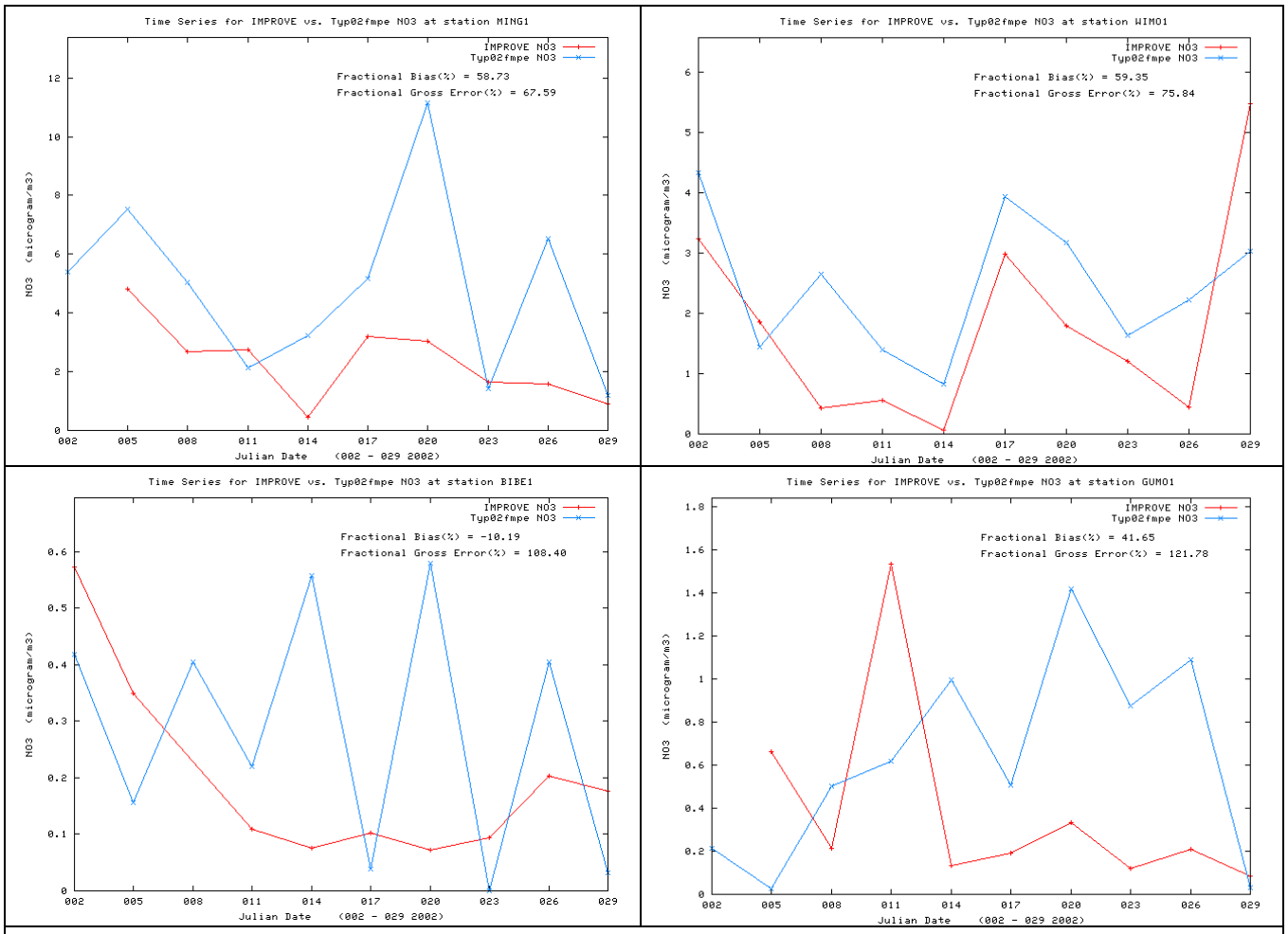


Figure C-10b. Time series of predicted and observed 24-hour nitrate (NO3) concentrations at CENRAP IMPROVE CLASS I AREA sites in January 2002 for CMAQ 2002 36 km Base F base case simulation.

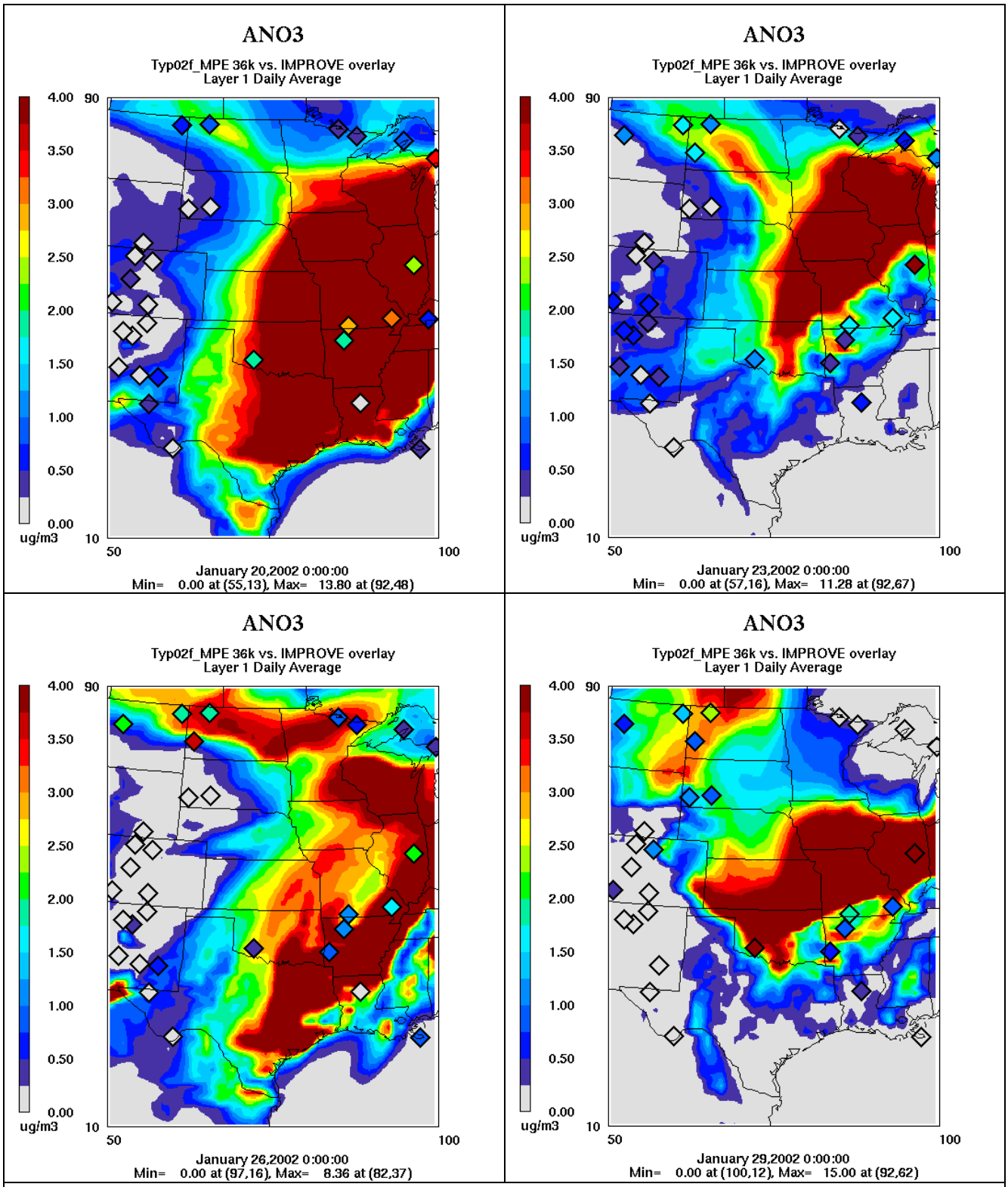


Figure C-10c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour NO3 concentrations for January 20, 23, 26 and 29, 2002.

C.3.2.2 NO3 in April 2002

Unlike the NO3 overestimation bias of January, the April NO3 performance is characterized by an underestimation bias (Figure C-11a). This under-prediction bias appears to be driven by near zero model predictions when the observed values are small (< 1 $\mu g/m^3$), but positive. This effect is especially noticeable in the NO3 time series (Figure C-11b) where at several sites the modeled NO3 concentrations foes to zero (e.g., BRET, BIBE, GUMO), whereas the observed values has an approximately 0.2 μg/m3 floor. The spatial maps suggest that the large April NO3 under-prediction bias indicated by the performance statistics is not as bad as they suggest (Figure C-11c). Mostly the model is predicting low NO3 values where low values are observed, just that the model approaches zero which results in a large relative difference with the observe values.

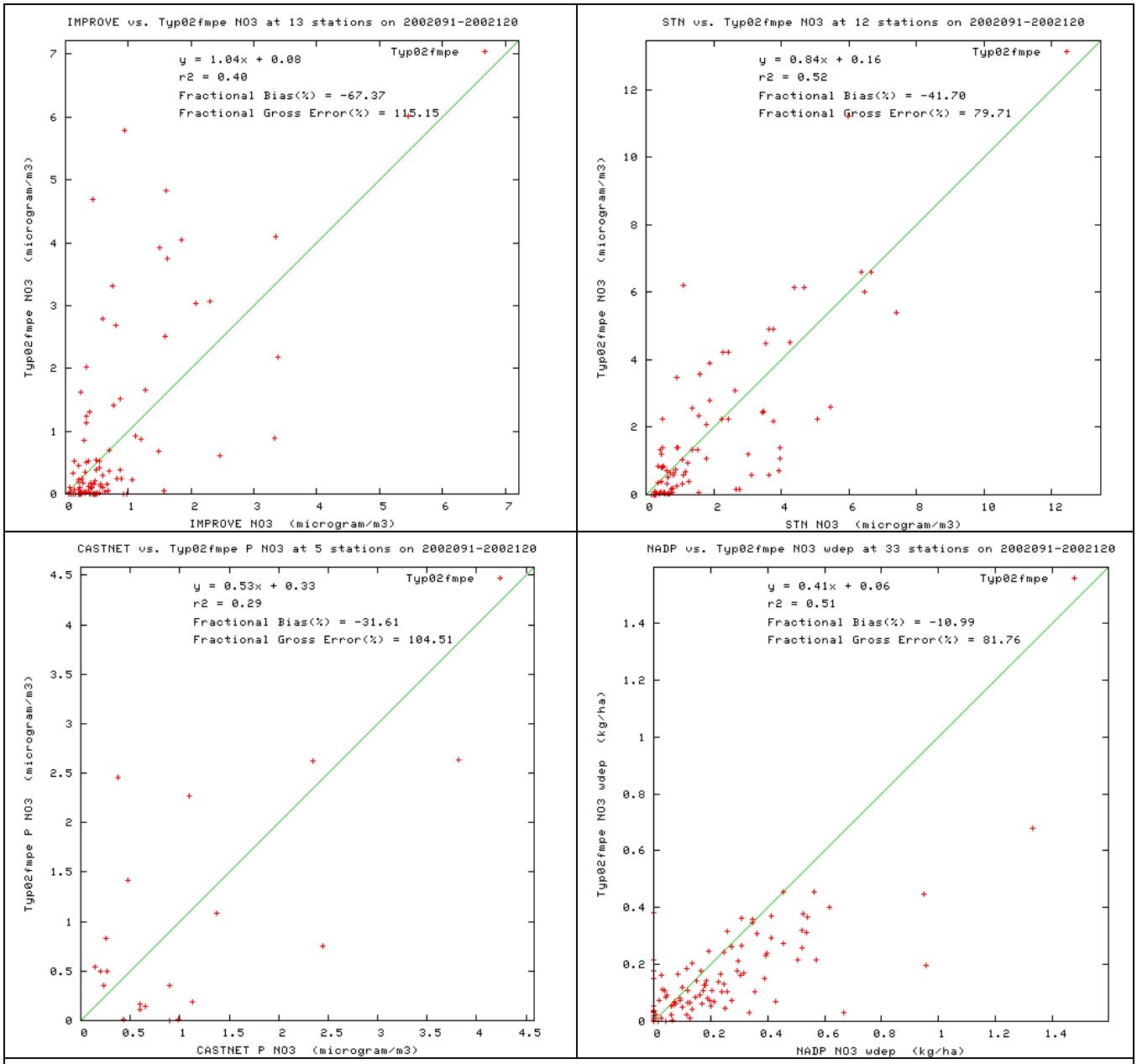
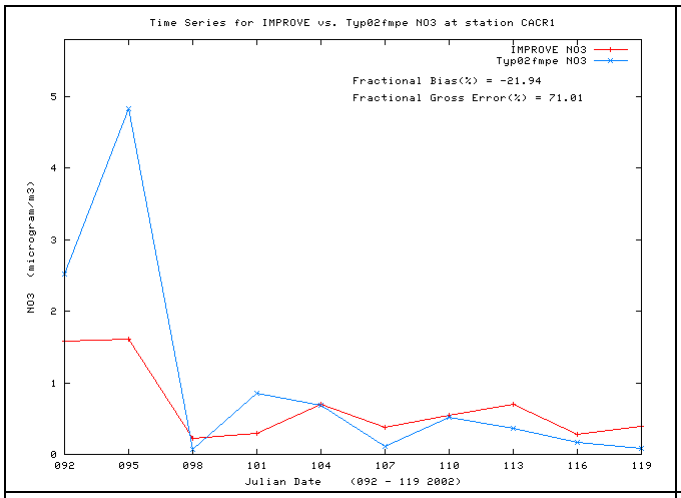
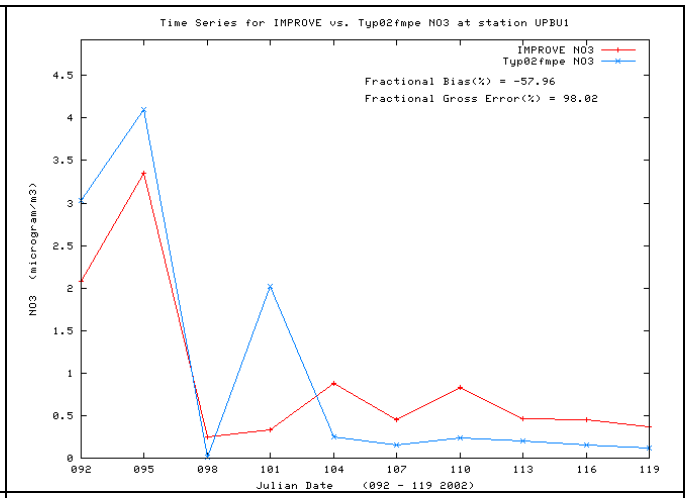
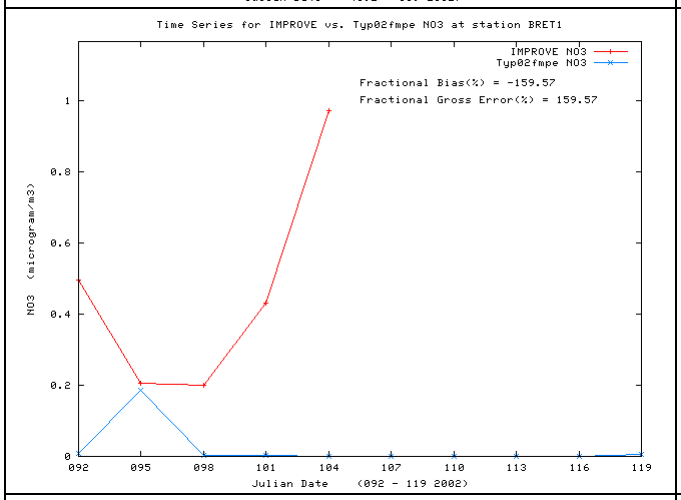
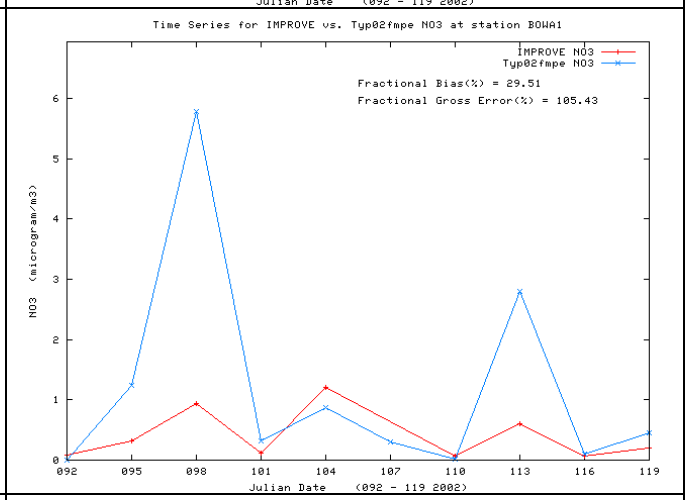


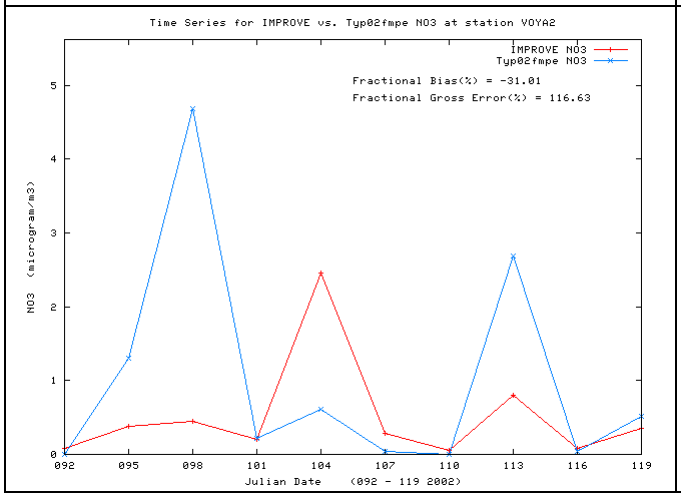
Figure C-11a. Scatter plots of predicted and observed nitrate (NO3) concentrations for April 2002 and sites in the CENRAP region using IMPROVE (top left), STN (top right), CASTNet (bottom left) and NADP monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

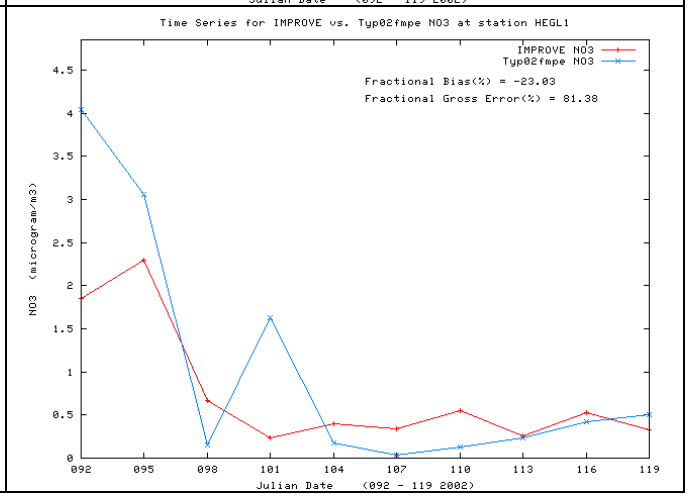

Time Series for IMPROVE vs. Typ02fmpe NO3 at station CACR1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -21.94
Fractional Gross Error(%) = 71.01
NO3 (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station UPBU1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -57.96
Fractional Gross Error(%) = 98.02
NO3 (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station BRET1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -159.57
Fractional Gross Error(%) = 159.57
NO3 (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station BOWA1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 29.51
Fractional Gross Error(%) = 105.43
NO3 (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station VOYA2
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -31.01
Fractional Gross Error(%) = 116.63
NO3 (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station HEGL1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -23.03
Fractional Gross Error(%) = 81.38
NO3 (microgram/m3)
Julian Date (092 - 119 2002)

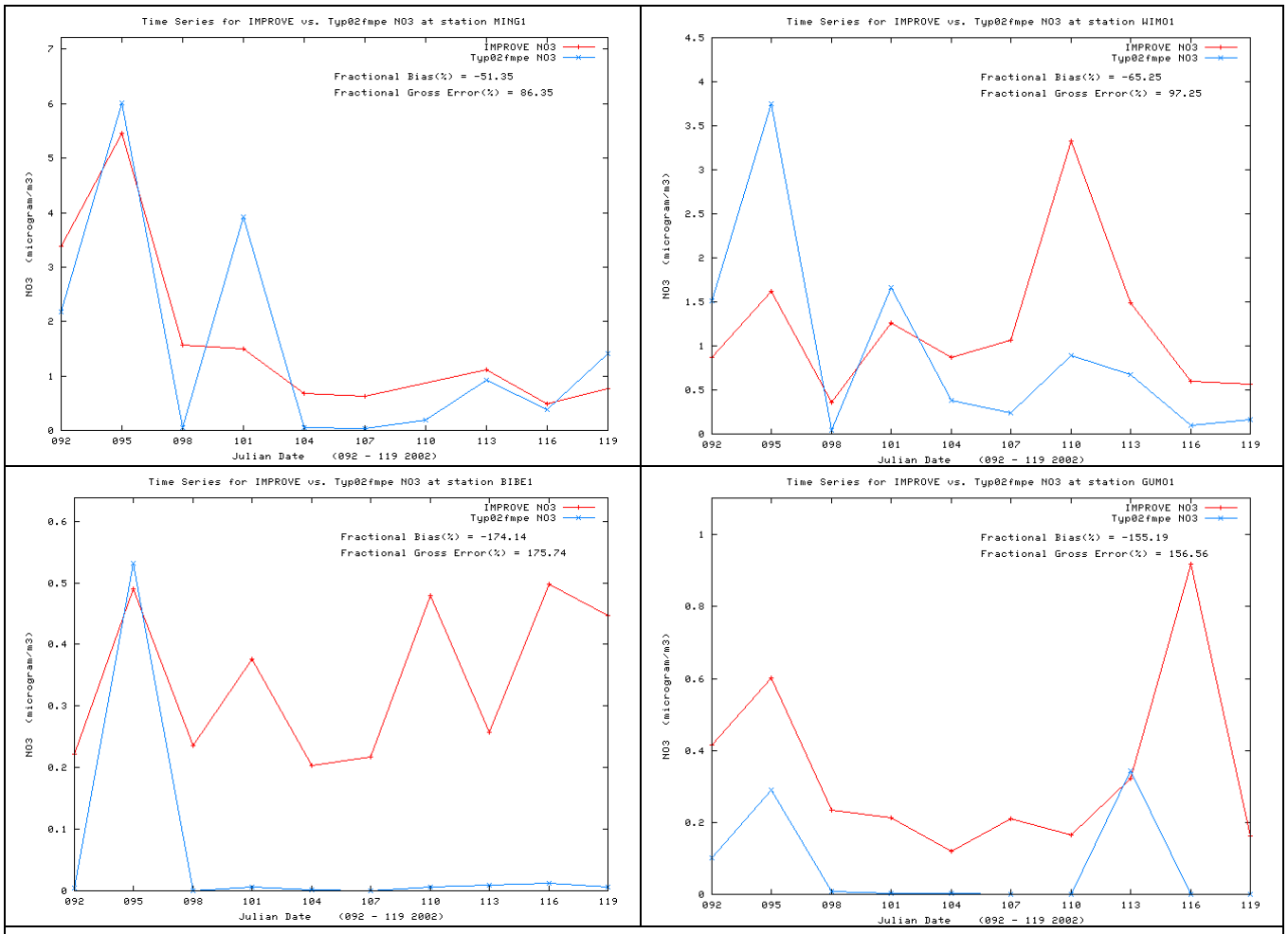


Figure C-11b. Time series of predicted and observed 24-hour nitrate (NO3) concentrations at CENRAP IMPROVE CLASS I AREA sites in April 2002 for CMAQ 2002 36 km Base F base case simulation.

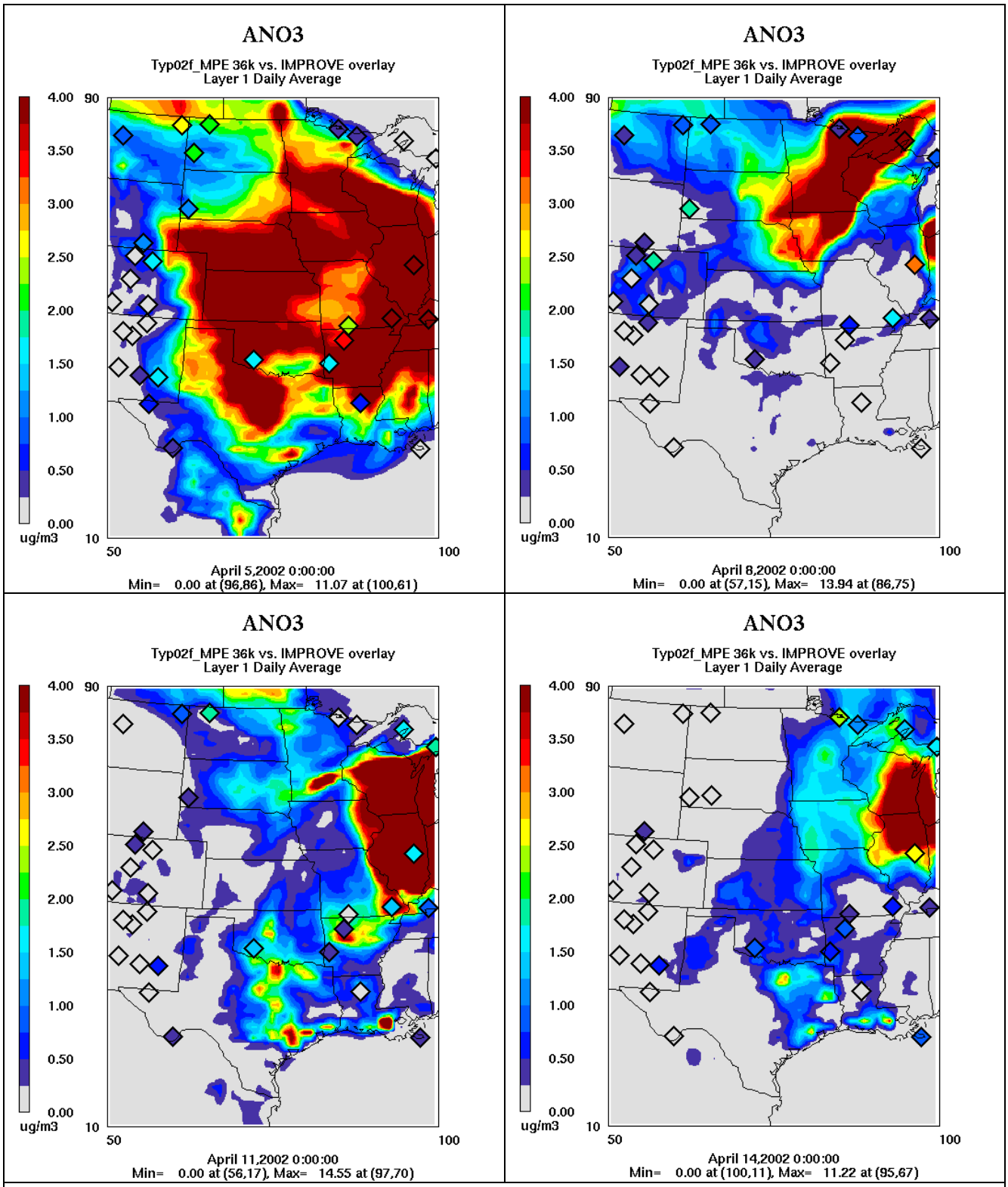


Figure C-11c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour NO3 concentrations for April 5, 8, 11 and 14, 2002.

C.3.2.3 NO3 in July 2002

NO3 performance in July 2002 is also characterized by a large under-prediction bias that is driven by the frequent occurrence of near zero modeled values (Figure C-12). Both the model and observations agree that NO3 is mostly extremely low in July, just the model produces near zero values and resultant poor performance statistics.

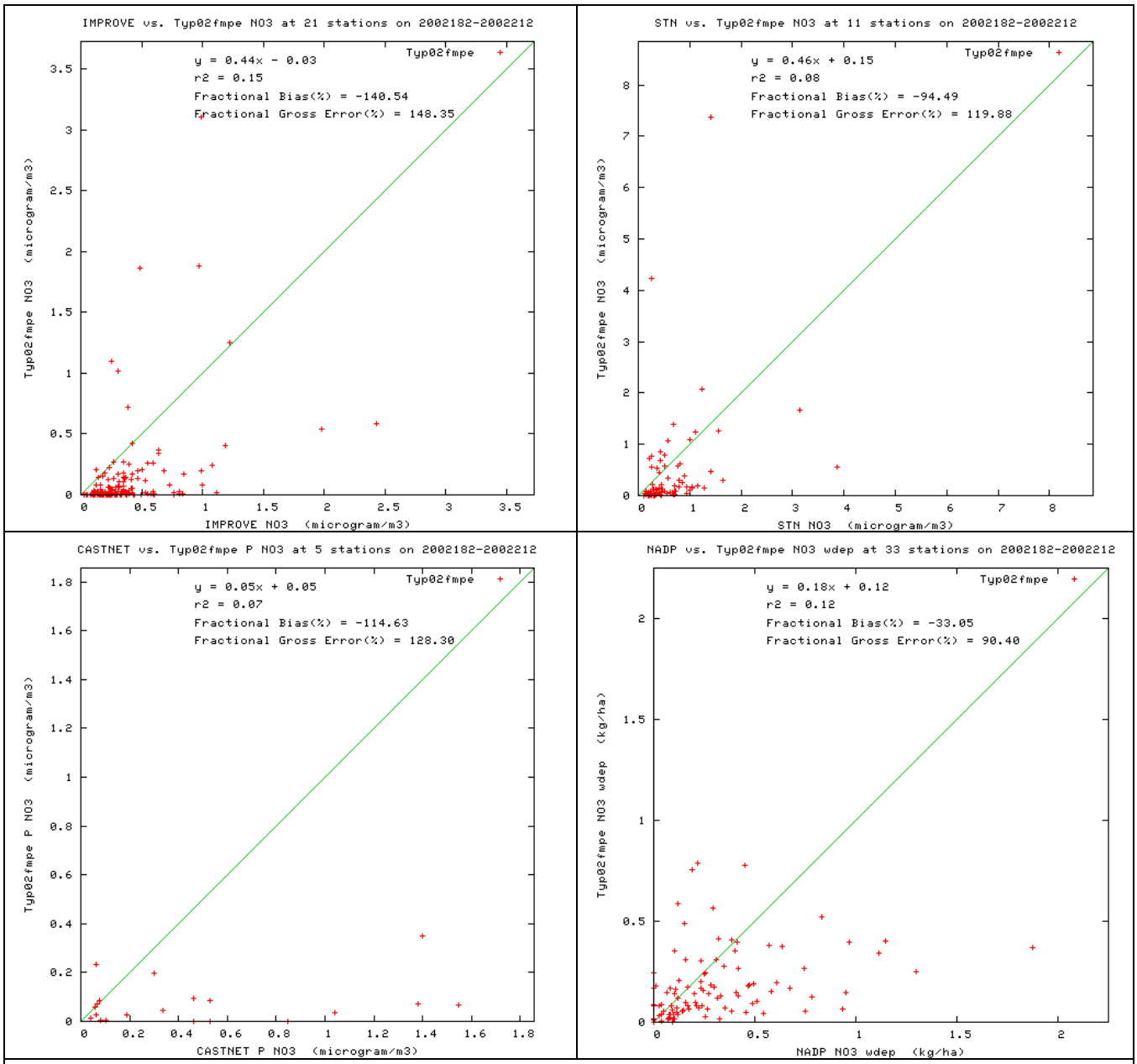
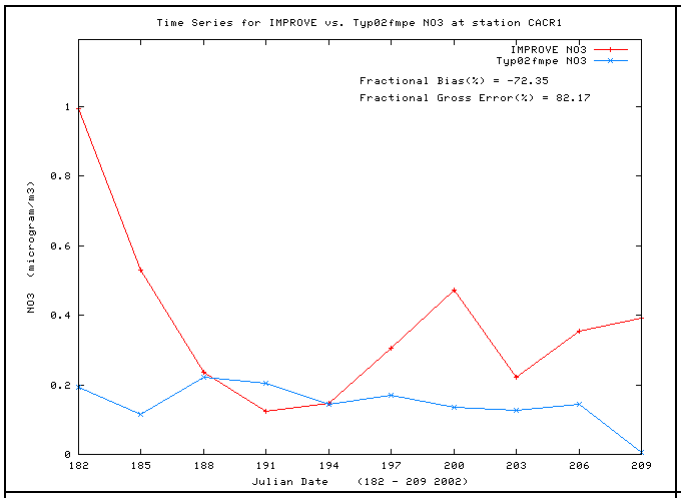
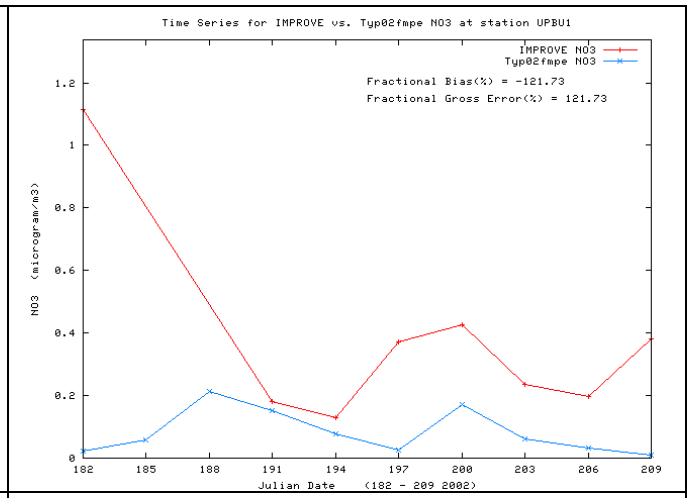
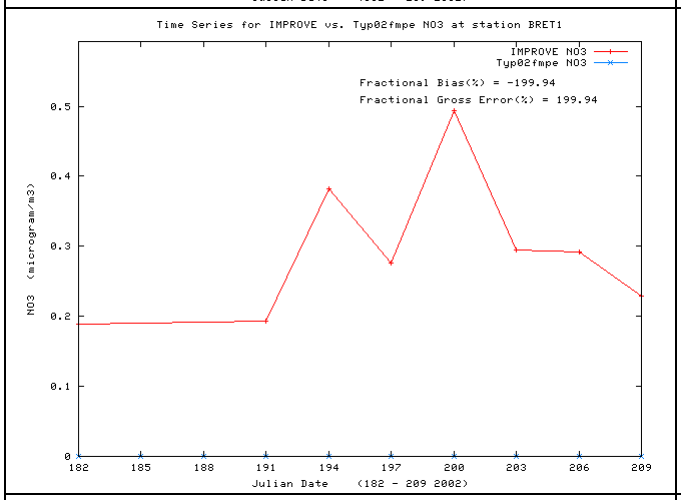
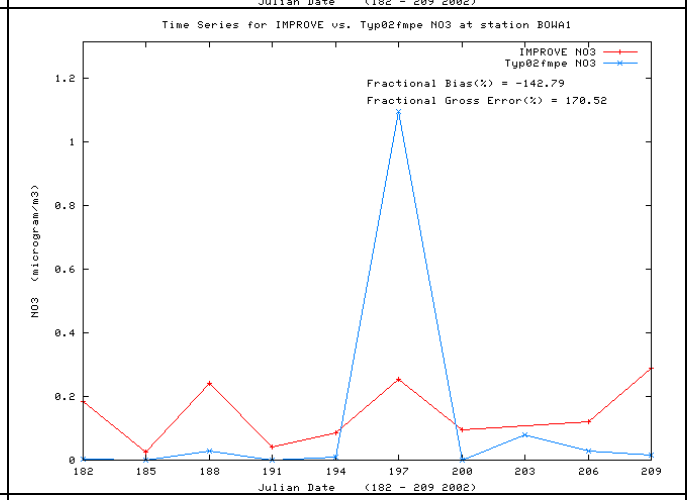


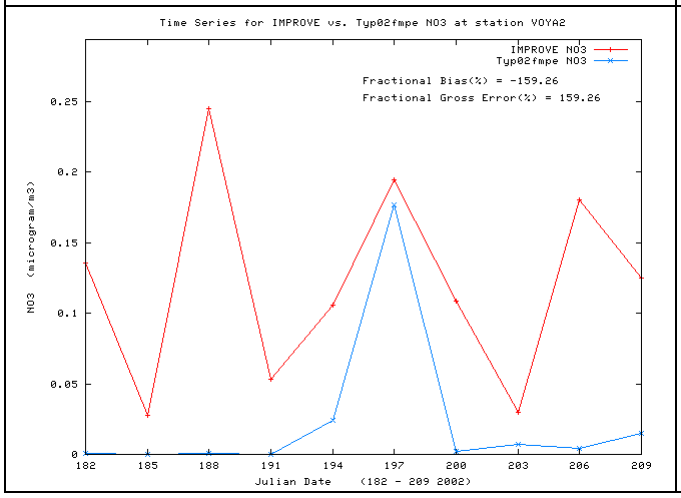
Figure C-12a. Scatter plots of predicted and observed nitrate (NO3) concentrations for July 2002 and sites in the CENRAP region using IMPROVE (top left), STN (top right), CASTNet (bottom left) and NADP monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

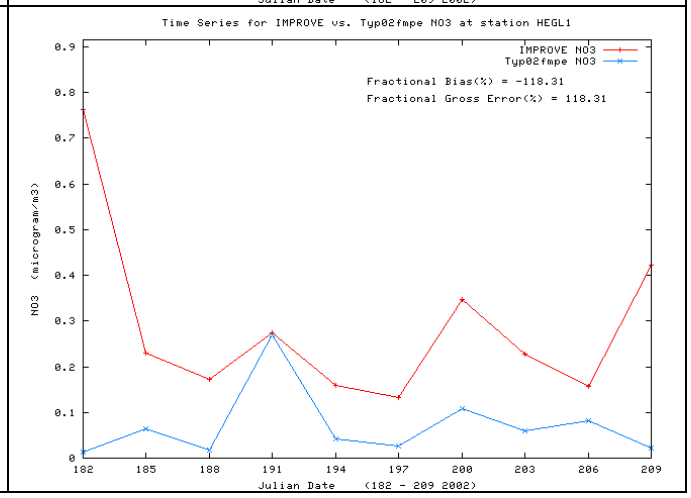

Time Series for IMPROVE vs. Typ02fmpe NO3 at station CACR1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -72.35
Fractional Gross Error(%) = 82.17
NO3 (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station UPBU1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -121.73
Fractional Gross Error(%) = 121.73
NO3 (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station BRET1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -199.94
Fractional Gross Error(%) = 199.94
NO3 (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station BOWA1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -142.79
Fractional Gross Error(%) = 170.52
NO3 (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station VOYA2
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -159.26
Fractional Gross Error(%) = 159.26
NO3 (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station HEGL1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -118.31
Fractional Gross Error(%) = 118.31
NO3 (microgram/m3)
Julian Date (182 - 209 2002)

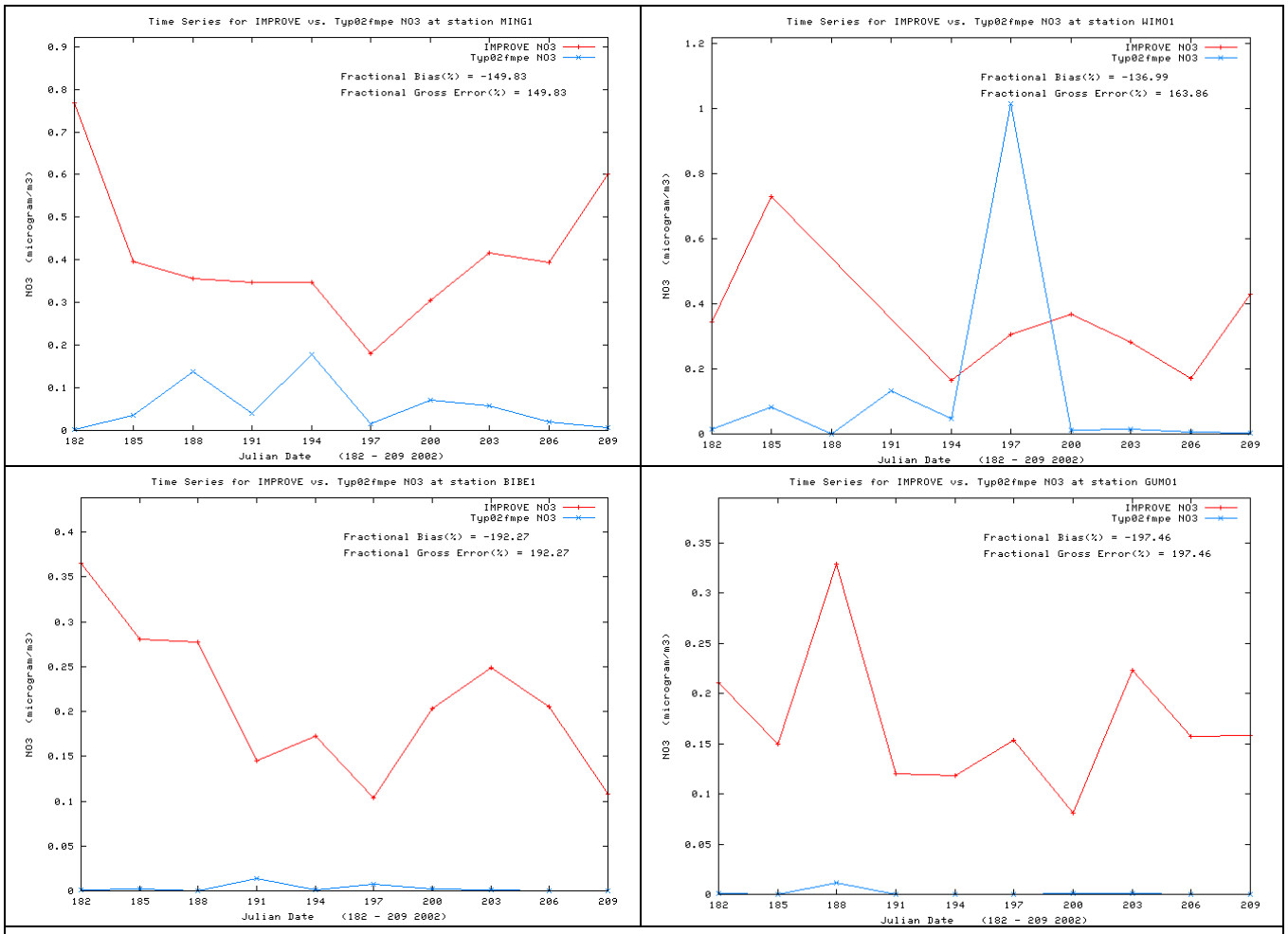


Figure C-12b. Time series of predicted and observed 24-hour nitrate (NO3) concentrations at CENRAP IMPROVE CLASS I AREA sites in July 2002 for CMAQ 2002 36 km Base F base case simulation.

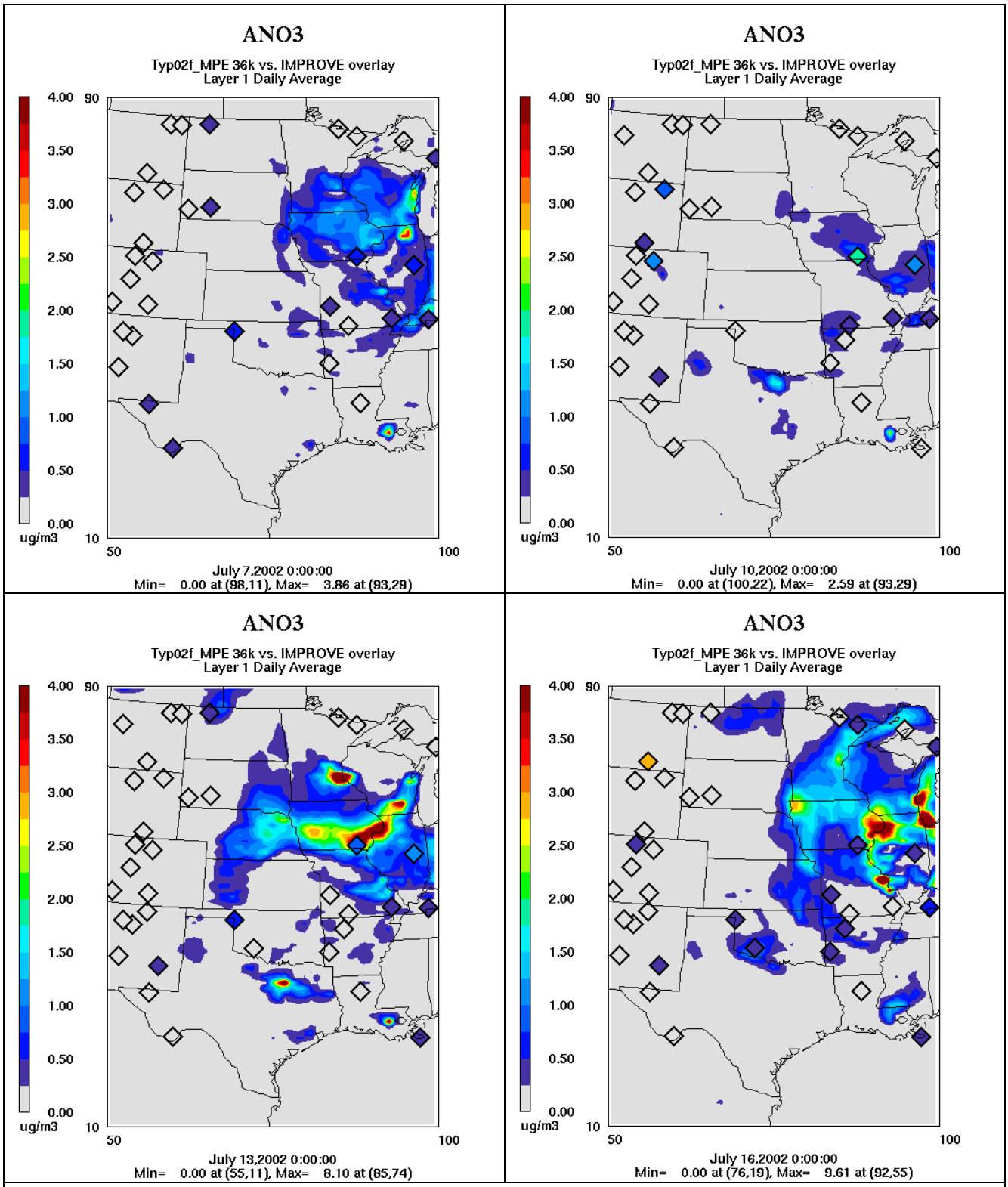


Figure C-12c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour NO3 concentrations for July 7, 10, 13 and 16, 2002.

C.3.2.4 NO3 in October 2002

Like January and unlike April and July, in October the model has a net NO3 overestimation bias of about 30%-40% (Figure C-13a). This overestimation bias occurs at all sites but BRET, BIBE and GUMO that exhibit a NO3 underestimation bias (Figure C-13b). The spatial maps suggest that the modeled elevated NO3 concentrations are more wide-spread and less spotty than observed.

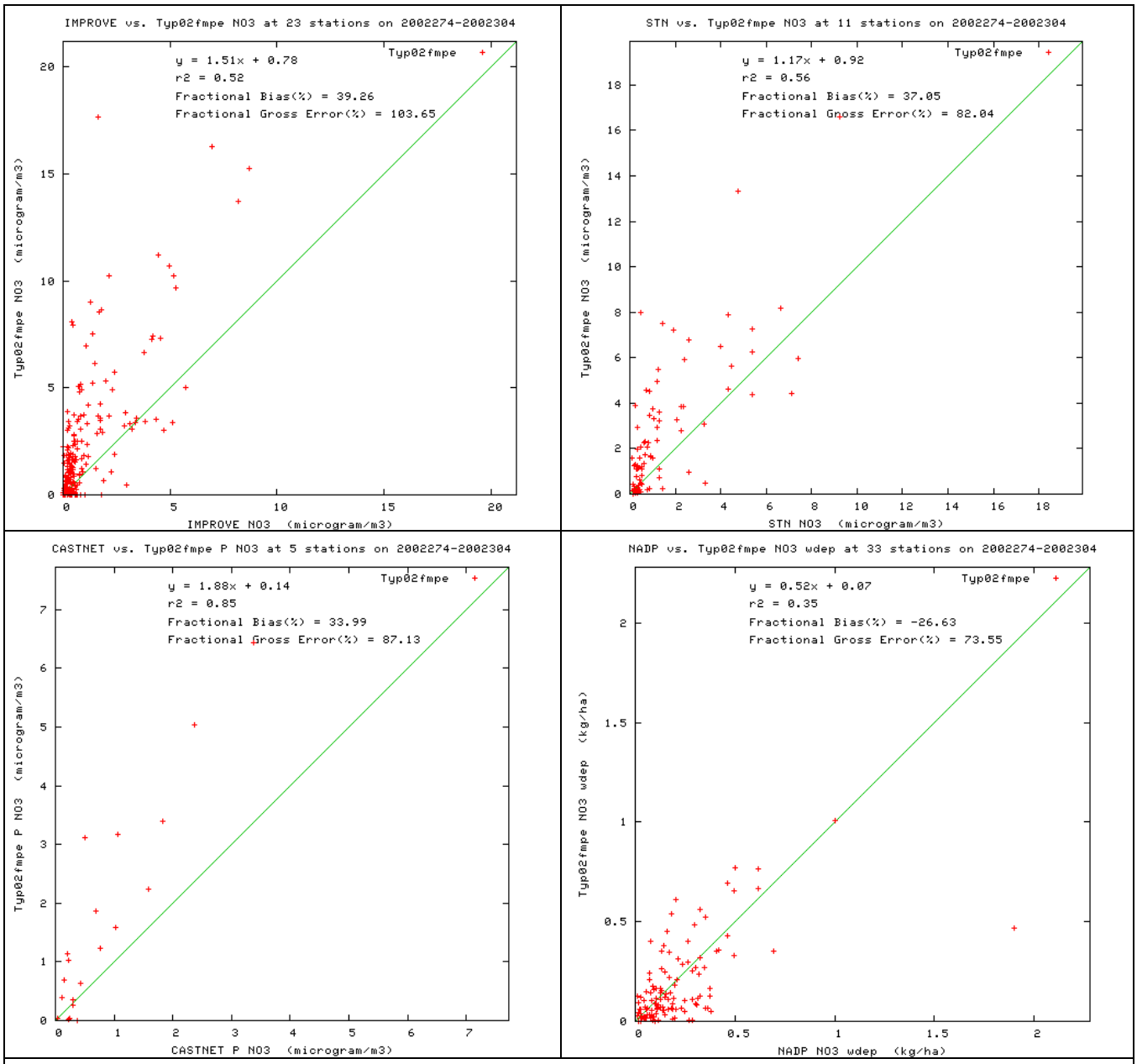
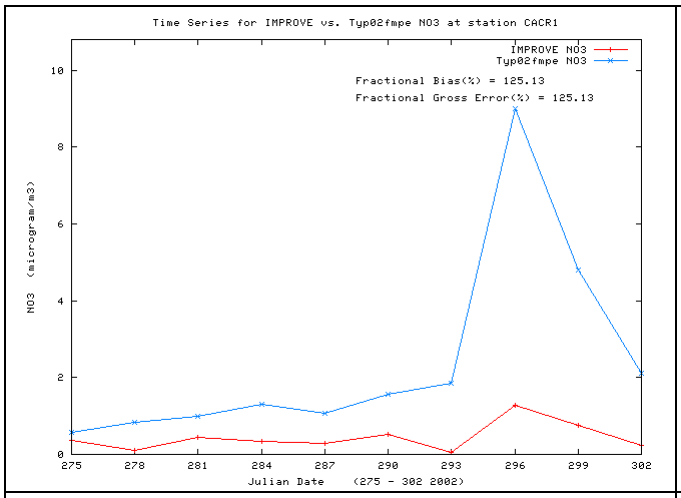
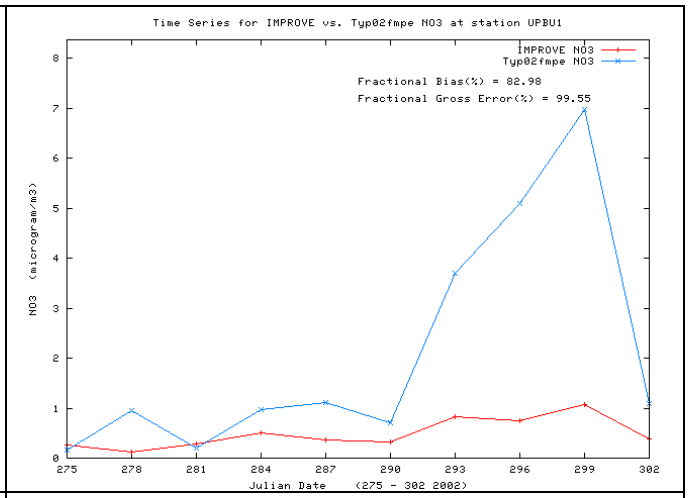
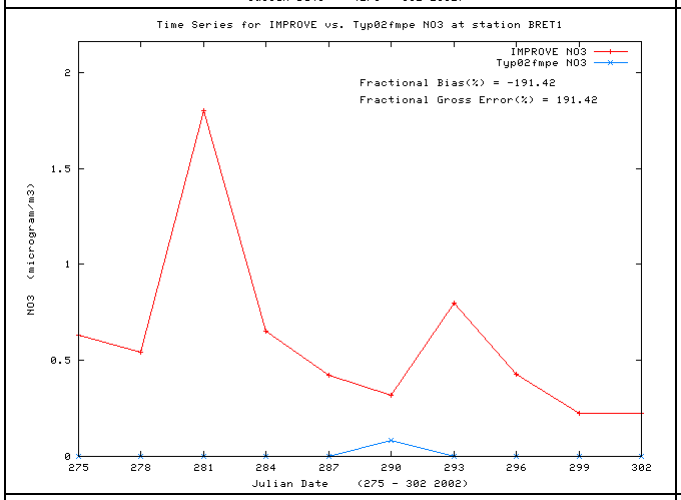
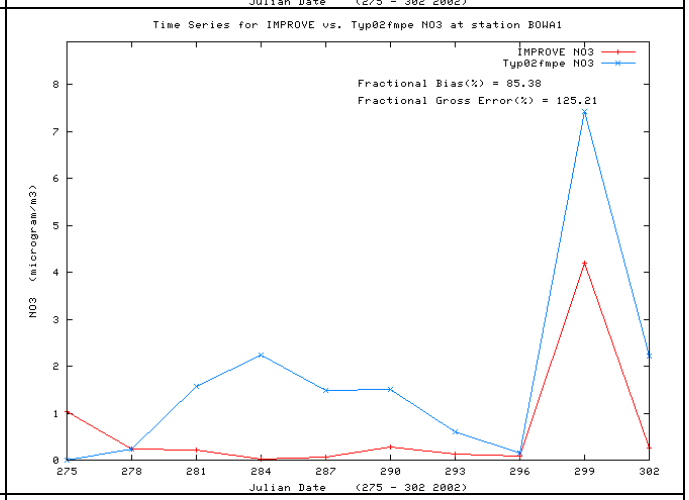


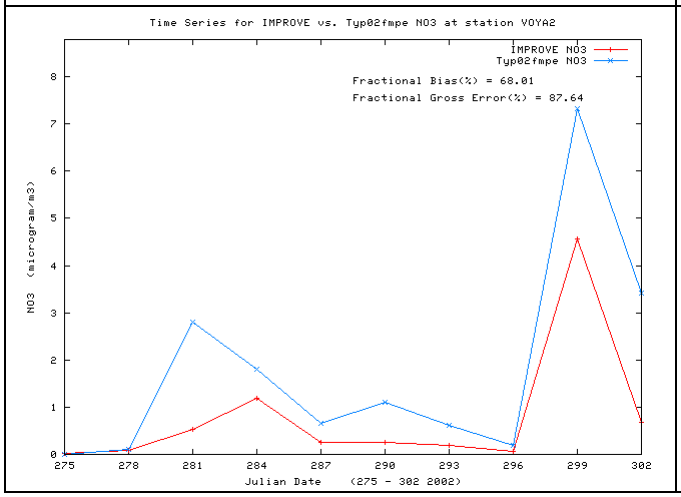
Figure C-13a. Scatter plots of predicted and observed nitrate (NO3) concentrations for October 2002 and sites in the CENRAP region using IMPROVE (top left), STN (top right), CASTNet (bottom left) and NADP monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

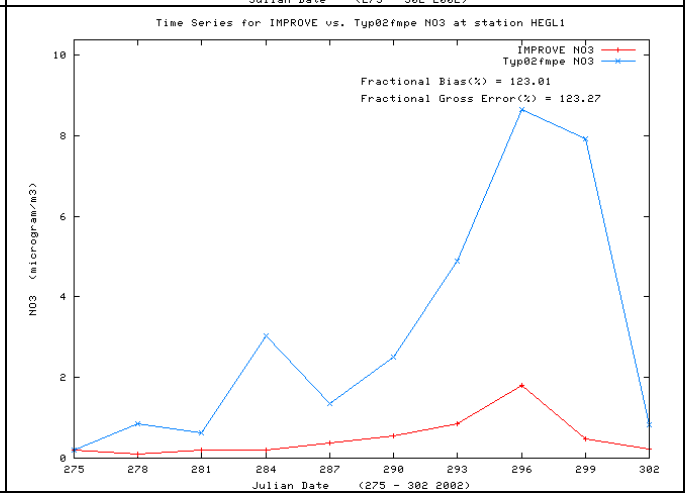

Time Series for IMPROVE vs. Typ02fmpe NO3 at station CACR1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 125.13
Fractional Gross Error(%) = 125.13
NO3 (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station UPBU1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 82.98
Fractional Gross Error(%) = 99.55
NO3 (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station BRET1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = -191.42
Fractional Gross Error(%) = 191.42
NO3 (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station BOWA1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 85.38
Fractional Gross Error(%) = 125.21
NO3 (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station VOYA2
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 68.01
Fractional Gross Error(%) = 87.64
NO3 (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe NO3 at station HEGL1
IMPROVE NO3
Typ02fmpe NO3
Fractional Bias(%) = 123.01
Fractional Gross Error(%) = 123.27
NO3 (microgram/m3)
Julian Date (275 - 302 2002)

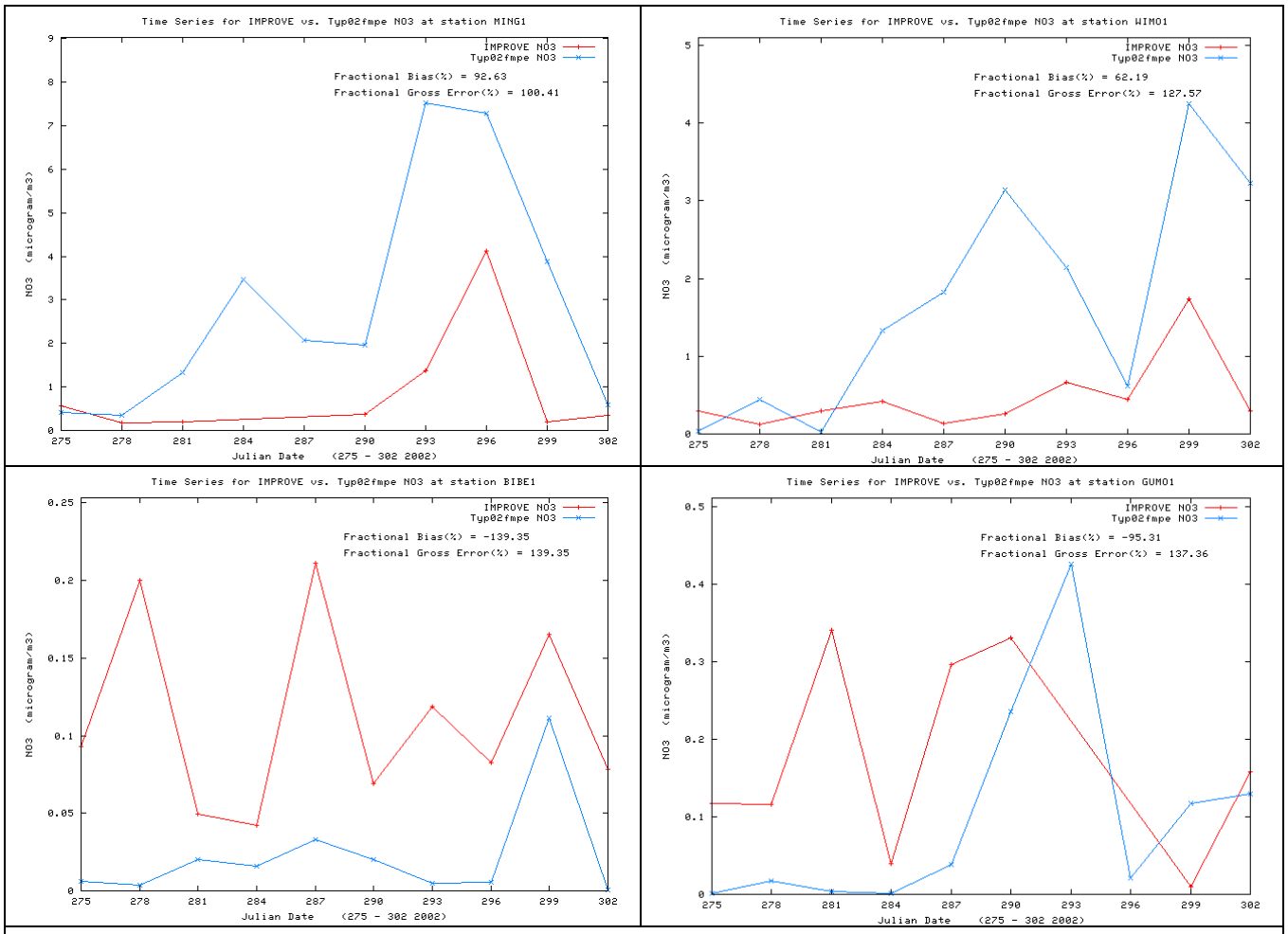


Figure C-13b. Time series of predicted and observed 24-hour nitrate (NO3) concentrations at CENRAP IMPROVE CLASS I AREA sites in October 2002 for CMAQ 2002 36 km Base F base case simulation.

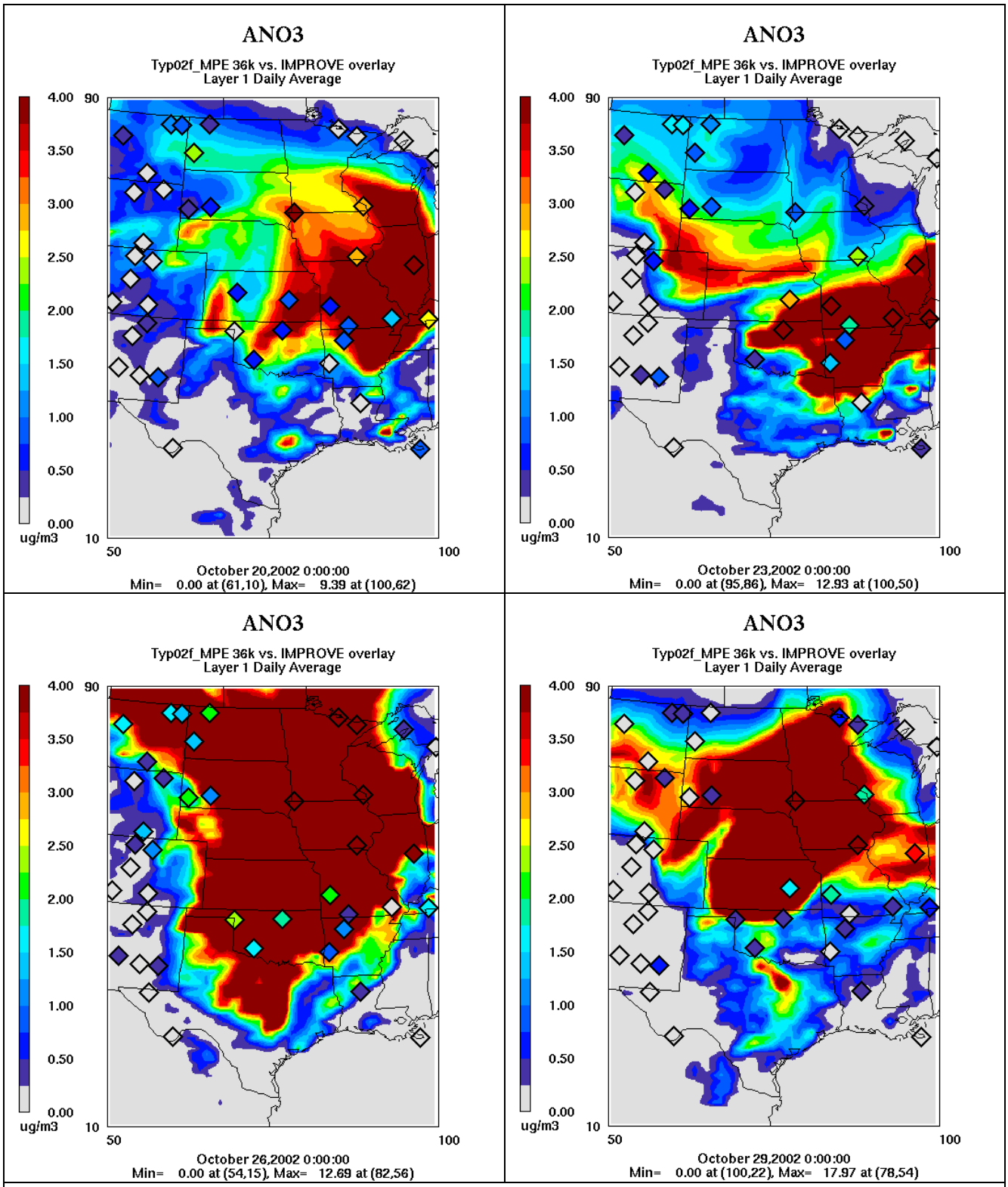


Figure C-13c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour NO3 concentrations for October 20, 23, 26 and 29, 2002.

C.3.2.5 NO3 Monthly Bias and Error

The monthly fractional bias values for NO3 clearly show the summer underestimation and winter overestimation bias (Figure C-14). The summer underestimation bias is more severe exceeding -100%, whereas the winter overestimation is closer to 50%. The fractional errors in the summer are also greater than in the winter with some values exceeding 100%. So based on statistics alone, it appears the summer underestimation bias is a bigger concern than the winter overestimation bias. However, the Bugle Plots in Figure C-15 paint a different picture entirely. The summer underestimation bias occurred when NO3 is low and is not an important component of PM and visibility impairment. These summer values occur in the flared horn part of the Bugle Plot and in fact the summer NO3 performance mostly achieves the model performance goal and always achieves the performance criteria. Whereas the winter overstated NO3 performance mostly doesn't meet the performance goal and there are even some months/networks that don't meet the performance criteria.

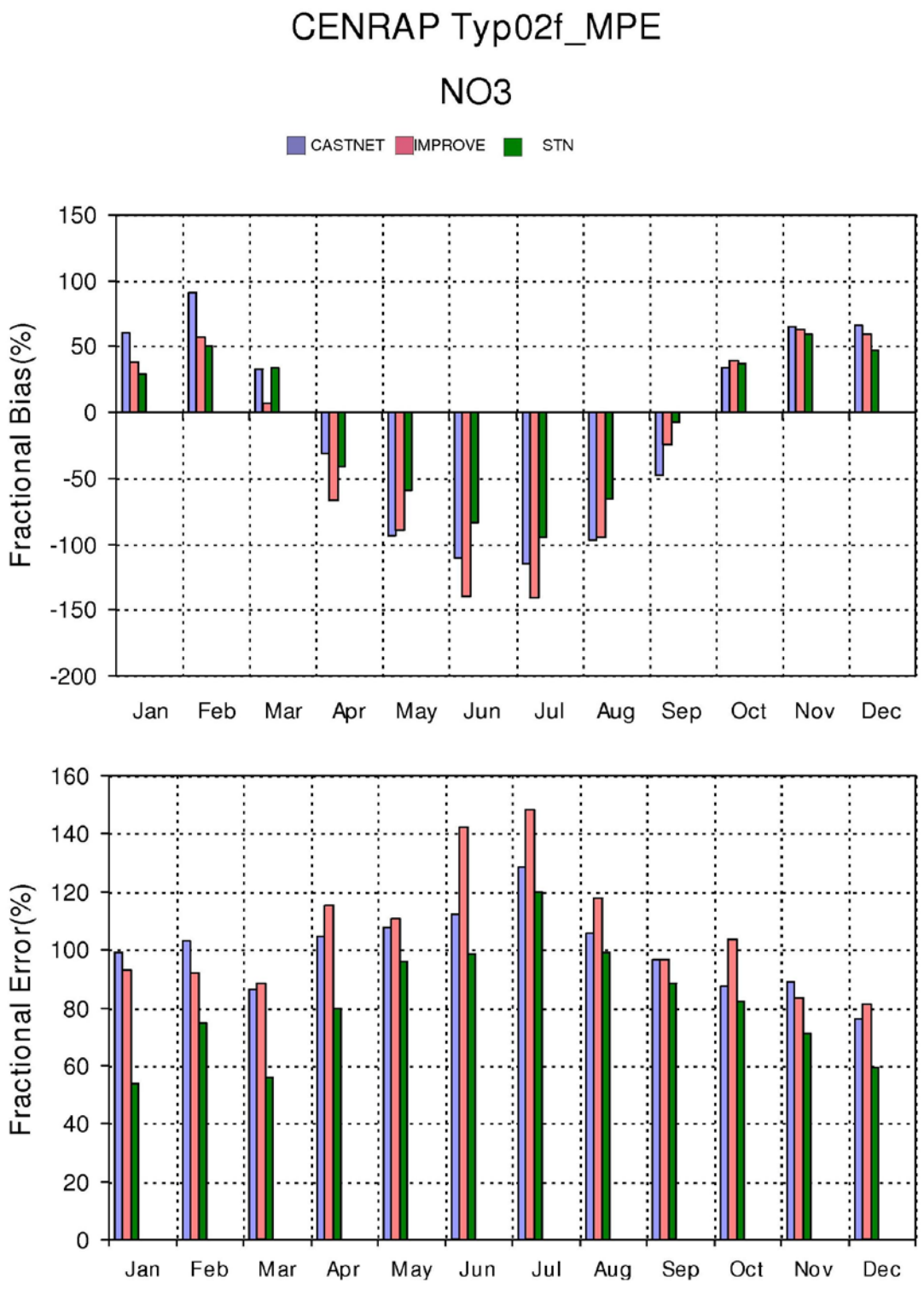


Figure C-14. Monthly NO3 fractional bias (top) and fractional gross error (bottom) statistical measures for IMPROVE, STN and CASTNet monitoring sites in the CENRAP region.

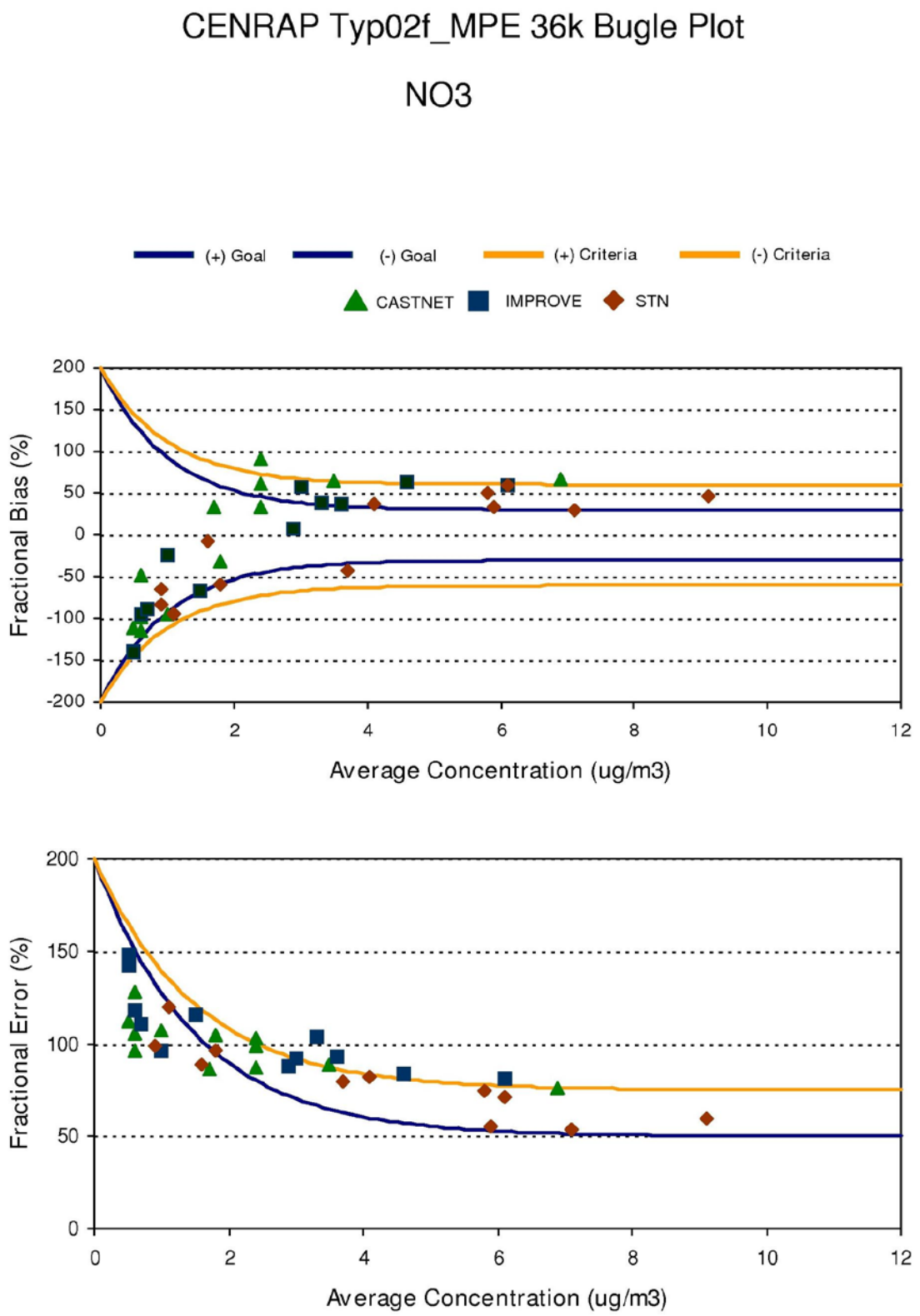


Figure C-15. Bugle Plots of monthly fractional bias (top) and fractional gross error (bottom) and comparisons with model performance goals and criteria for NO3 and IMPROVE, STN and CASTNet monitoring sites in the CENRAP region.

C.3.3 Organic Matter Carbon (OMC) Monthly Model Performance

Organic Matter Carbon (OMC) model performance is presented below. There is incommensurability between the observed and modeled OMC, the model provides estimates of OMC that includes Organic Carbon (OC) as well as other elements attached to the OC (e.g., oxygen), whereas the monitoring networks measure just the carbon component of OMC (i.e., OC). Consequently, the measured OC must be adjusted to OMC for comparison with the model to account for the additional elements attached to the carbon. The OMC/OC ratio is not constant and depends in part on the age of the OMC with fresh OMC having lower OMC/OC ratios than aged OMC. The original IMPROVE equation used an OMC/OC ratio of 1.4 based mainly on urban-oriented measurements. The new IMPROVE equation uses an OMC/OC ratio of 1.8 reflecting the fact that OMC at the more rural IMPROVE monitors is more aged than urban OMC. Thus, selecting a single OMC/OC ratio for adjusting the measured OC to OMC for the model evaluation is somewhat problematic when we have both urban (STN) and rural (IMPPROVE) monitors. In addition, measured OC also has substantial uncertainty with different measurement techniques differing by as much as 50% (Solomon et al., 2005). A 1.4 OMC/OC ratio was used to convert the measured OC to OMC for the model performance evaluation.

C.3.3.1 OMC in January 2002

Figure C-16a displays scatter plots and performance statistics for January OMC model performance across the IMPROVE and STN sites in the CENRAP region. OMC model performance is fairly with near zero bias across the IMPROVE sites, -38% underestimation bias across the STN sites and errors of ~50%. The underestimation of OMC at the urban STN sites is a common occurrence in air quality modeling and may indicate a missing source of urban OMC. With the exception of an underestimation bias at Breton Island and an over-prediction bias at the two Texas IMPORVE sites (BIBE and GUMO), the model reproduces the observed OMC time series in January fairly well. The modeled spatial distribution of OMC is in general agreement with the observations although it sometimes captures the elevated values on some days (e.g., January 29, 2002 in central Illinois) and misses it on others (e.g., January 26, 2002 at Mingo).

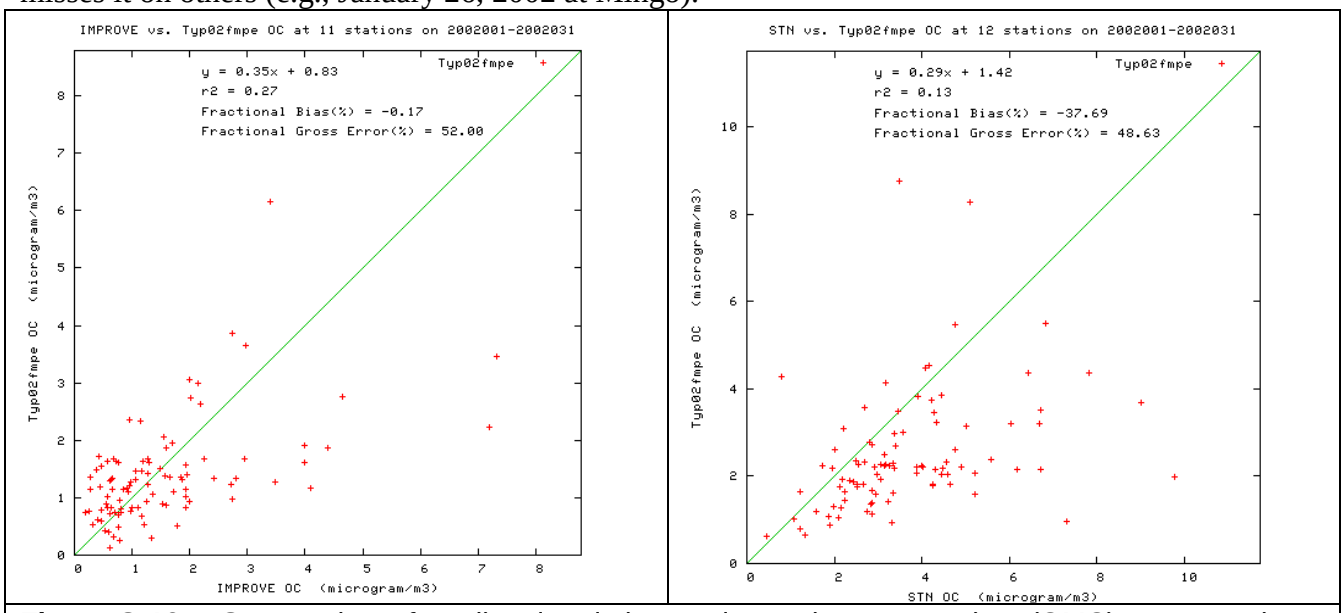
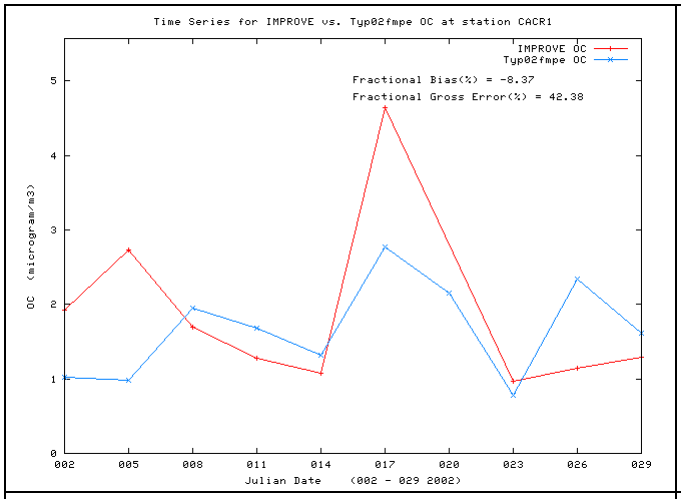
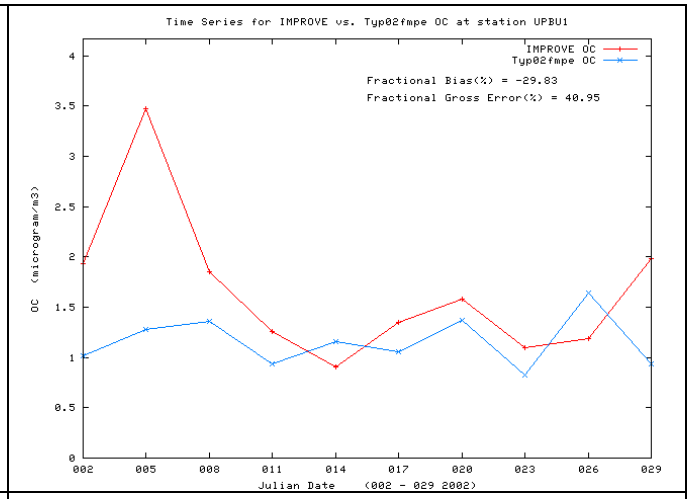
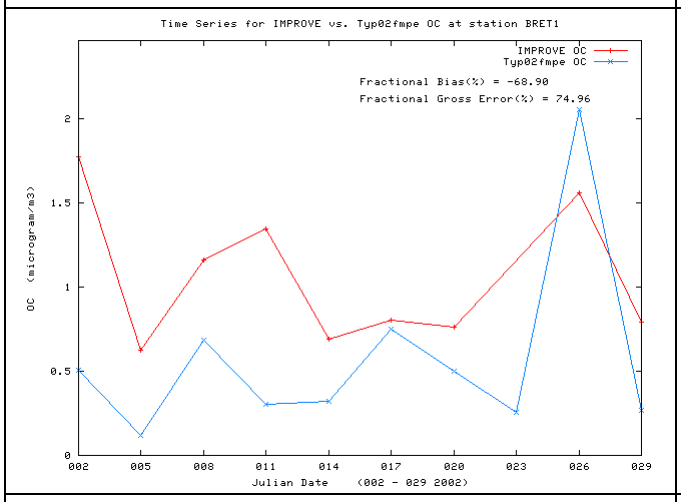
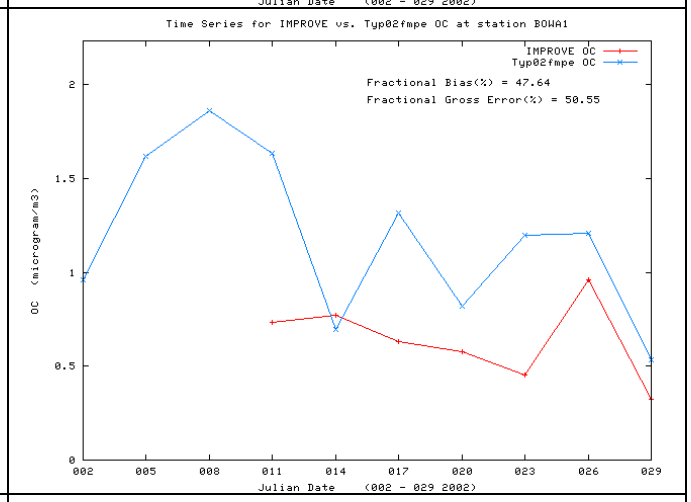


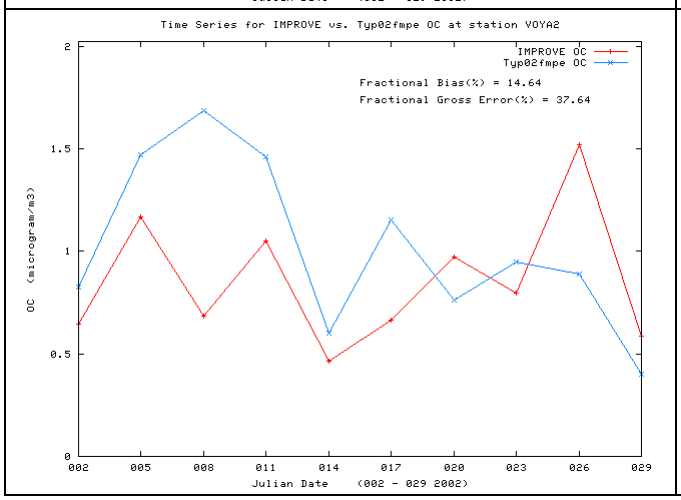
Figure C-16a. Scatter plots of predicted and observed organic matter carbon (OMC) concentrations for January 2002 and sites in the CENRAP region using IMPROVE (left) and STN (right) monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

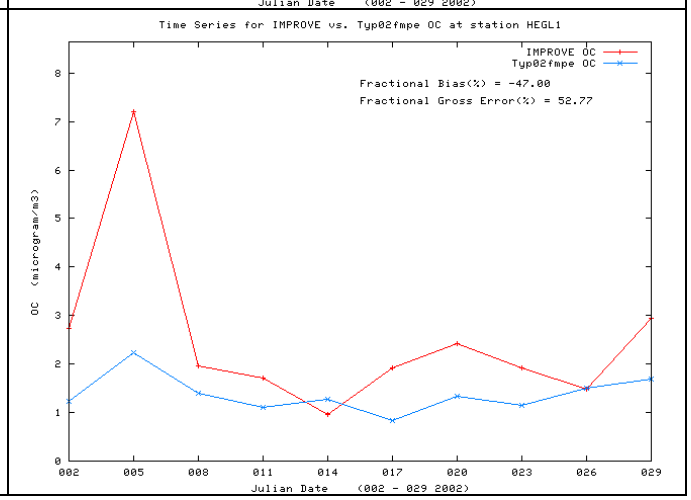

Time Series for IMPROVE vs. Typ02fmpe OC at station CACR1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -8.37
Fractional Gross Error(%) = 42.38
OC (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station UPBU1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -29.83
Fractional Gross Error(%) = 40.95
OC (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station BRET1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -68.90
Fractional Gross Error(%) = 74.96
OC (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station BOWA1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 47.64
Fractional Gross Error(%) = 50.55
OC (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station VOYA2
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 14.64
Fractional Gross Error(%) = 37.64
OC (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station HEGL1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -47.00
Fractional Gross Error(%) = 52.77
OC (microgram/m3)
Julian Date (002 - 029 2002)

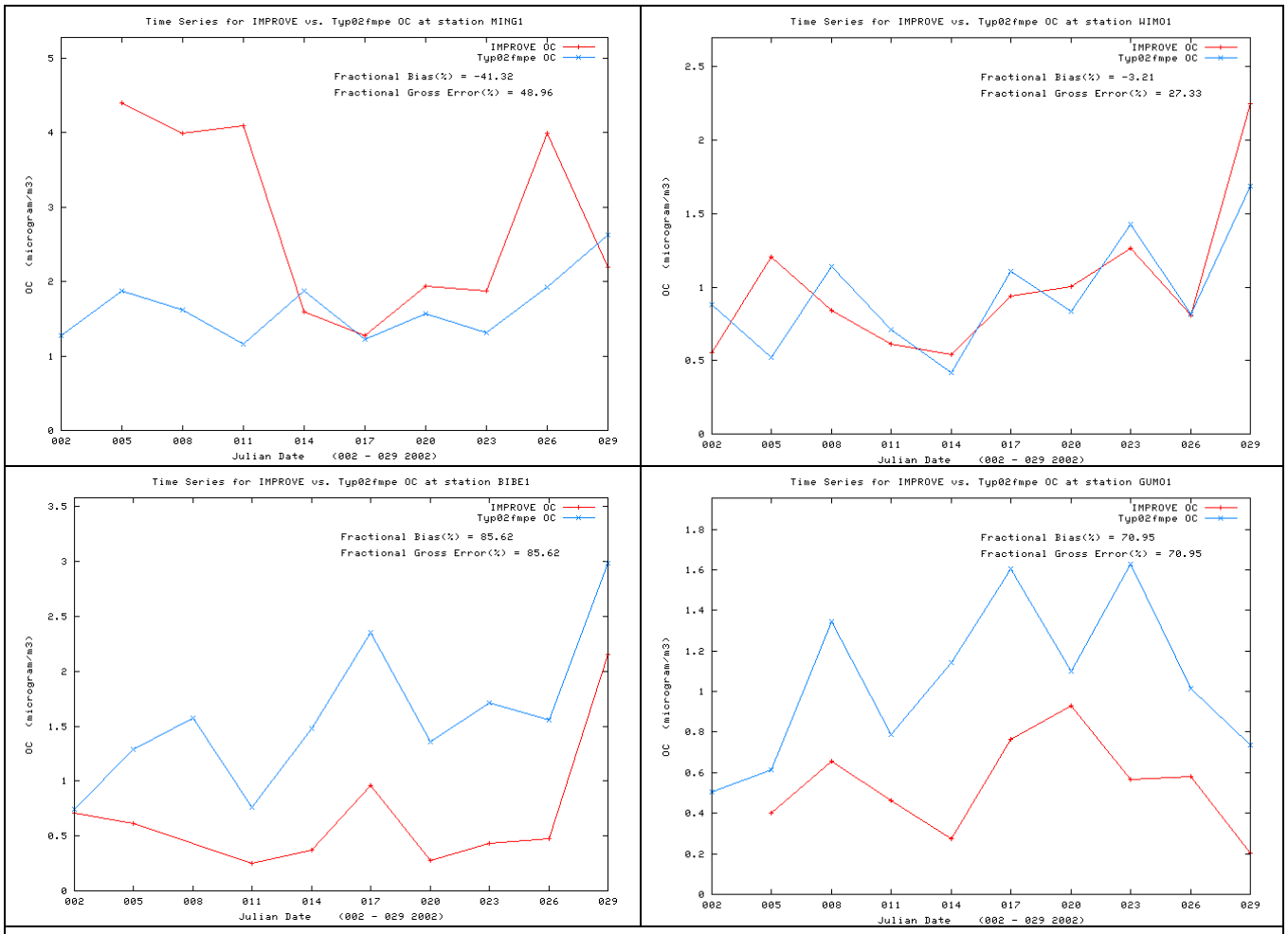


Figure C-16b. Time series of predicted and observed 24-hour organic matter carbon (OMC) concentrations at CENRAP IMPROVE CLASS I AREA sites in January 2002 for CMAQ 2002 36 km Base F base case simulation.

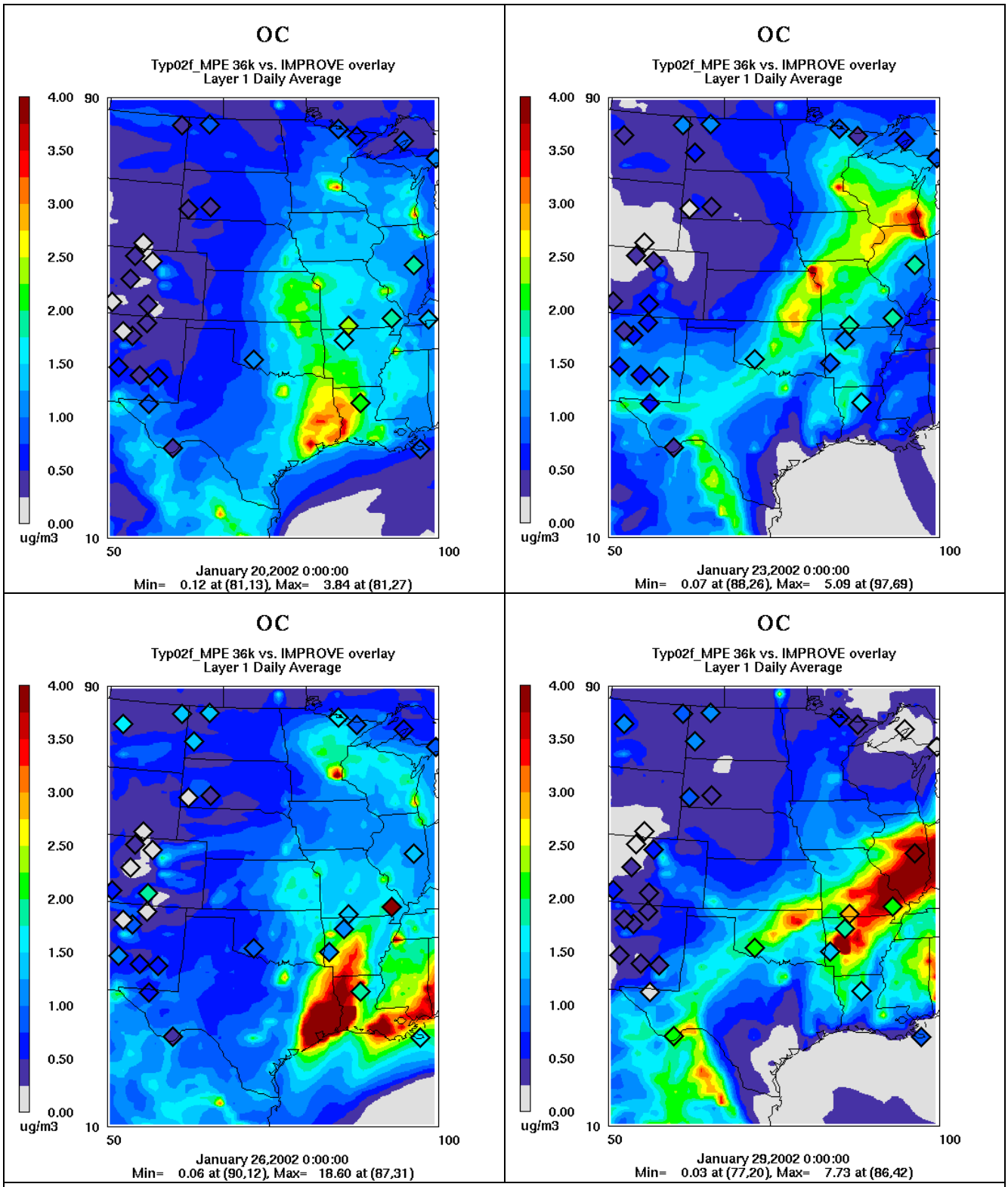


Figure C-16c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour OMC concentrations for January 20, 23, 26 and 29, 2002.

C.3.3.2 OMC in April 2002

The OMC performance in April is also fairly reasonable, again bias across the IMPROVE monitors is near zero (-7%), an underestimation bias exists across the STN sites (-30%) and errors are near 50% (Figure C-17a). The time series comparisons (Figure C-17b) are also reasonable with the model generally agreeing on the magnitudes of the observed OMC, but with an underestimation bias at several sites (e.g., MING and WIMO). The observed spatial distribution of OMCV appears to be much spottier than predicted (Figure C-17c). Thus, when the model reproduces an elevated observed OMC value like at UPBU on April 5th, it overestimates OMC at neighboring sites that have lower values (e.g., HEGL).

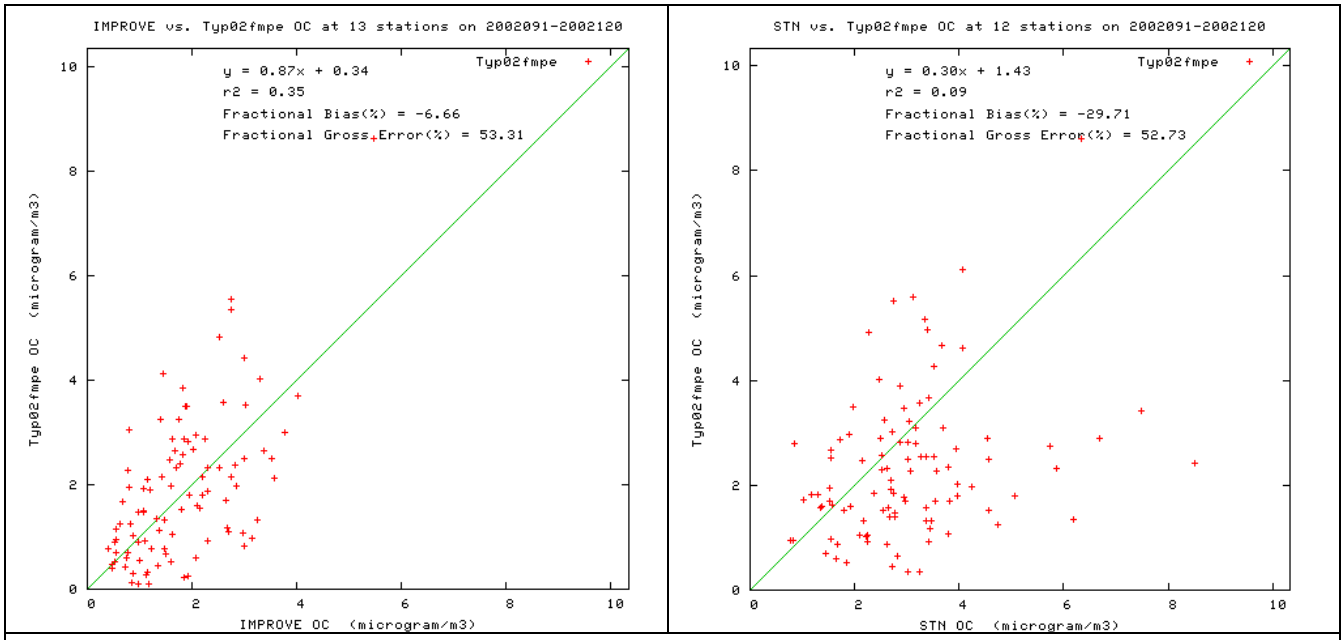
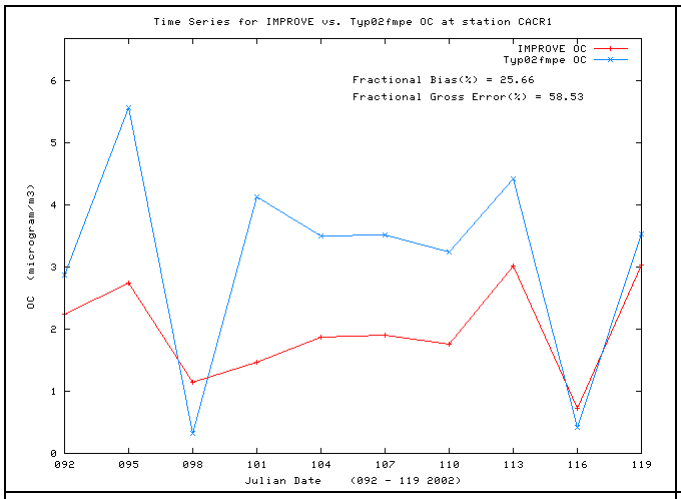
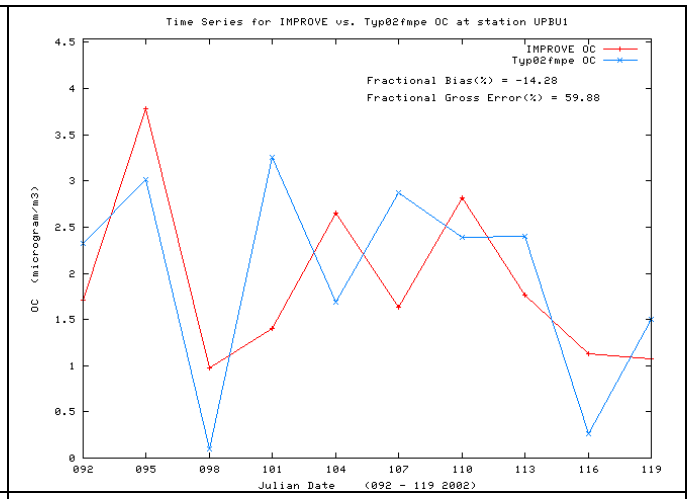
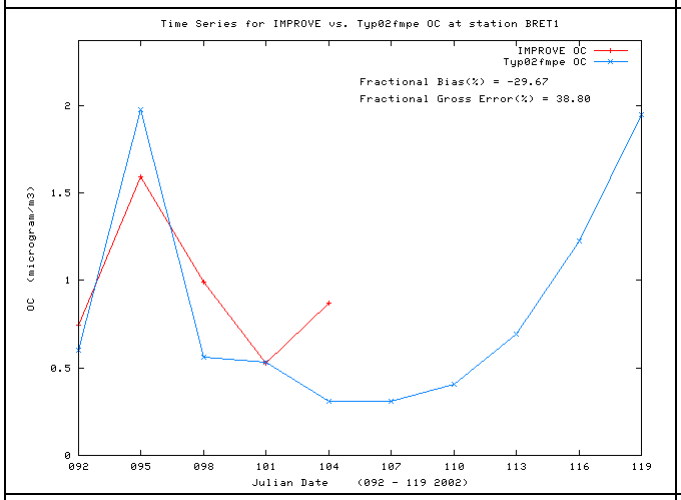
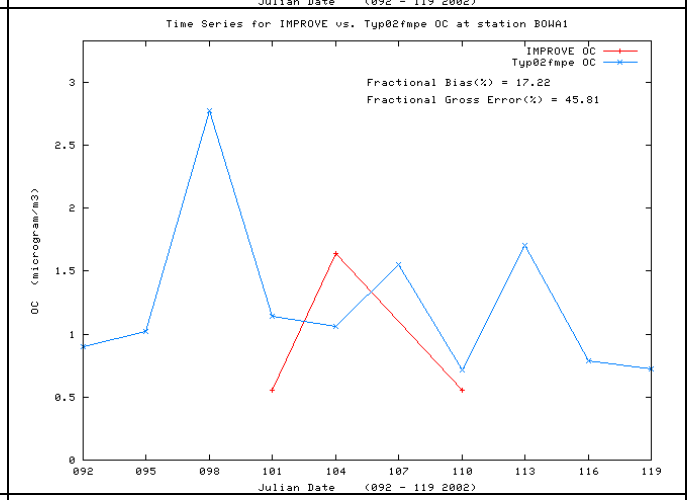


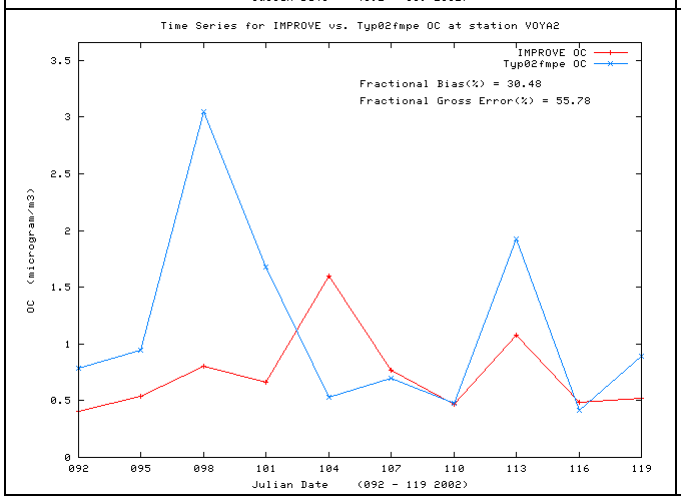
Figure C-17a. Scatter plots of predicted and observed organic matter carbon (OMC) concentrations for April 2002 and sites in the CENRAP region using IMPROVE (left) and STN (right) monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

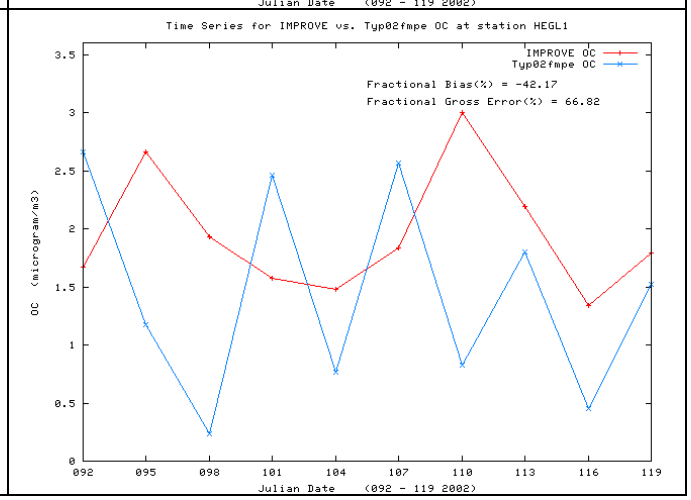

Time Series for IMPROVE vs. Typ02fmpe OC at station CACR1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 25.66
Fractional Gross Error(%) = 58.53
OC (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station UPBU1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -14.28
Fractional Gross Error(%) = 59.88
OC (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station BRET1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -29.67
Fractional Gross Error(%) = 38.80
OC (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station BOWA1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 17.22
Fractional Gross Error(%) = 45.81
OC (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station VOYA2
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 30.48
Fractional Gross Error(%) = 55.78
OC (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station HEGL1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -42.17
Fractional Gross Error(%) = 66.82
OC (microgram/m3)
Julian Date (092 - 119 2002)

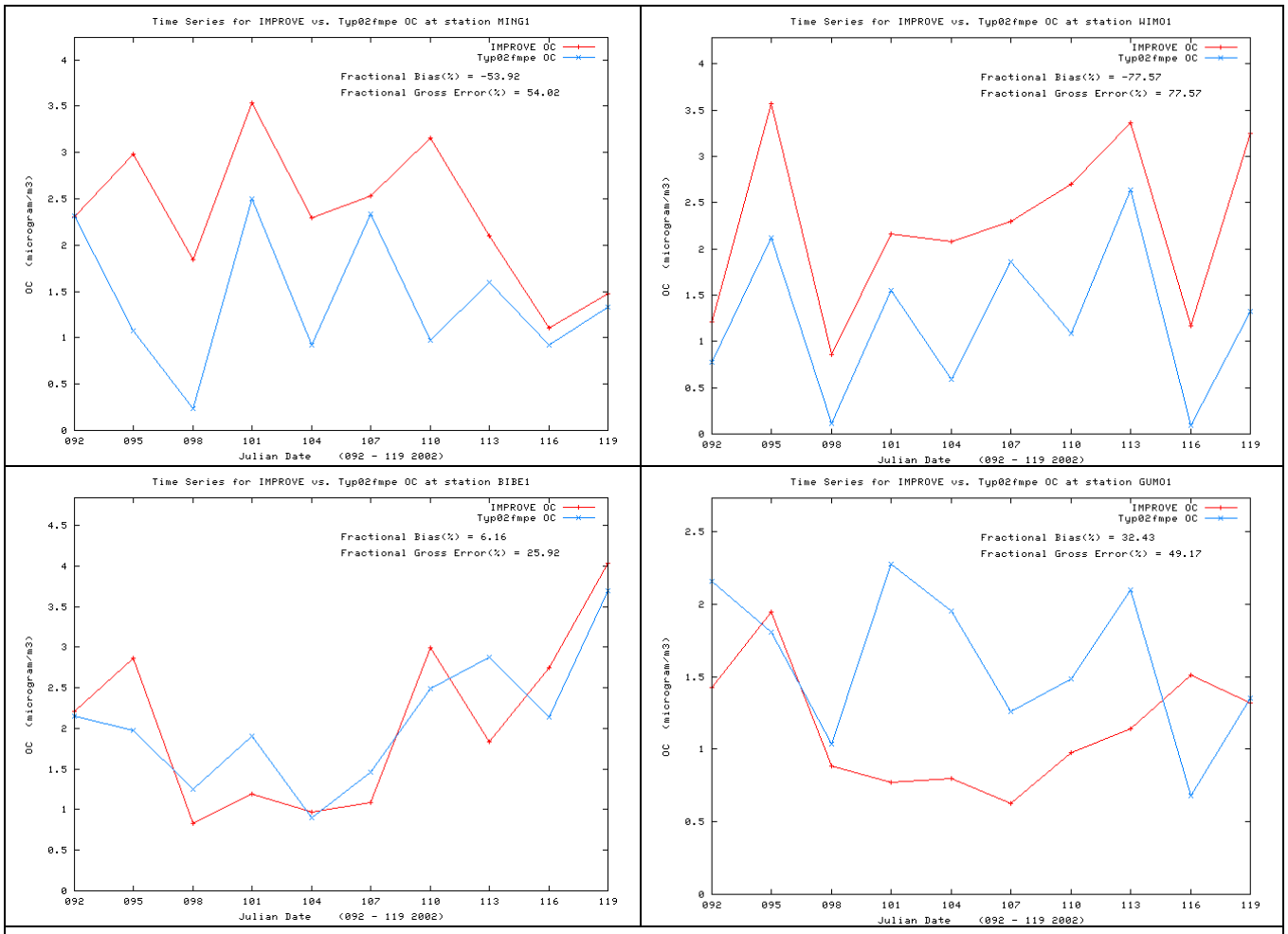


Figure C-17b. Time series of predicted and observed 24-hour organic matter carbon (OMC) concentrations at CENRAP IMPROVE CLASS I AREA sites in April 2002 for CMAQ 2002 36 km Base F base case simulation.

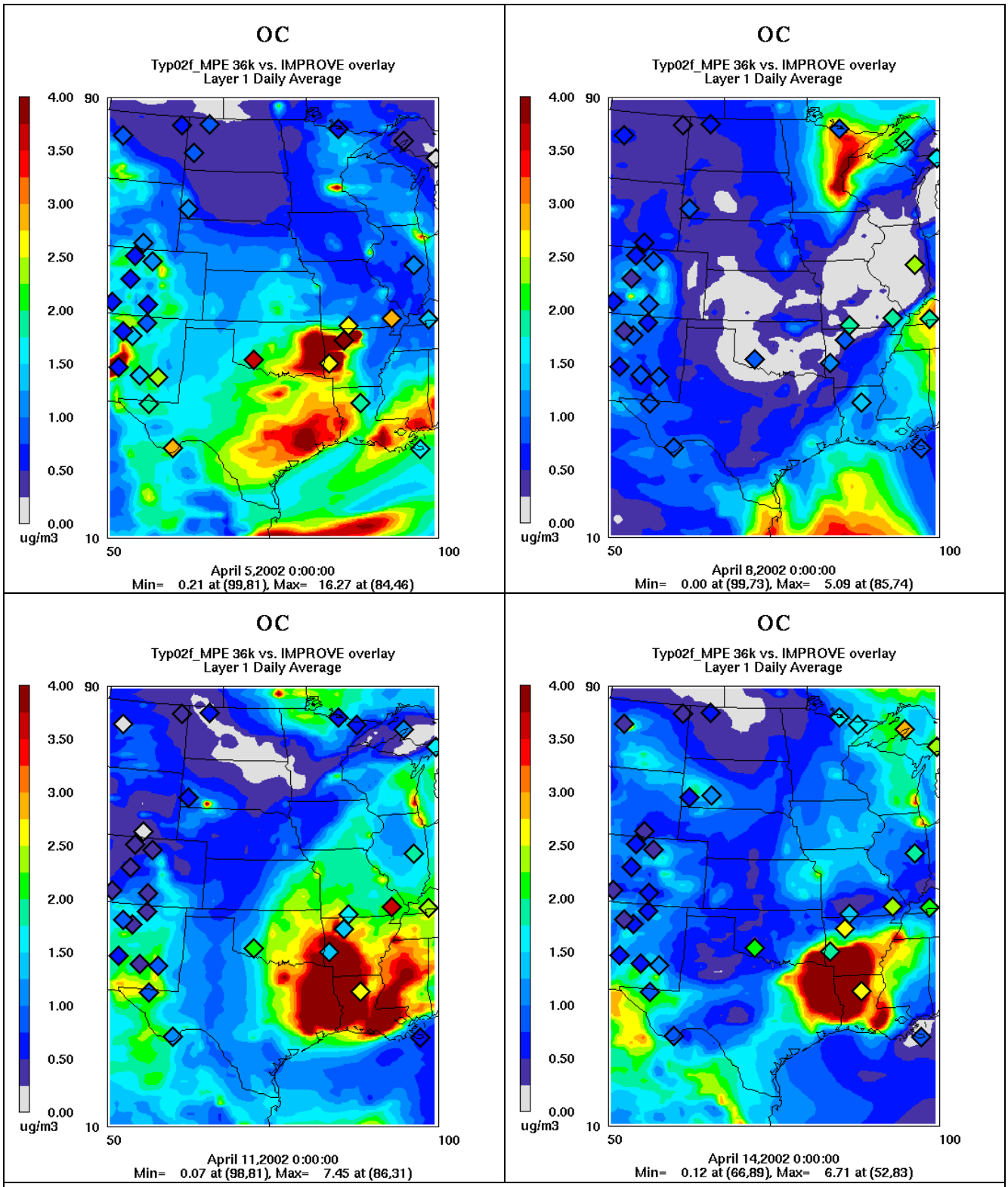


Figure C-17c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour OMC concentrations for April 5, 8, 11 and 14, 2002.

C.3.3.3 OMC in July 2002

Modeled and observed OMC are higher in July due to the impacts of more secondary organic aerosols (SOA) and fires. OMC bias values of -18% and -41% exist across the IMPROVE and STN networks in July (Figure C-18a). Two of the observed OMC values at the IMPROVE sites are very high (> 15 μg/m^3). An examination of the time series plots (Figure C-18b) reveals that these two values occur on Julian Day 200 and the two northern Minnesota sites (VOYA and BOWA) and are likely due to fire impacts. The model is also estimating elevated OMC at these sites on these two days, but not as high as observed. At most sites the model is racking the temporal variation of the observed OMC reasonably well. OMC data for MING were missing in July 2002. The model reproduces the observed high OMC in northern Minnesota and centered on Louisiana and adjacent areas on July 7 and 10 quite well, but also predicts elevated OMC in the Denver area that is not reflected in the observations (Figure C-18c). The model is exhibiting less skill in predicting the spatial distribution of the observed OMC on July 13 and 16.

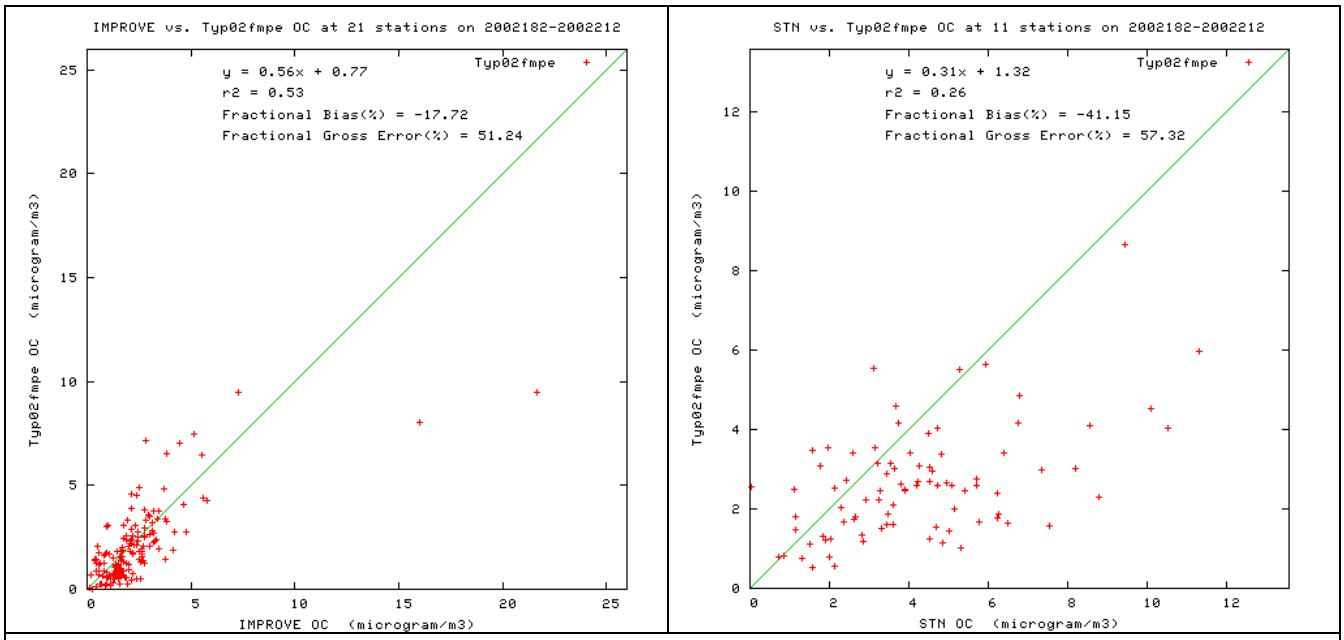
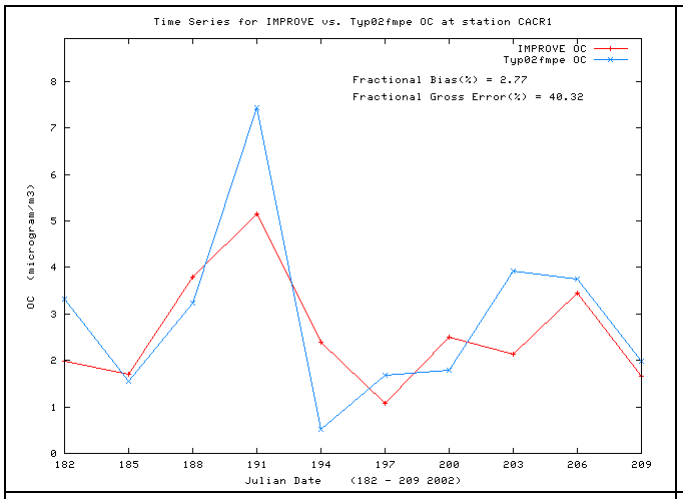
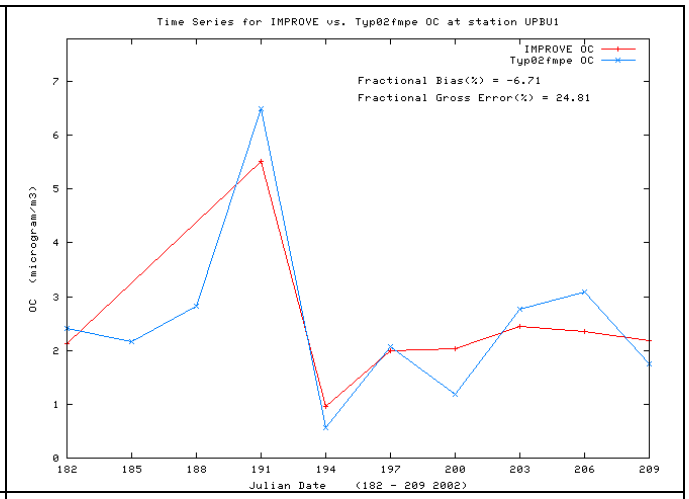
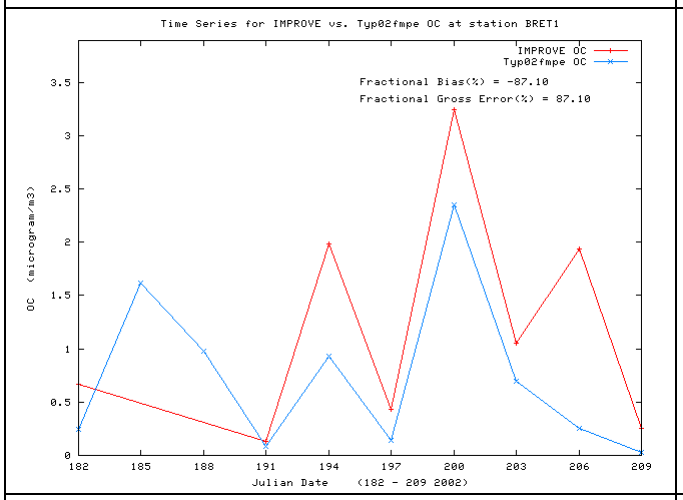
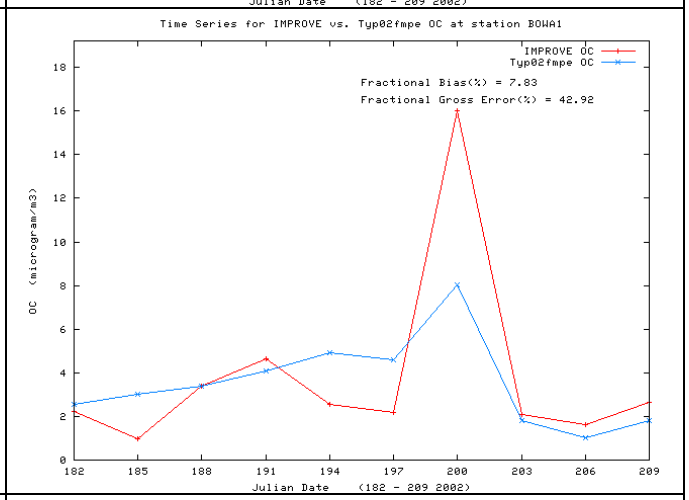


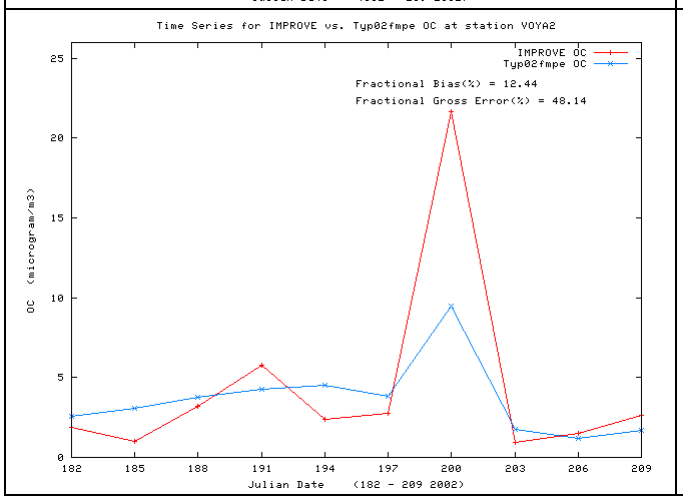
Figure C-18a. Scatter plots of predicted and observed organic matter carbon (OMC) concentrations for July 2002 and sites in the CENRAP region using IMPROVE (left) and STN (right) monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

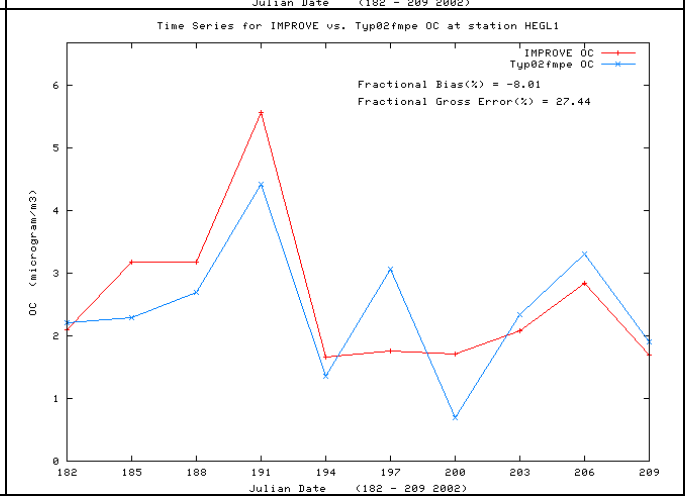

Time Series for IMPROVE vs. Typ02fmpe OC at station CACR1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 2.77
Fractional Gross Error(%) = 40.32
OC (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station UPBU1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -6.71
Fractional Gross Error(%) = 24.81
OC (microgram/m3)
Julian Date (182 - 209 2002)

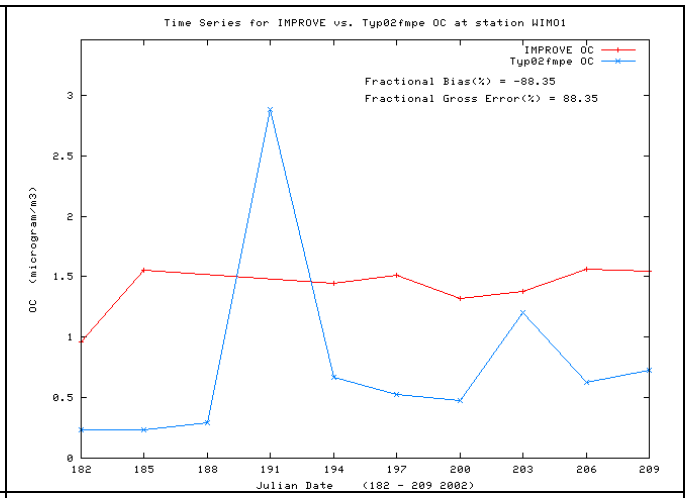

Time Series for IMPROVE vs. Typ02fmpe OC at station BRET1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -87.10
Fractional Gross Error(%) = 87.10
OC (microgram/m3)
Julian Date (182 - 209 2002)

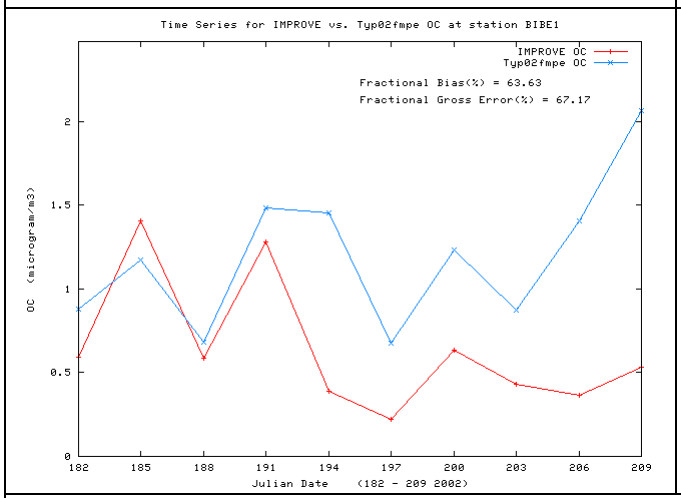

Time Series for IMPROVE vs. Typ02fmpe OC at station BOWA1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 7.83
Fractional Gross Error(%) = 42.92
OC (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station VOYA2
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 12.44
Fractional Gross Error(%) = 48.14
OC (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station HEGL1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -8.01
Fractional Gross Error(%) = 27.44
OC (microgram/m3)
Julian Date (182 - 209 2002)

No Data for Mingo (MING)





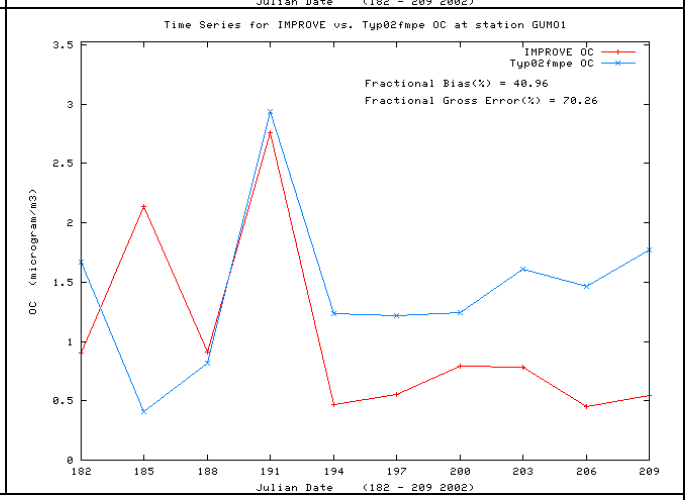


Figure C-18b. Time series of predicted and observed 24-hour organic matter carbon (OMC) concentrations at CENRAP IMPROVE CLASS I AREA sites in July 2002 for CMAQ 2002 36 km Base F base case simulation.

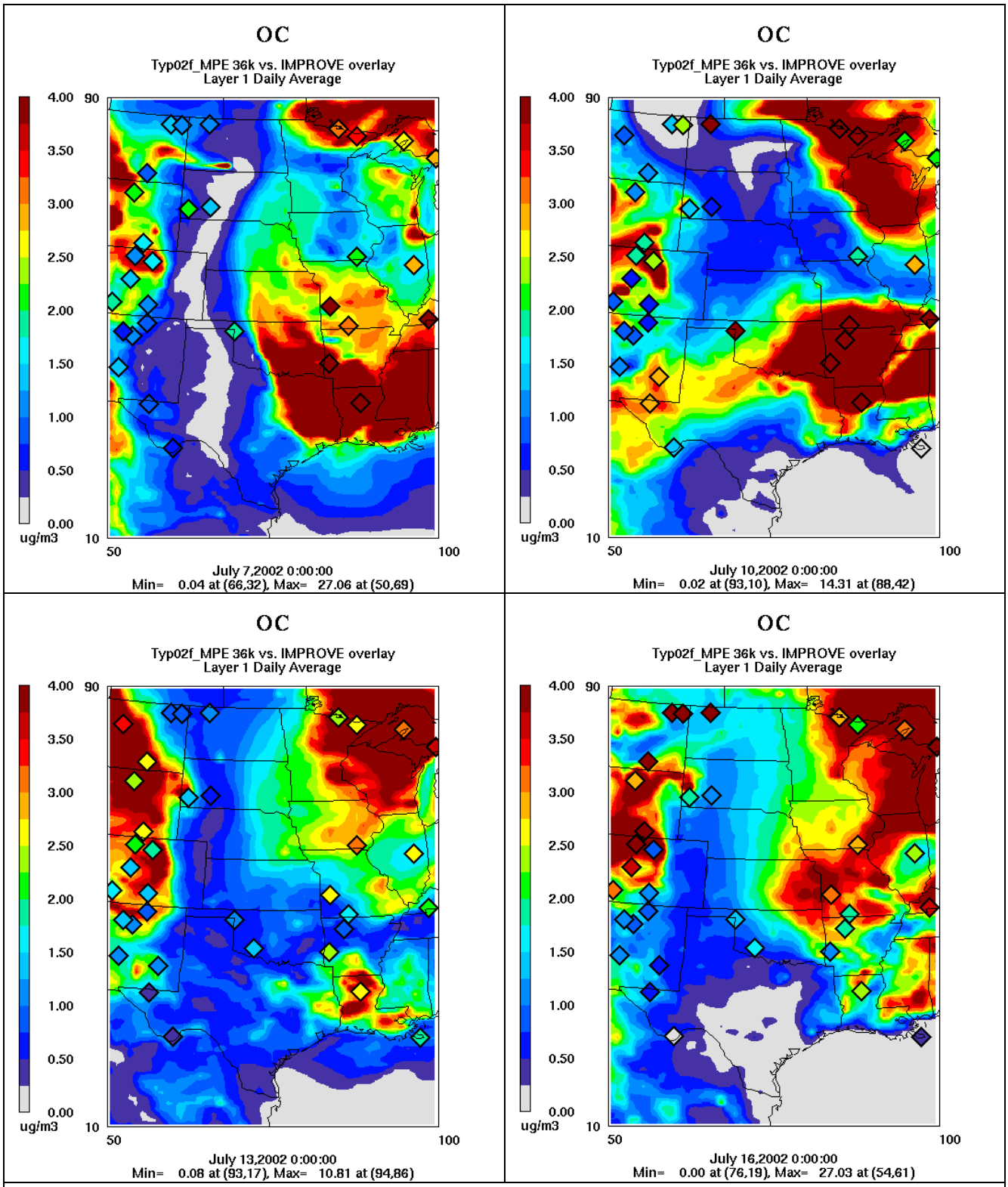


Figure C-18c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour OMC concentrations for July 7, 10, 13 and 16, 2002.

C.3.3.4 OMC in October 2002

OMC model performance in October 2002 is similar to the other months with near zero bias across the IMPROVE sites and an underestimation bias across the STN sites in the CENRAP region (Figure C-19a). Although OMC overestimation bias occurs at the Texas sites (BIBE and GUMO), the model is exhibiting remarkable ability to reproduce the observed temporal variation in OMC at several of the sites (e.g., CACR, UPBU, VOYA and HEGL; Figure C-19b). The model also performs reasonable well in reproducing the day to day and spatial variability in the observed OMC (Figure C-19c).

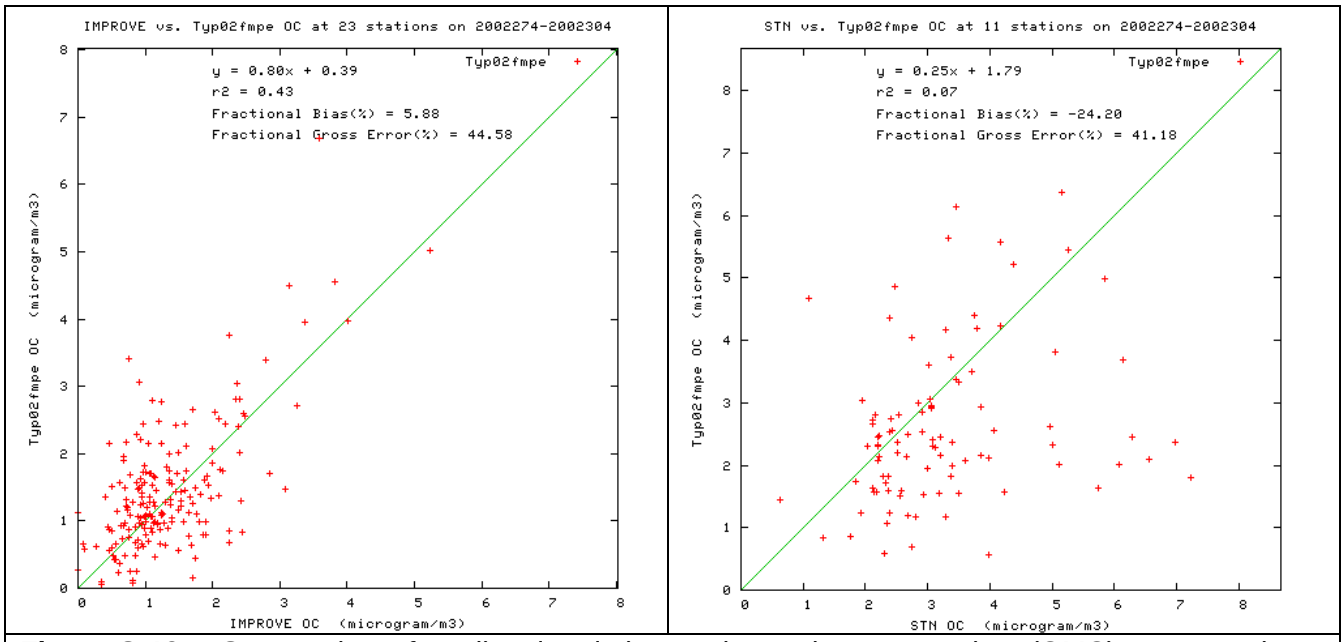
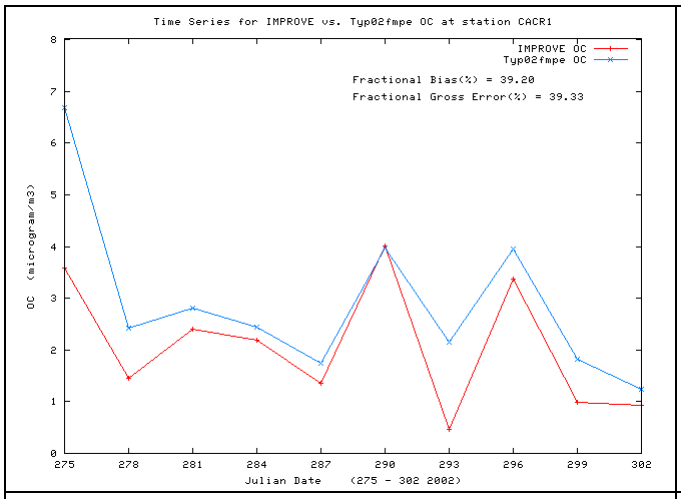
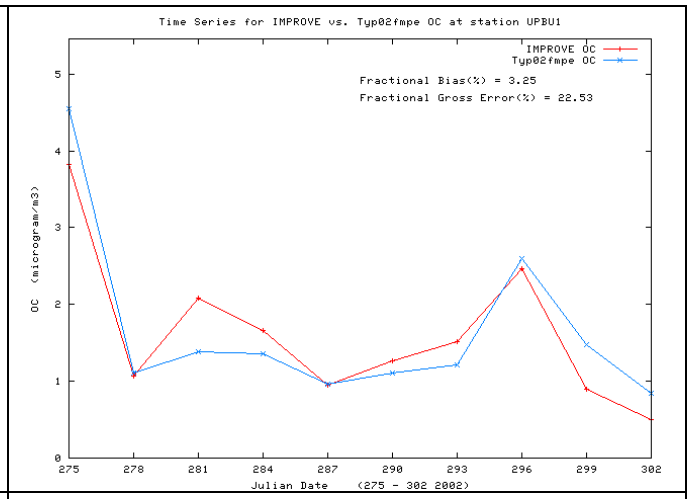
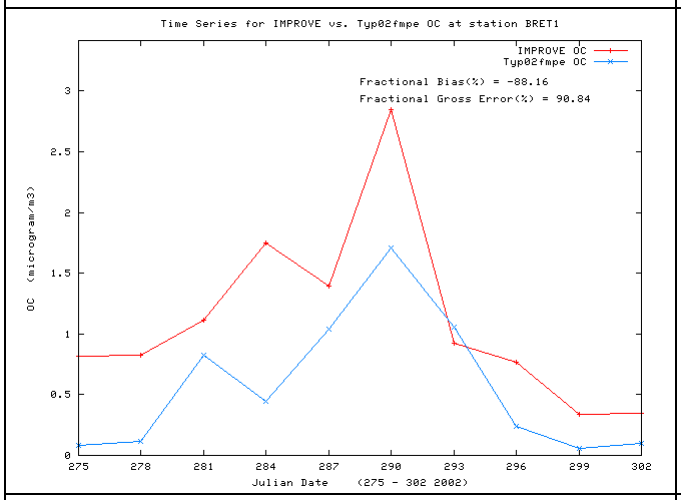
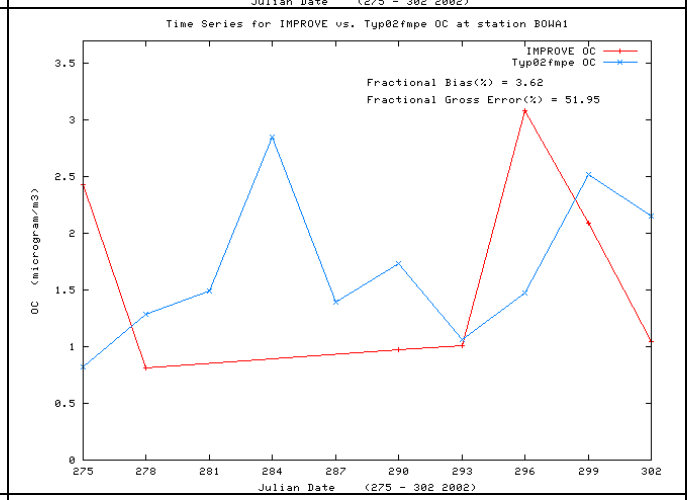


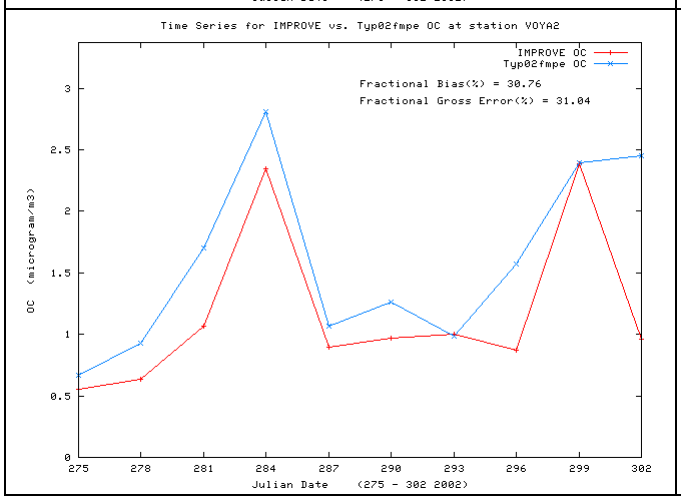
Figure C-19a. Scatter plots of predicted and observed organic matter carbon (OMC) concentrations for October 2002 and sites in the CENRAP region using IMPROVE (left) and STN (right) monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

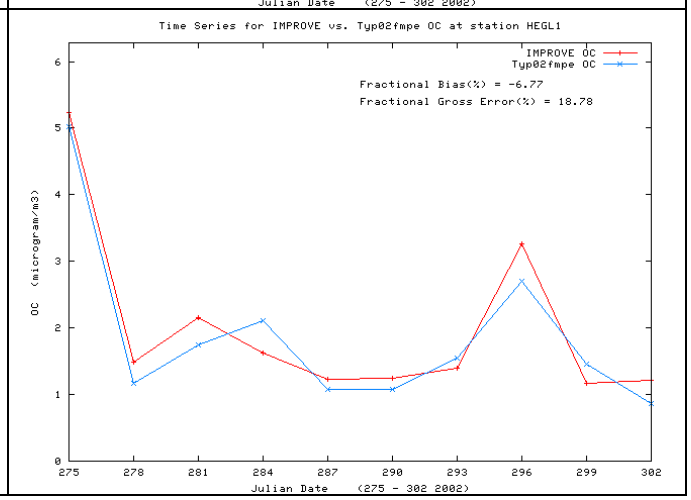

Time Series for IMPROVE vs. Typ02fmpe OC at station CACR1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 39.20
Fractional Gross Error(%) = 39.33
OC (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station UPBU1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 3.25
Fractional Gross Error(%) = 22.53
OC (microgram/m3)
Julian Date (275 - 302 2002)

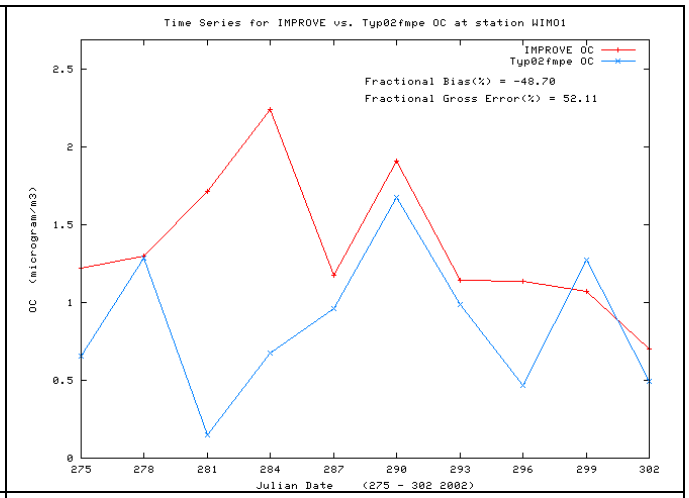

Time Series for IMPROVE vs. Typ02fmpe OC at station BRET1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -88.16
Fractional Gross Error(%) = 90.84
OC (microgram/m3)
Julian Date (275 - 302 2002)

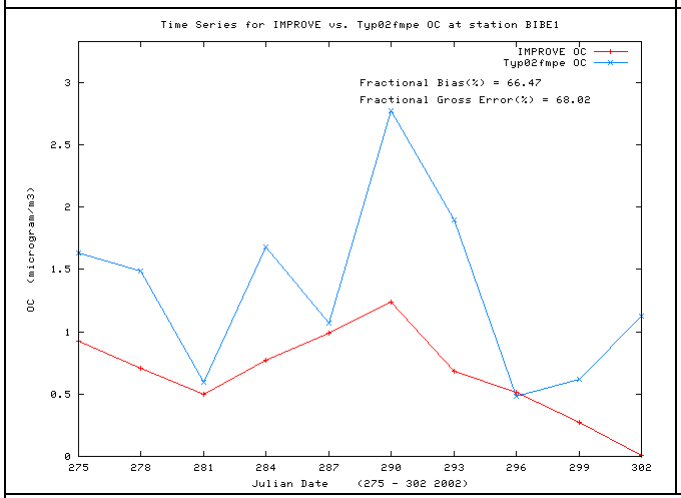

Time Series for IMPROVE vs. Typ02fmpe OC at station BOWA1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 3.62
Fractional Gross Error(%) = 51.95
OC (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station VOYA2
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = 30.76
Fractional Gross Error(%) = 31.04
OC (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe OC at station HEGL1
IMPROVE OC
Typ02fmpe OC
Fractional Bias(%) = -6.77
Fractional Gross Error(%) = 18.78
OC (microgram/m3)
Julian Date (275 - 302 2002)

No Data for Mingo (MING)





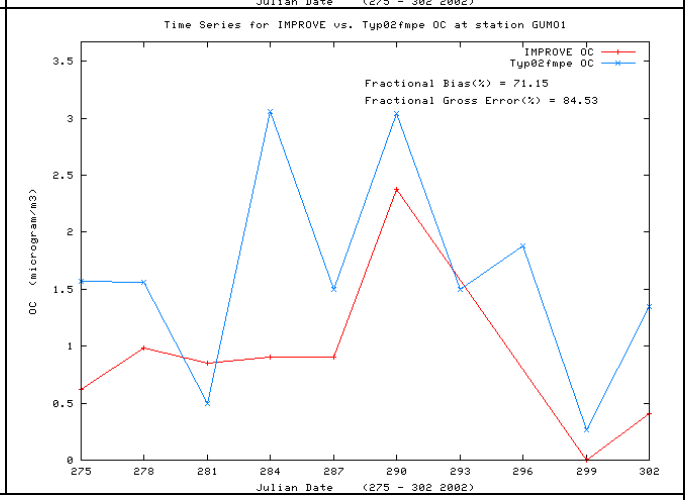


Figure C-19b. Time series of predicted and observed 24-hour organic matter carbon (OMC) concentrations at CENRAP IMPROVE CLASS I AREA sites in October 2002 for CMAQ 2002 36 km Base F base case simulation.

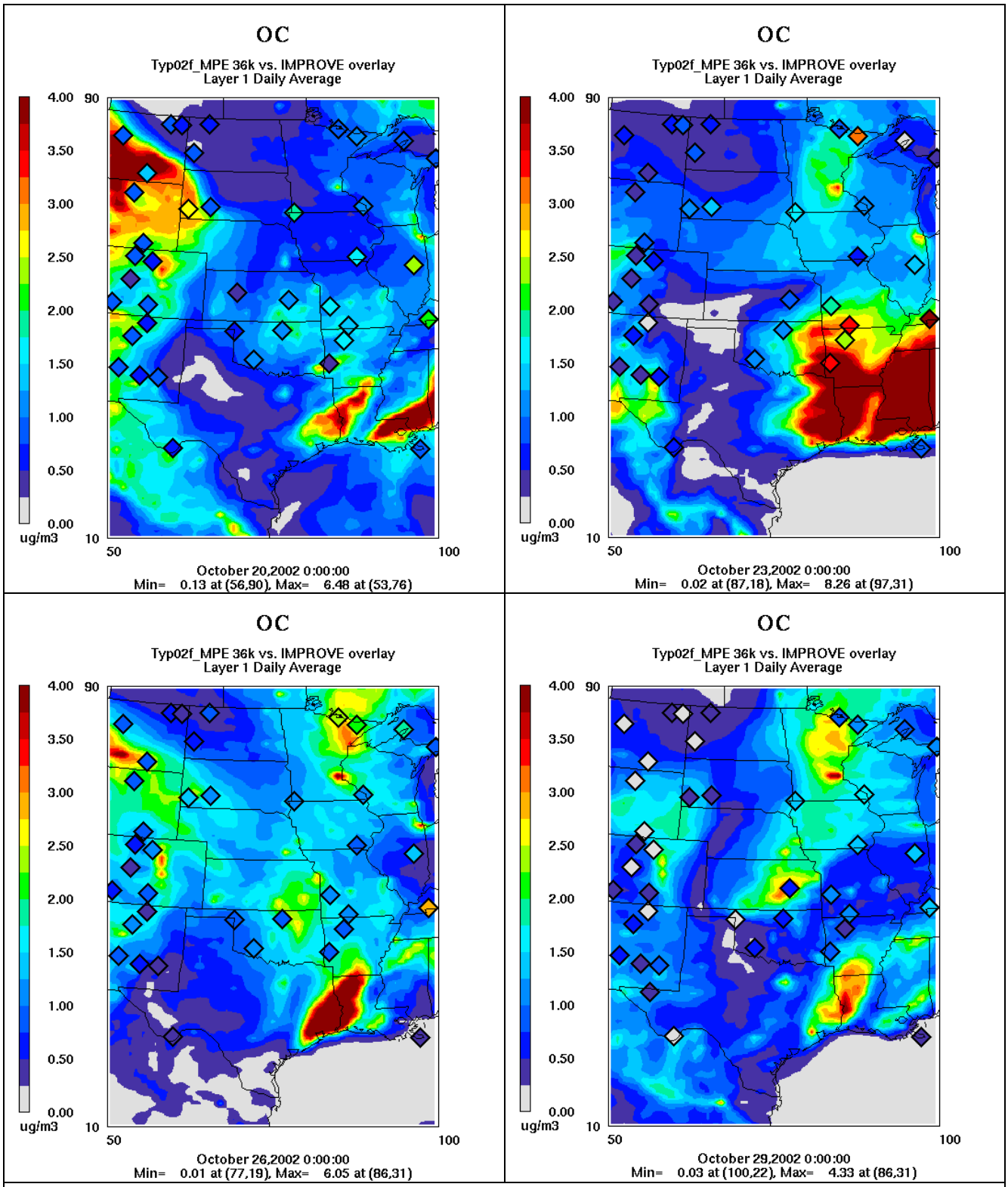


Figure C-19c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour OMC concentrations for October 20, 23, 26 and 29, 2002.

C.3.3.5 OMC Monthly Bias and Error

The OMC monthly bias and error across IMPROVE and STN sites in the CENRAP region are shown in Figure C-20. The bias performance for OMC at the IMPROVE sites are quite good throughout the year with values generally within ±20%, albeit with a slight winter overestimation and summer underestimation bias. At the urban STN sites the model exhibits an underestimation bias throughout the year that ranges from -20% to -50%. Fractional errors are mostly within 40% to 60% with the STN network generally exhibiting more error than IMPROVE.

The good performance of the model for OMC at the IMPROVE sites is also reflected in the Bugle Plot (Figure C-21) with the bias and error achieving the proposed PM model performance goal for all months of the year. At the STN sites, however, the OMC bias falls between the proposed PM model performance goal and criteria, with error right at the goal for most months.

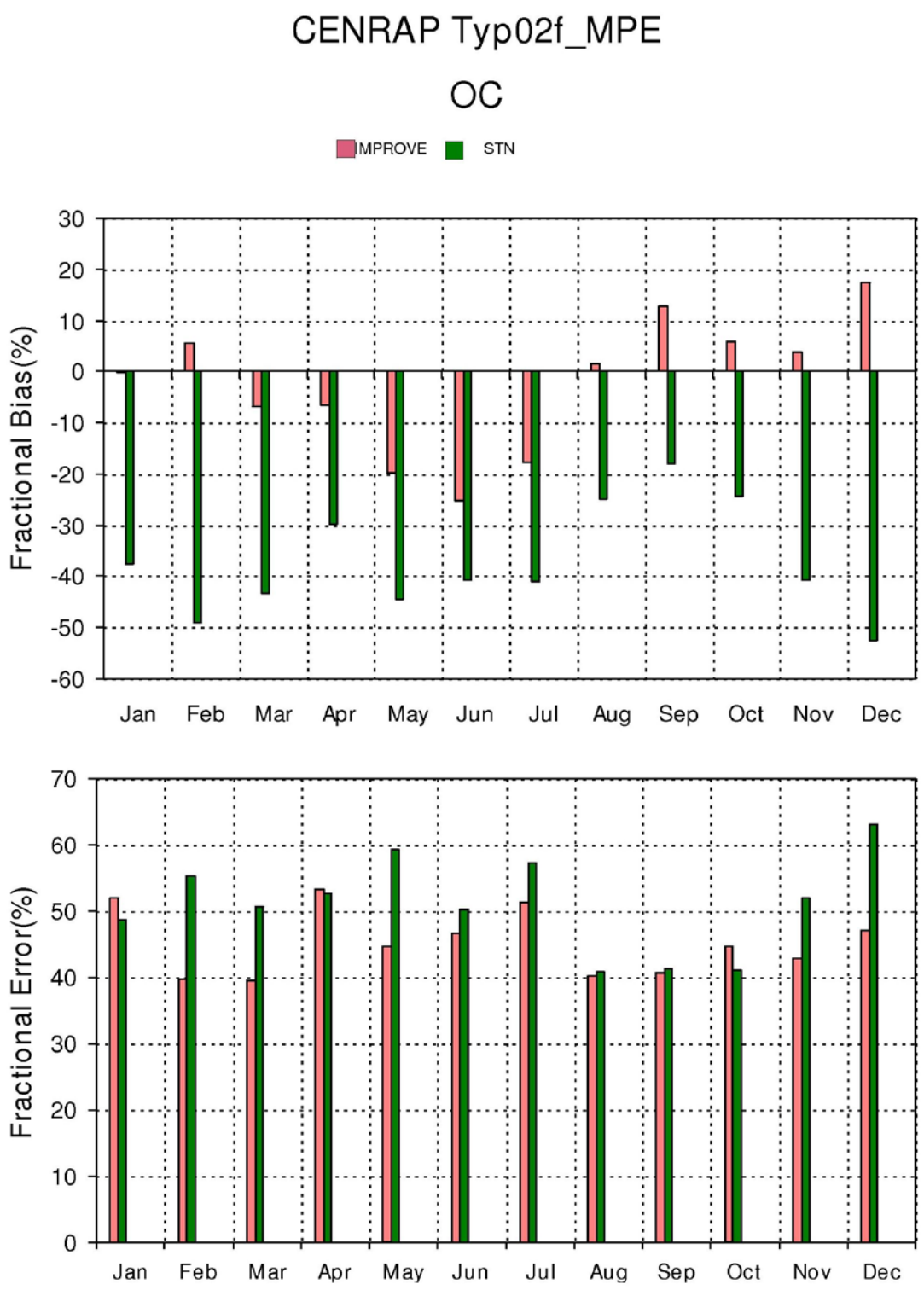


Figure C-20. Monthly OMC fractional bias (top) and fractional gross error (bottom) statistical measures for IMPROVE and STN monitoring sites in the CENRAP region.

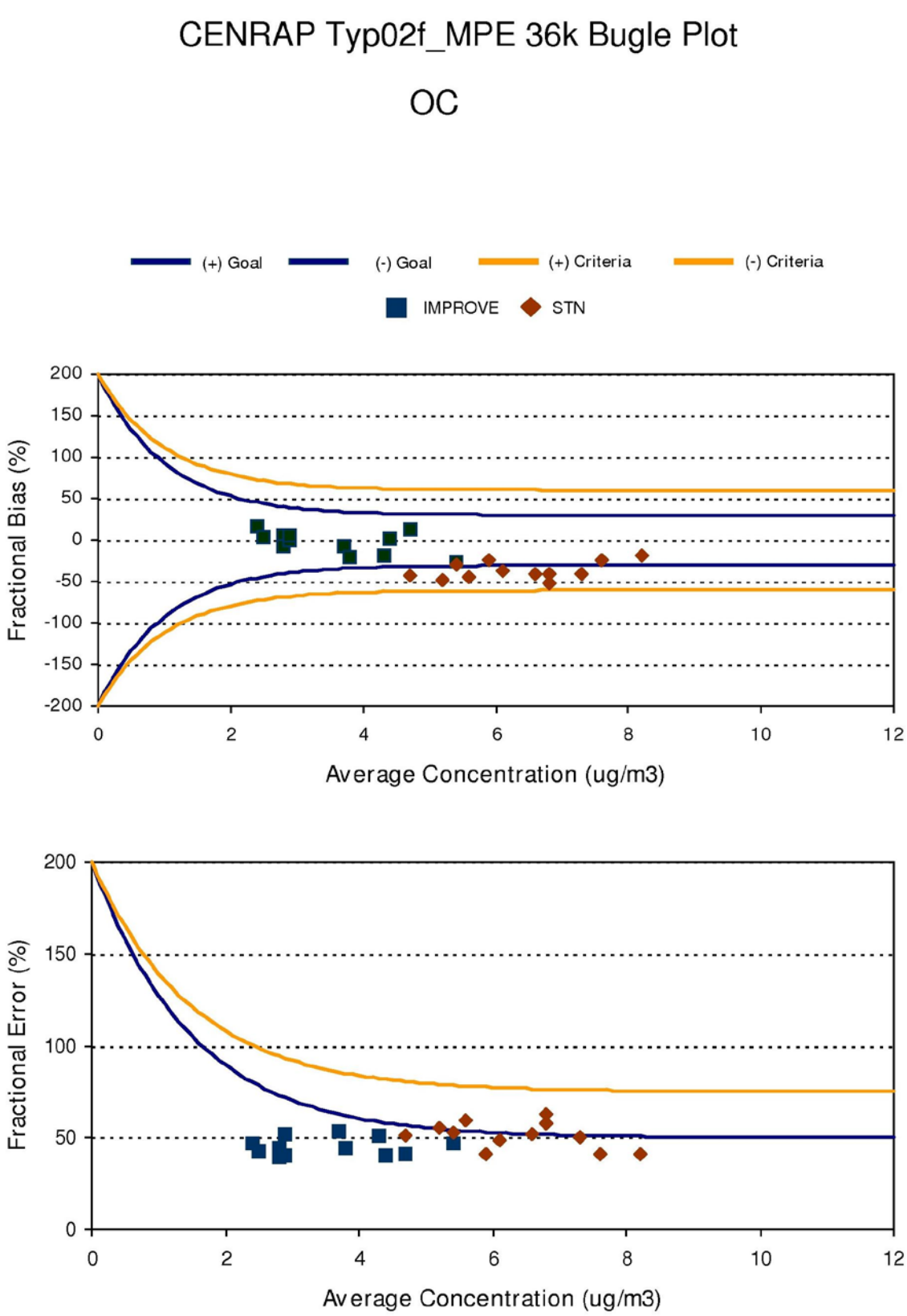


Figure C-21. Bugle Plots of monthly fractional bias (top) and fractional gross error (bottom) and comparisons with model performance goals and criteria for OMC and IMPROVE and STN monitoring sites in the CENRAP region.

C.3.4 Elemental Carbon (EC) Monthly Model Performance

Elemental Carbon (EC) measurements are also uncertain, with the IMPROVE and STN using different measurement technologies with different measurement artifacts.

C.3.4.1 EC in January 2002

Although there is a lot of scatter in the January EC scatter plots at the IMPROVE and STN sites, the bias is fairly low (-24% and 1%) with errors in the 40%-50% range (Figure C-22a). The time series comparisons (Figure C-22b) suggest an EC underestimation bias at BRET and an overestimation bias at the northern Minnesota sites (VOYA and BOWA). The model generally agrees with the observed spatial distribution of EC in January with higher values on the eastern than western portions of the CENRAP region (Figure C-22c).

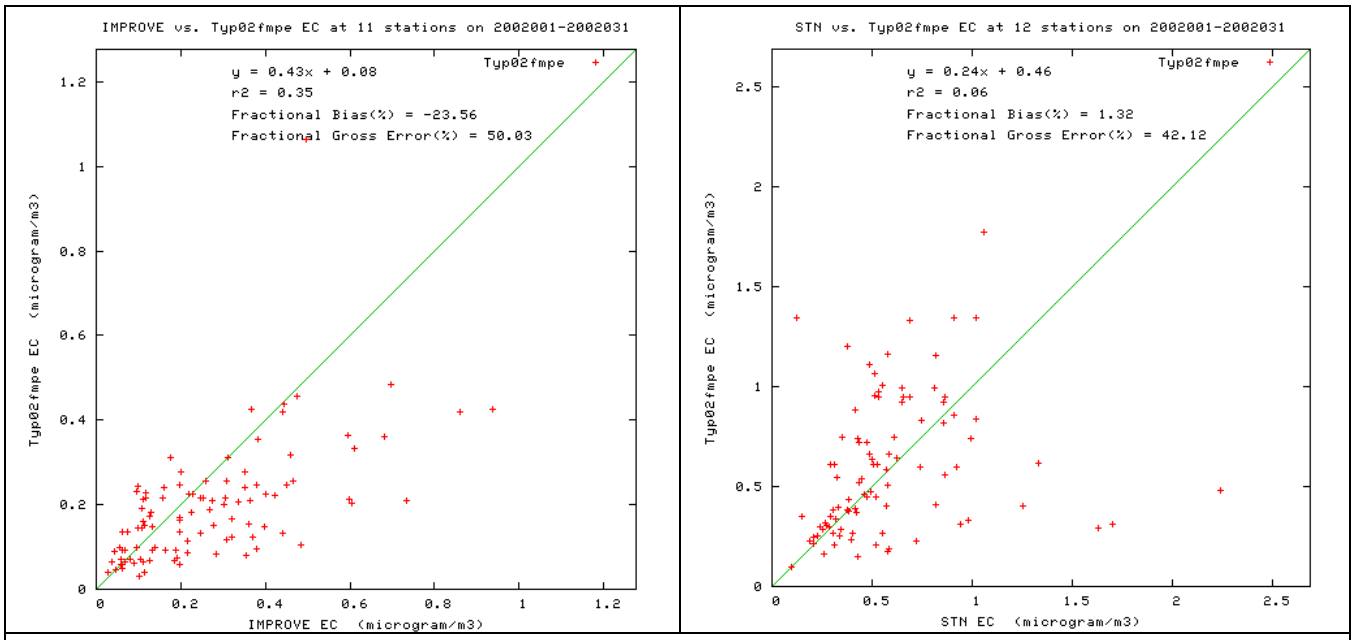
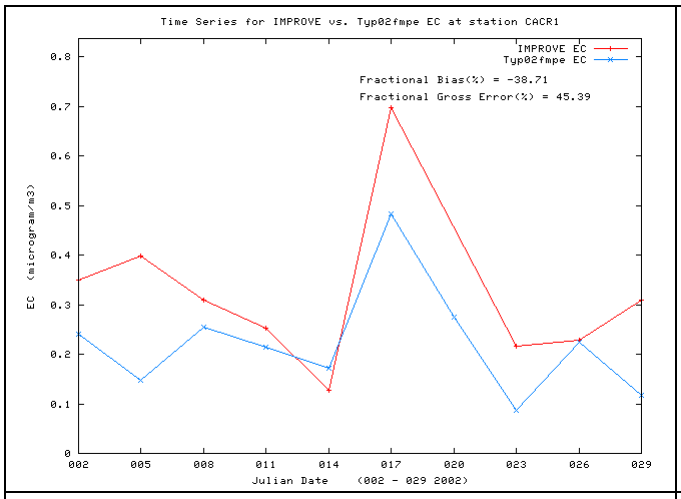
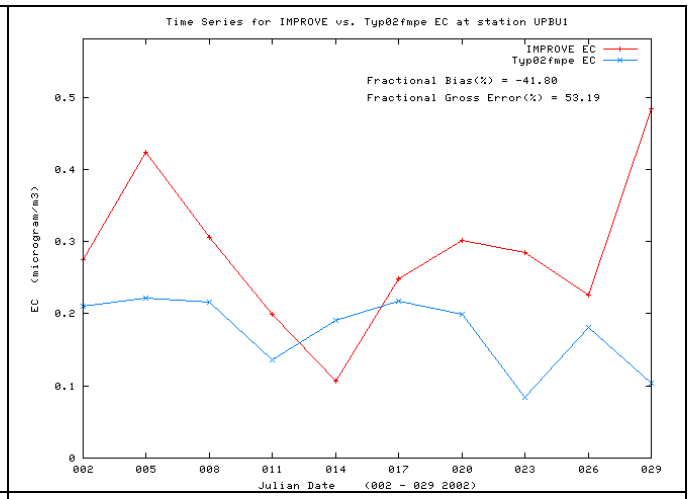
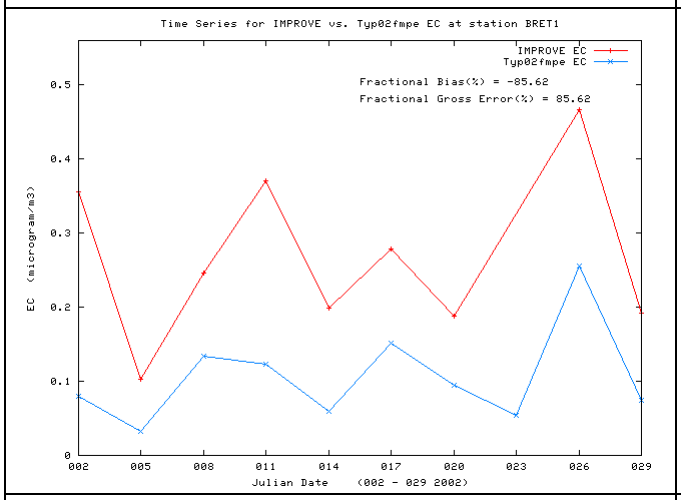
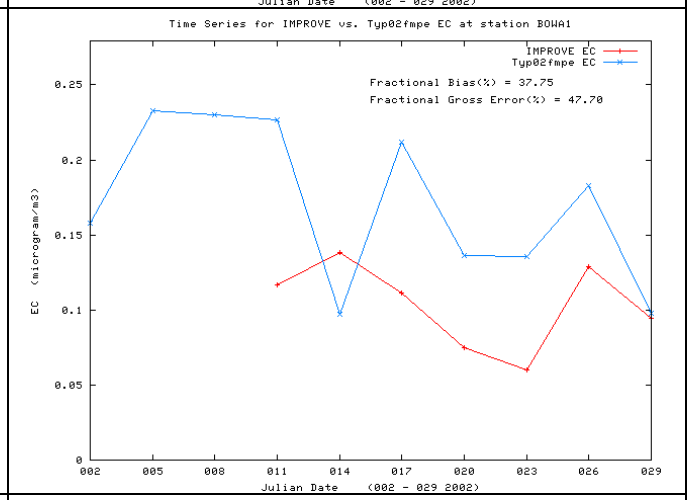


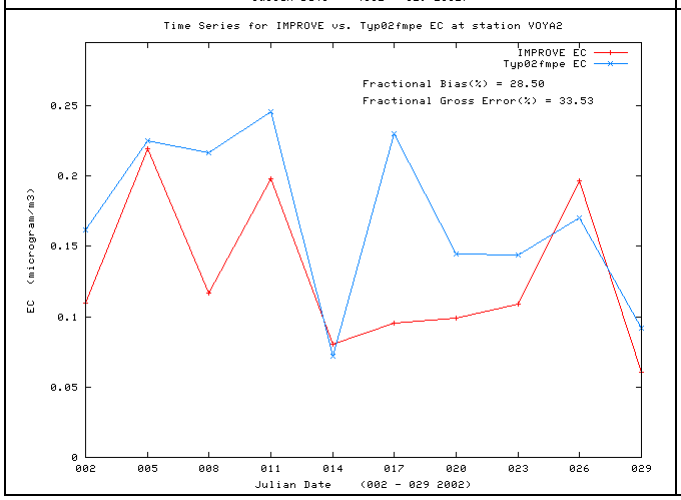
Figure C-22a. Scatter plots of predicted and observed elemental carbon (EC) concentrations for January 2002 and sites in the CENRAP region using IMPROVE (left) and STN (right) monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

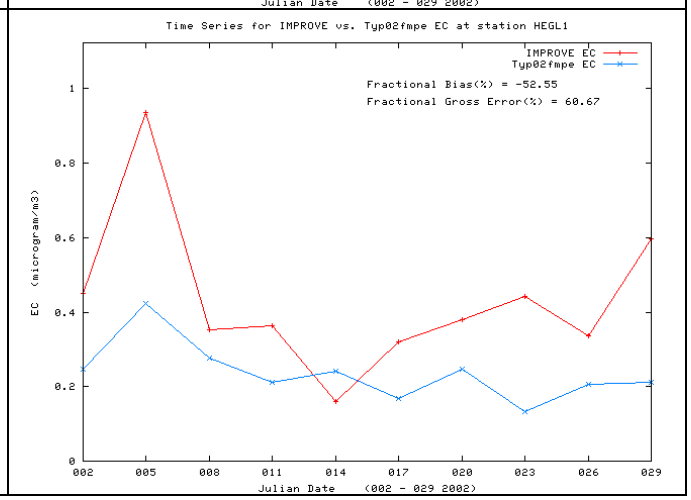

Time Series for IMPROVE vs. Typ02fmpe EC at station CACR1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -38.71
Fractional Gross Error(%) = 45.39
EC (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station UPBU1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -41.80
Fractional Gross Error(%) = 53.19
EC (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station BRET1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -85.62
Fractional Gross Error(%) = 85.62
EC (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station BOWA1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = 37.75
Fractional Gross Error(%) = 47.70
EC (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station VOYA2
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = 28.50
Fractional Gross Error(%) = 33.53
EC (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station HEGL1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -52.55
Fractional Gross Error(%) = 60.67
EC (microgram/m3)
Julian Date (002 - 029 2002)

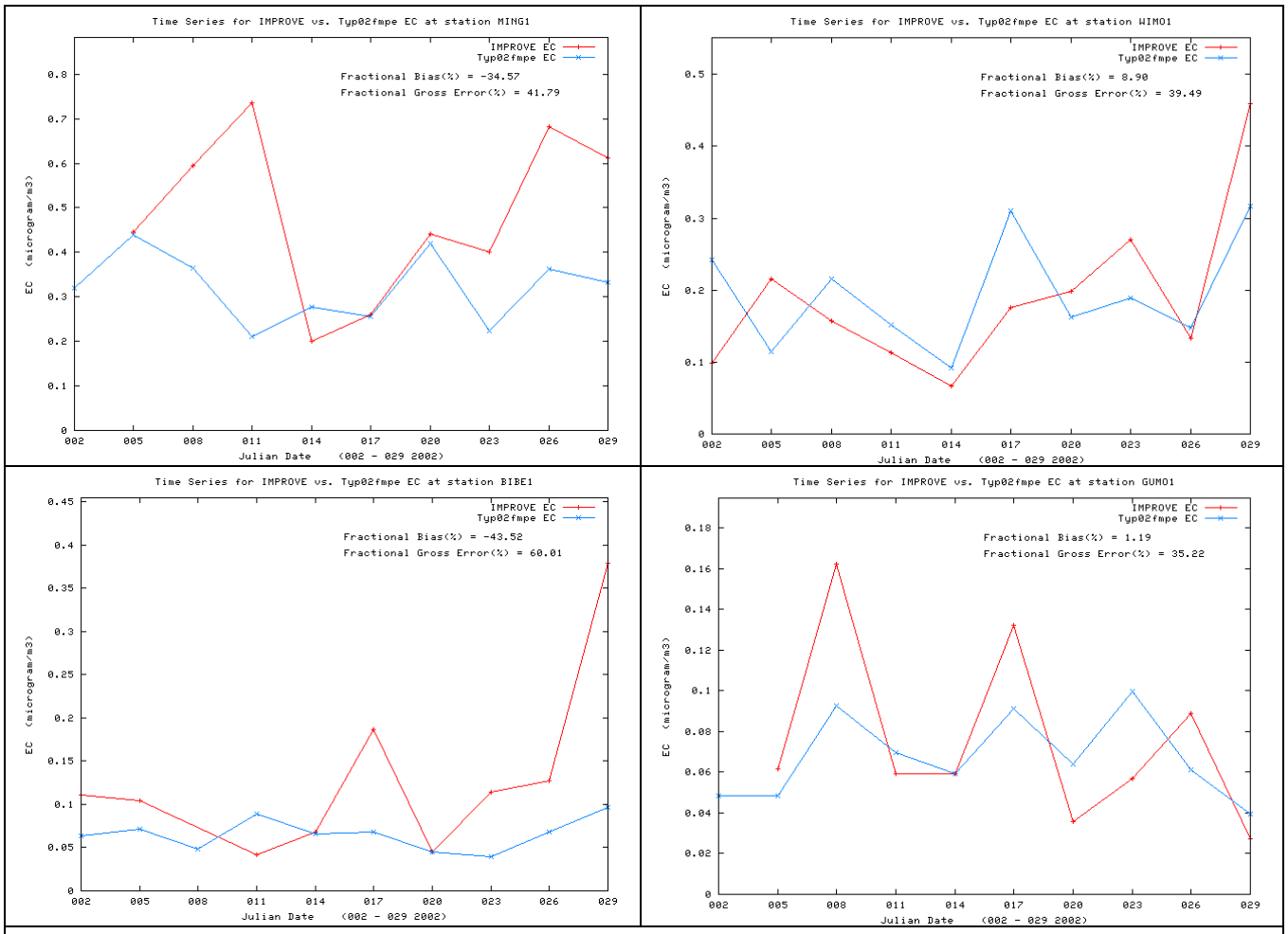


Figure C-22b. Time series of predicted and observed 24-hour elemental carbon (EC) concentrations at CENRAP IMPROVE CLASS I AREA sites in January 2002 for CMAQ 2002 36 km Base F base case simulation.

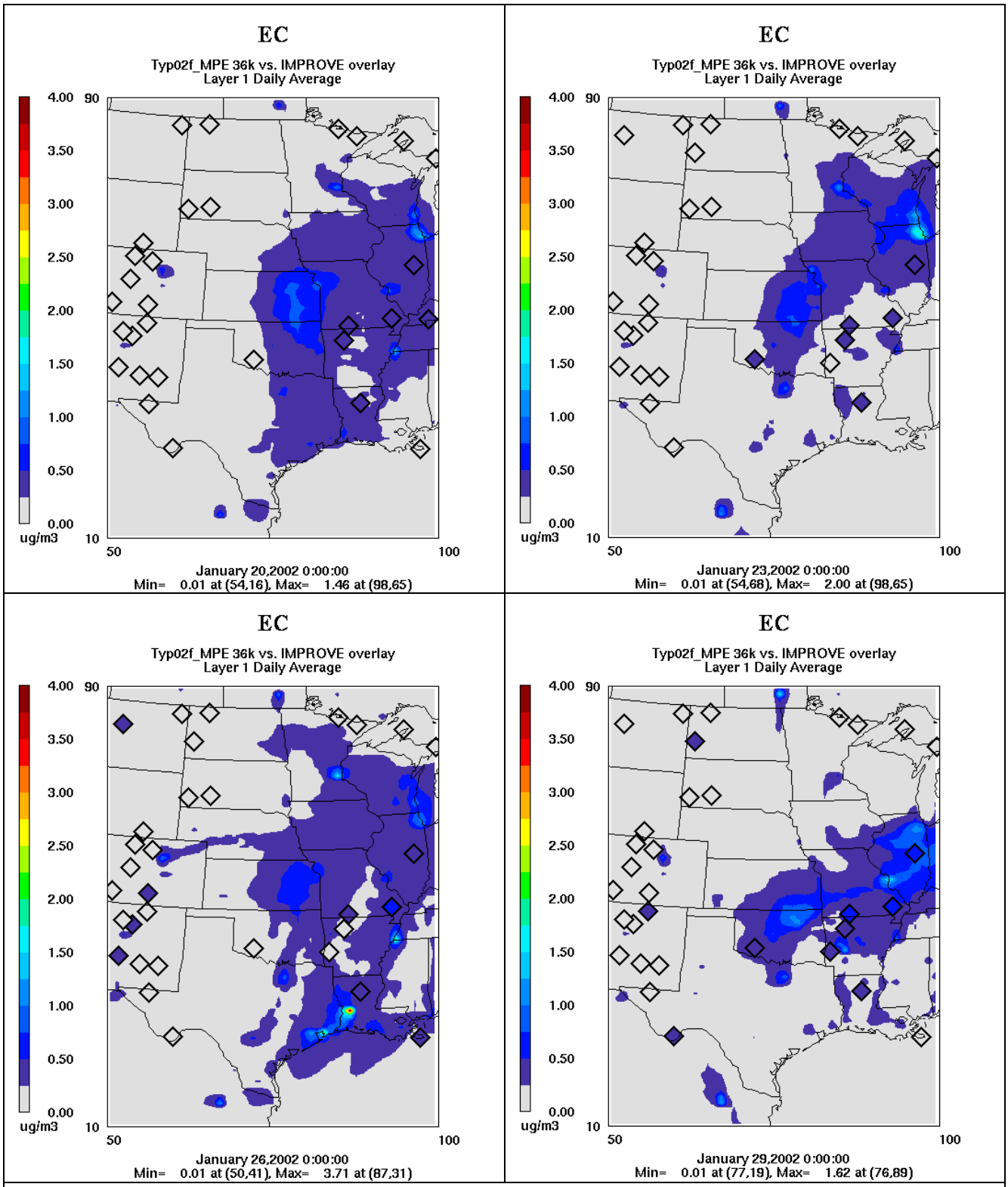


Figure C-22c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour EC concentrations for January 20, 23, 26 and 29, 2002.

C.3.4.2 EC in April 2002

EC is underestimated at the IMPROVE sites in April (bias of -48%), but reproduced well at the STN sites (bias of -13%). Although EC is underestimated at the IMPROVE sites both the model and observations agree that EC concentrations are very small and not a significant component of the PM budget. The model fails to capture the day-to-day variability in the observed EC at the IMPROVE sites and exhibits a systematic under-prediction tendency at some sites (Figure C-23b). On April 5 and 11 the model reproduces the spatial distribution of the observed EC reasonable well with higher values in the eastern than western portion of the CENRAP region. But on April 8 and 14 the model is much to clean in the eastern portion of the CENRAP region (Figure C-23c).

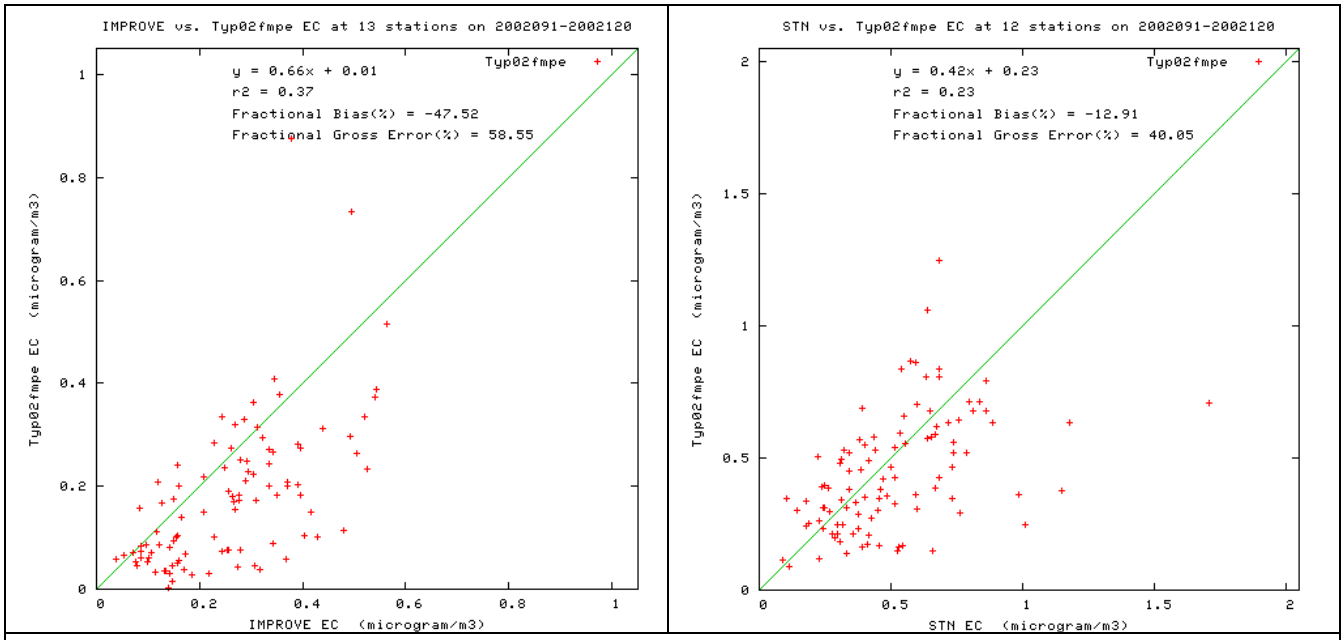
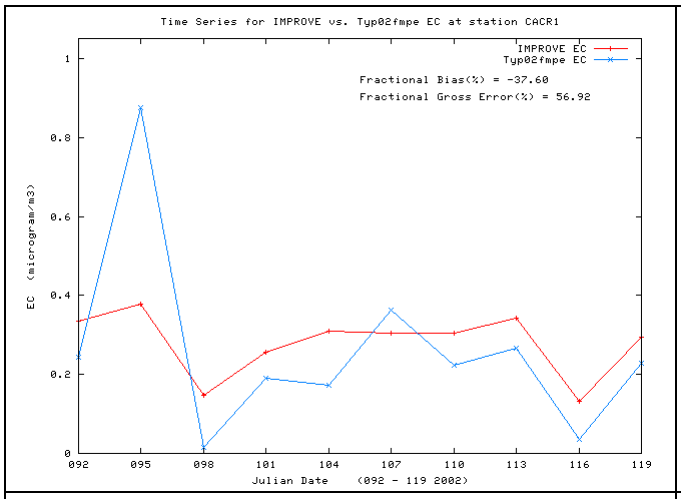
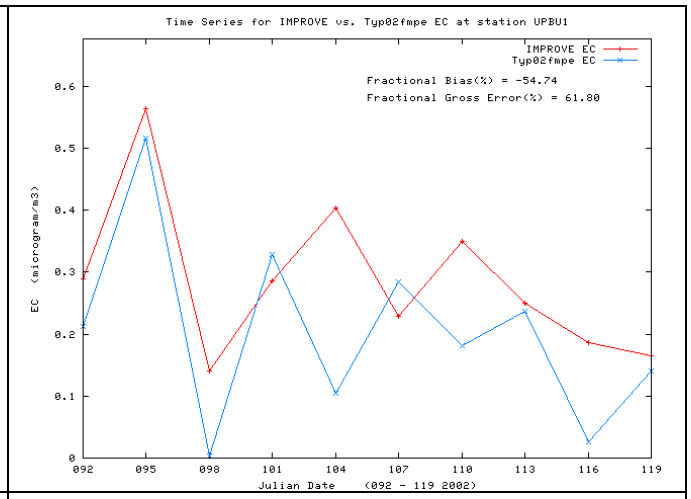
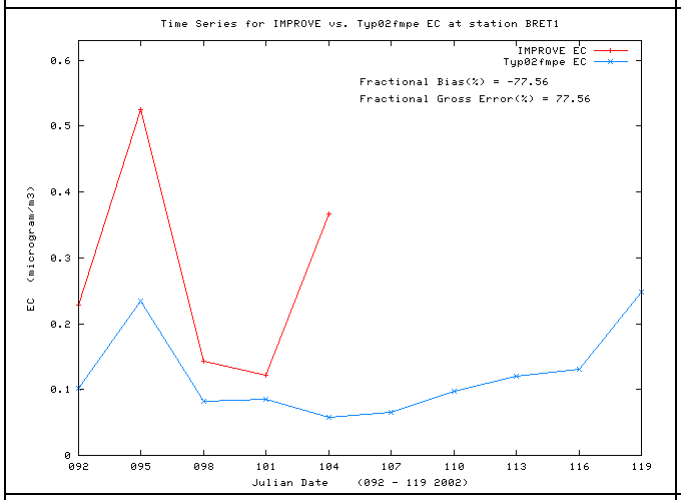
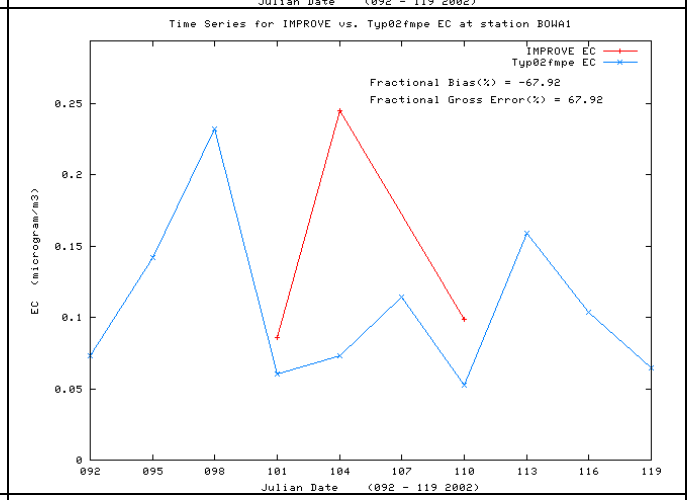


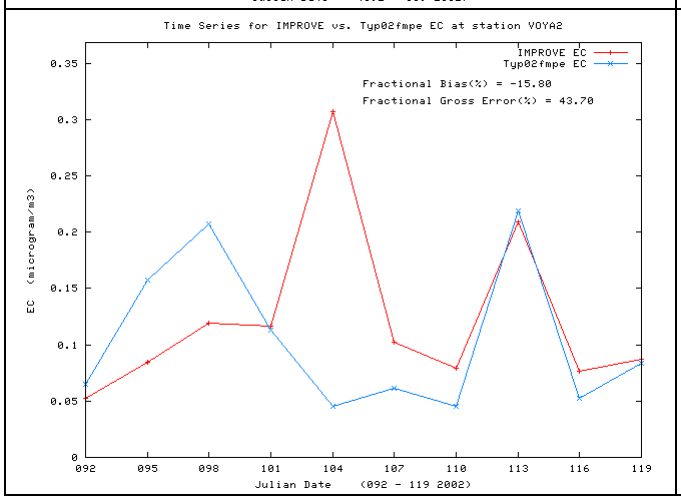
Figure C-23a. Scatter plots of predicted and observed elemental carbon (EC) concentrations for April 2002 and sites in the CENRAP region using IMPROVE (left) and STN (right) monitoring networks using the CMAQ 2002 36 km Base F base case simulation

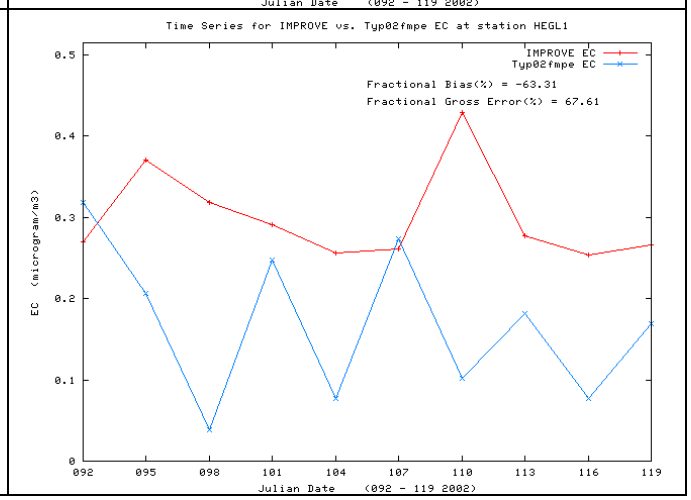

Time Series for IMPROVE vs. Typ02fmpe EC at station CACR1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -37.60
Fractional Gross Error(%) = 56.92
EC (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station UPBU1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -54.74
Fractional Gross Error(%) = 61.80
EC (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station BRET1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -77.56
Fractional Gross Error(%) = 77.56
EC (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station BOWA1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -67.92
Fractional Gross Error(%) = 67.92
EC (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station VOYA2
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -15.80
Fractional Gross Error(%) = 43.70
EC (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station HEGL1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -63.31
Fractional Gross Error(%) = 67.61
EC (microgram/m3)
Julian Date (092 - 119 2002)

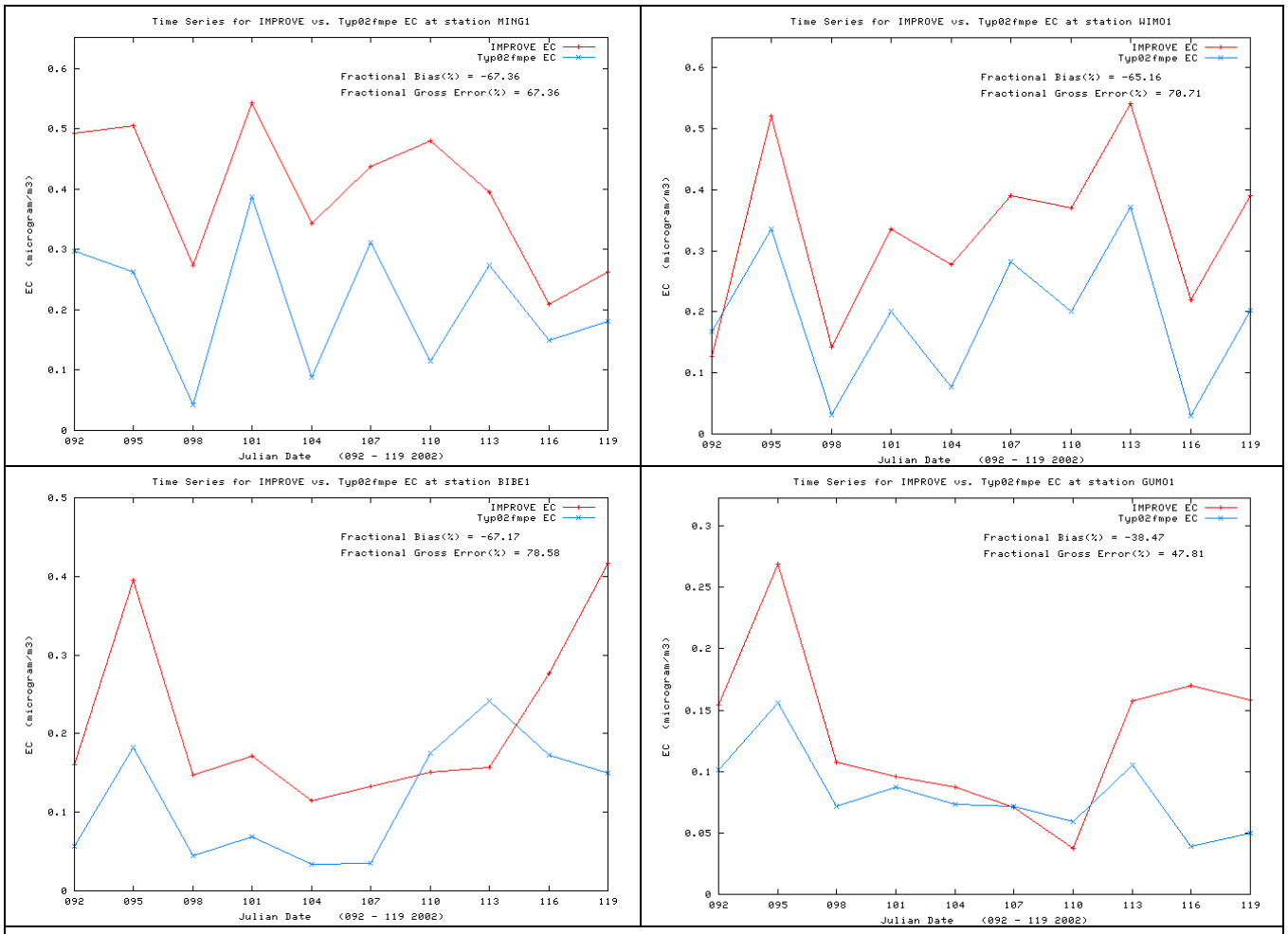


Figure C-23b. Time series of predicted and observed 24-hour elemental carbon (EC) concentrations at CENRAP IMPROVE CLASS I AREA sites in April 2002 for CMAQ 2002 36 km Base F base case simulation.

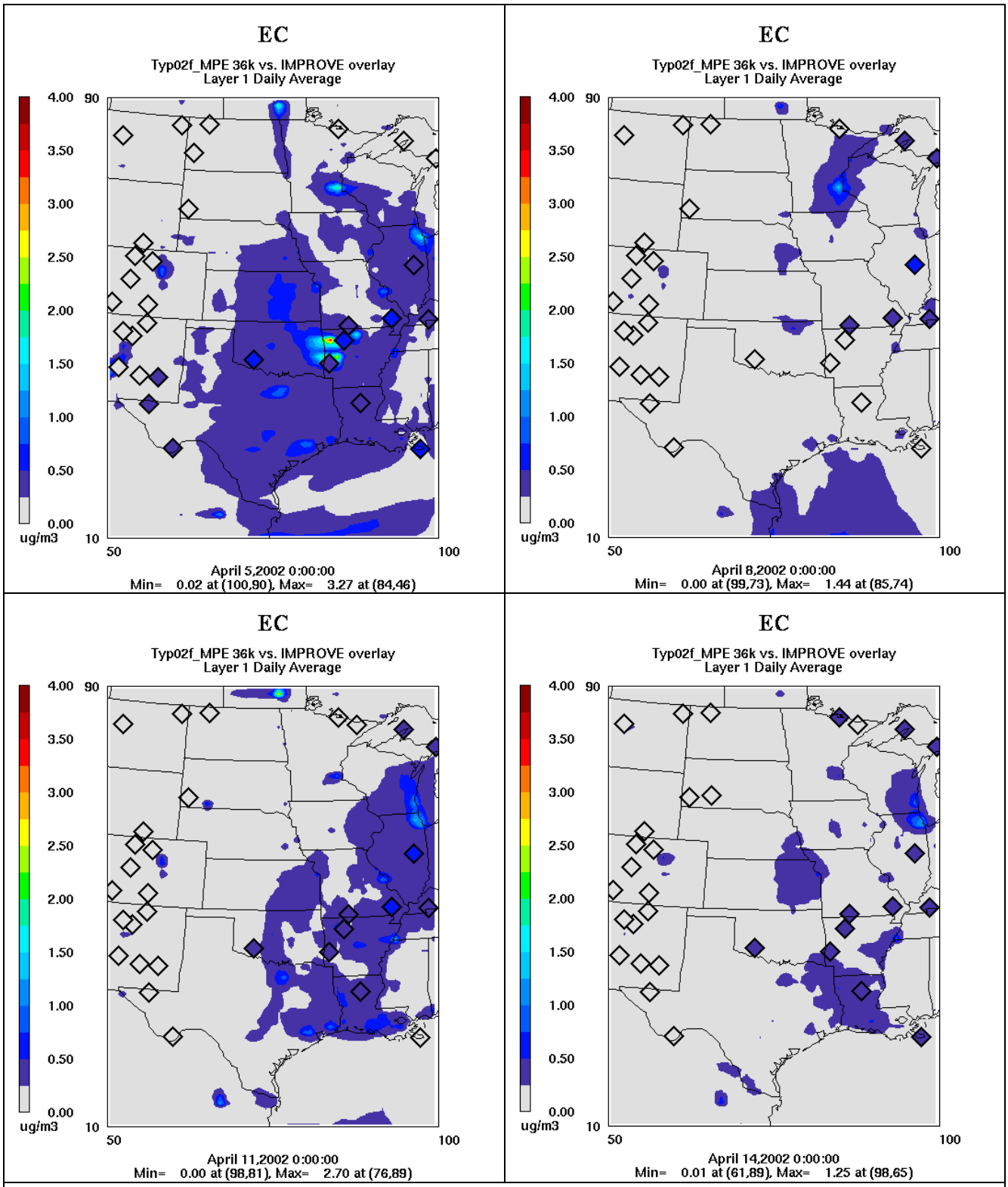


Figure C-23c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour EC concentrations for April 5, 8, 11 and 14, 2002.

C.3.3.3 EC in July 2002

July EC performance is similar to the other months with near zero bias across he STN sites and an underestimation bias across the IMPROVE sites (Figure C-24). Again the model and observations agree that EC is low in July and not a significant component of visibility impairment.

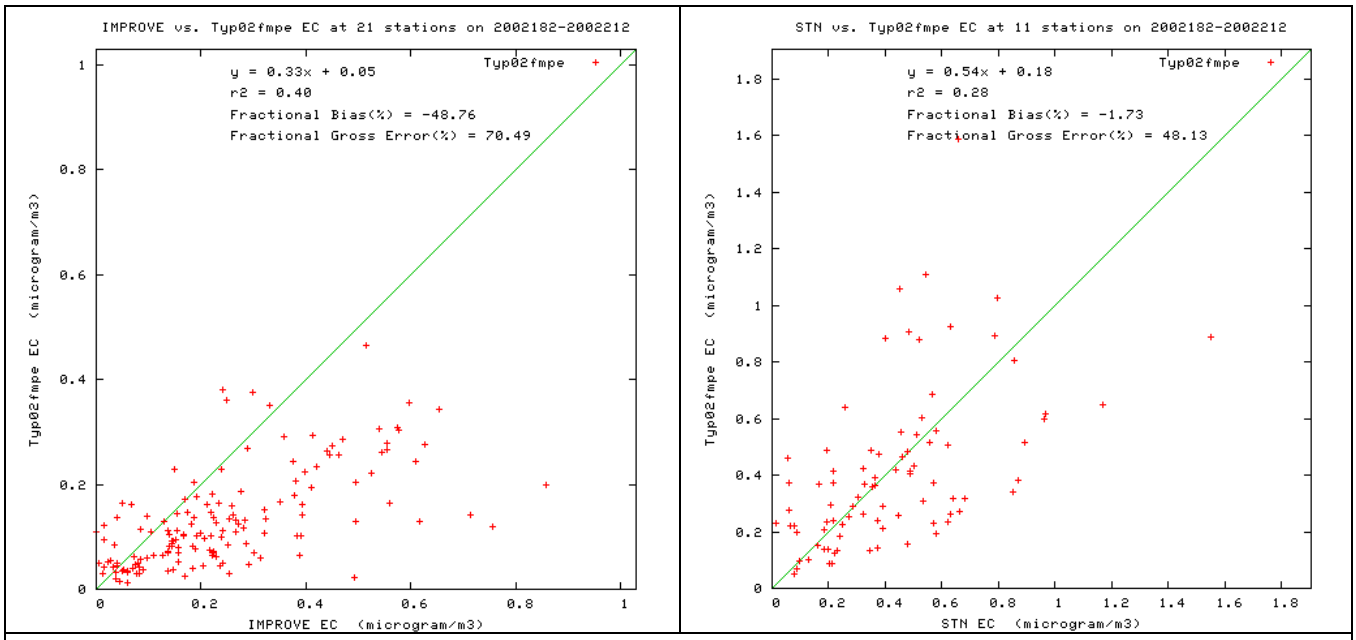
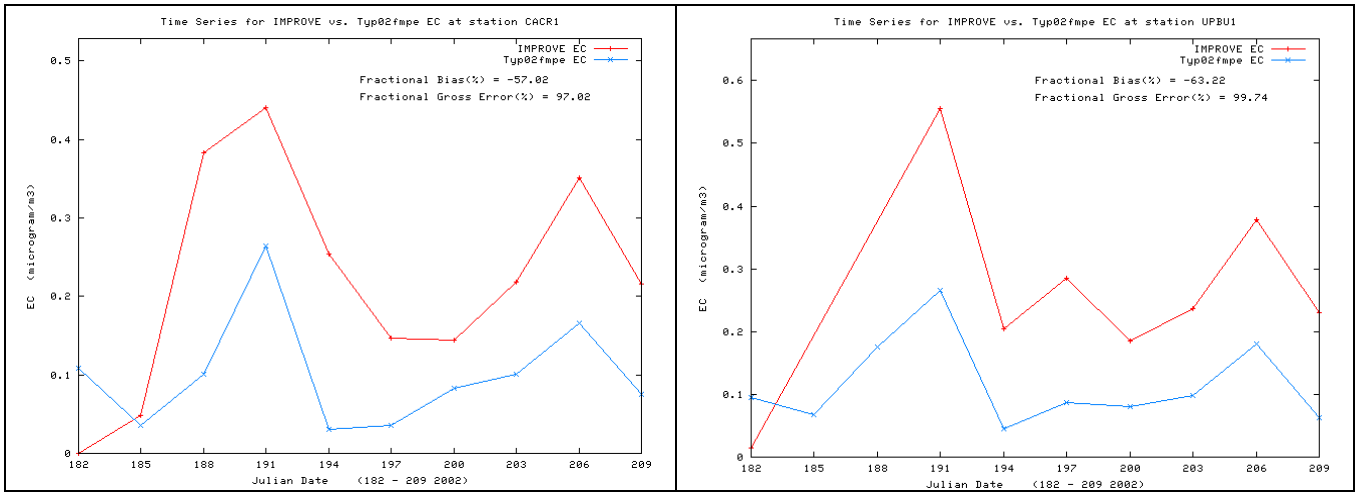
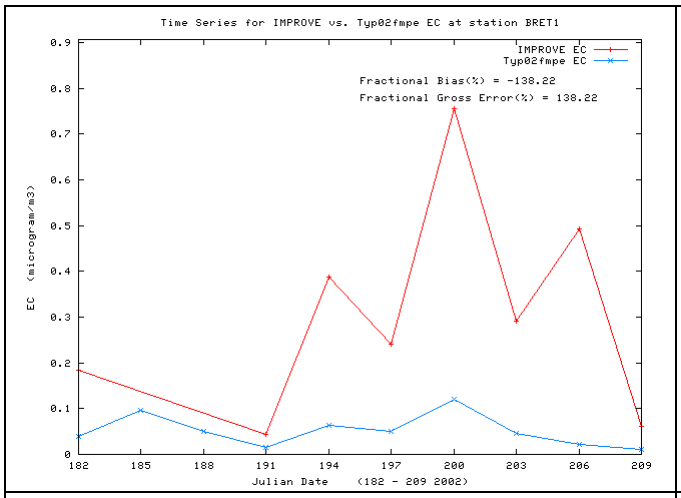
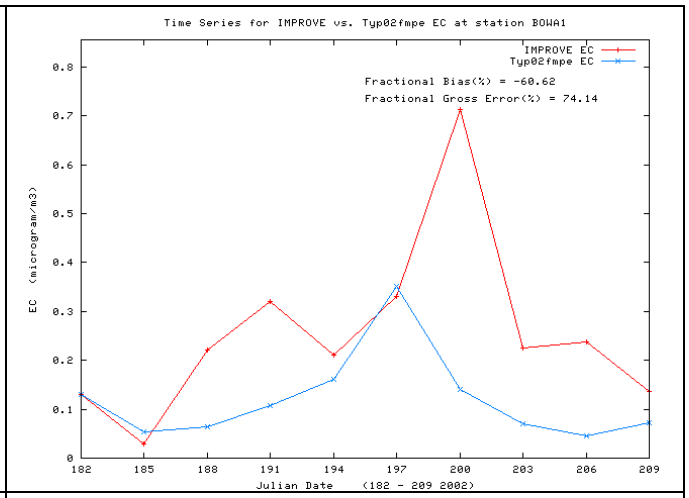
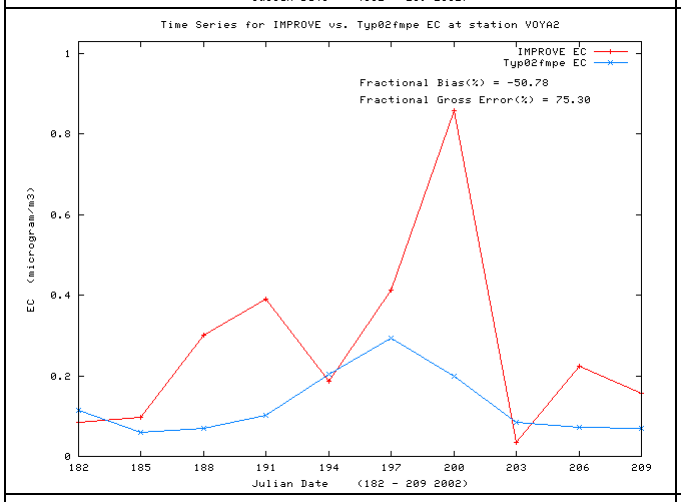


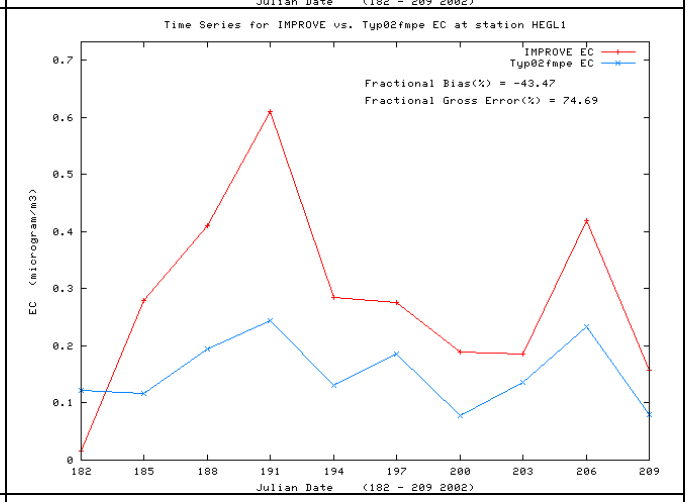
Figure C-24a. Scatter plots of predicted and observed elemental carbon (EC) concentrations for July 2002 and sites in the CENRAP region using IMPROVE (left) and STN (right) monitoring networks using the CMAQ 2002 36 km Base F base case simulation.



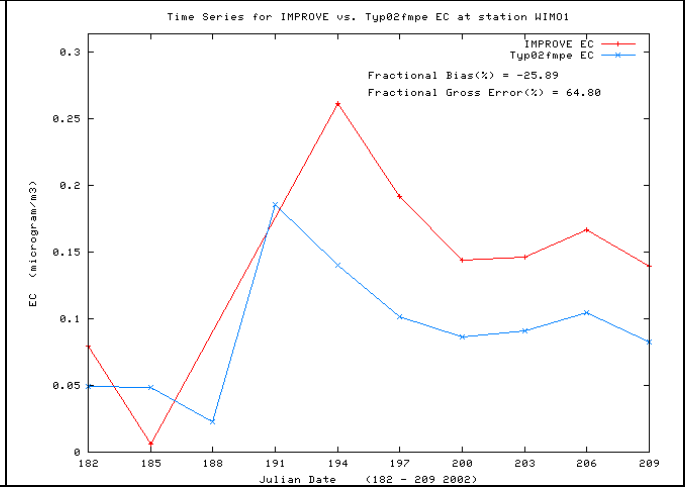








No Data for Mingo (MING)



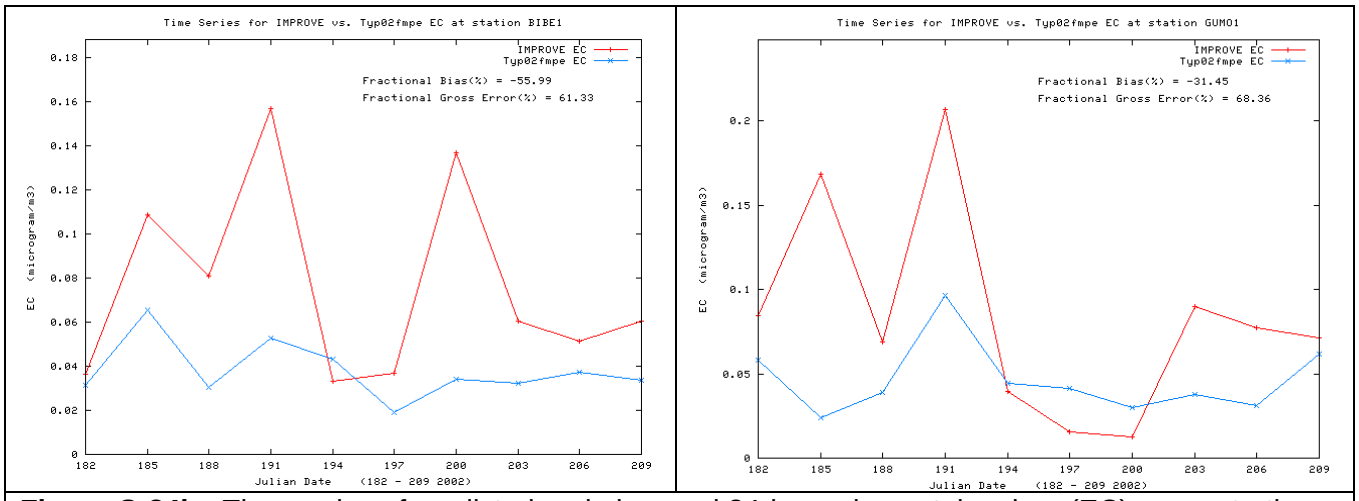


Figure C-24b. Time series of predicted and observed 24-hour elemental carbon (EC) concentrations at CENRAP IMPROVE CLASS I AREA sites in July 2002 for CMAQ 2002 36 km Base F base case simulation.

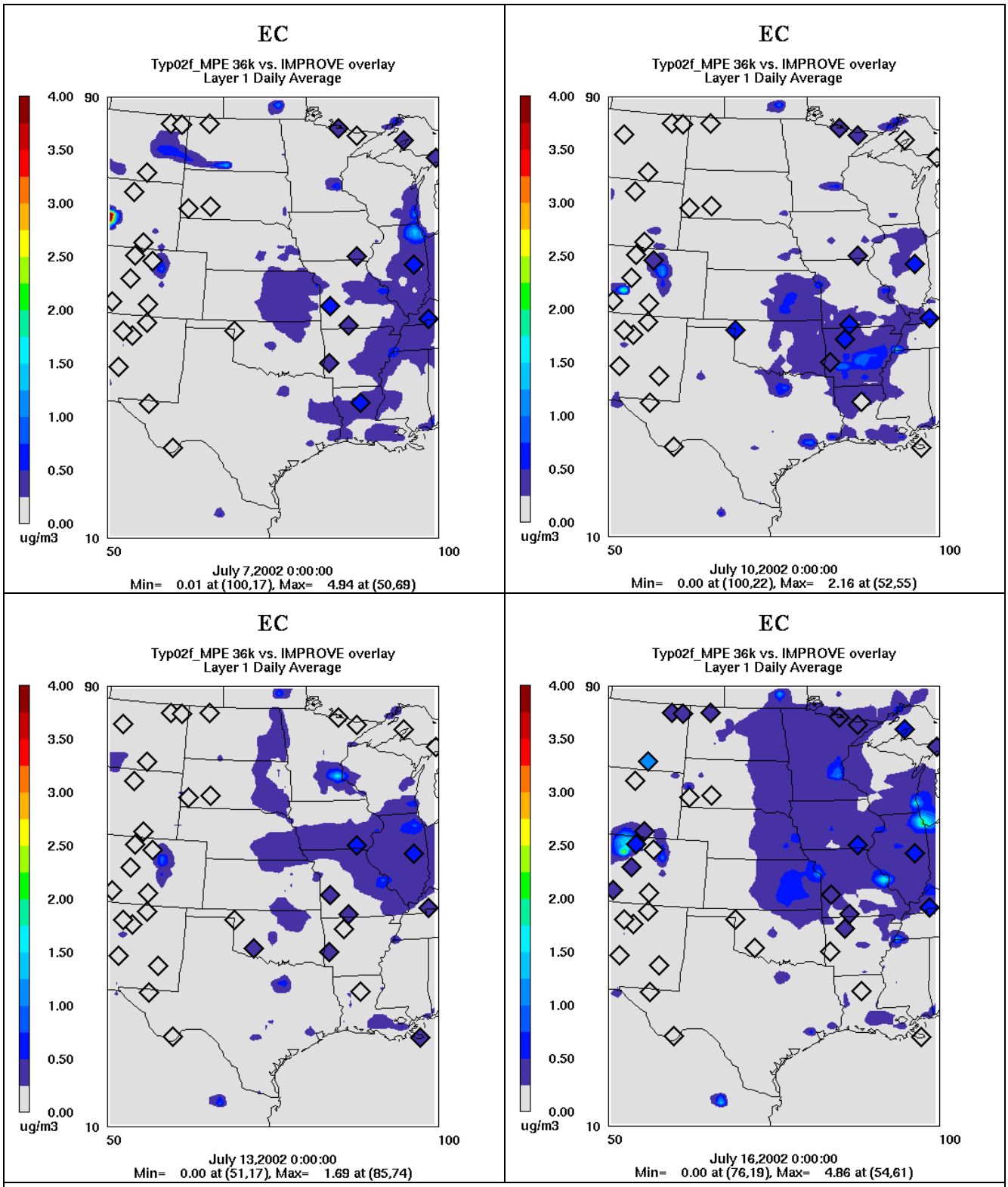


Figure C-24c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour EC concentrations for July 7, 10, 13 and 16, 2002.

C.3.4.4 EC in October 2002

EC performance is improved at the IMPROVE sites in October with lower bias (9%) than the previous months where an under-prediction tendency was seen (Figure C-25a). EC bias is also fairly low at the STN sites with errors across both networks of approximately 50%. Although there is a systematic underestimation of EC at BRET, the agreement between the predicted and observed October time series (Figure C-25b) is remarkable at several sites (e.g., CACR, UPBU, VOYA and HEGL).

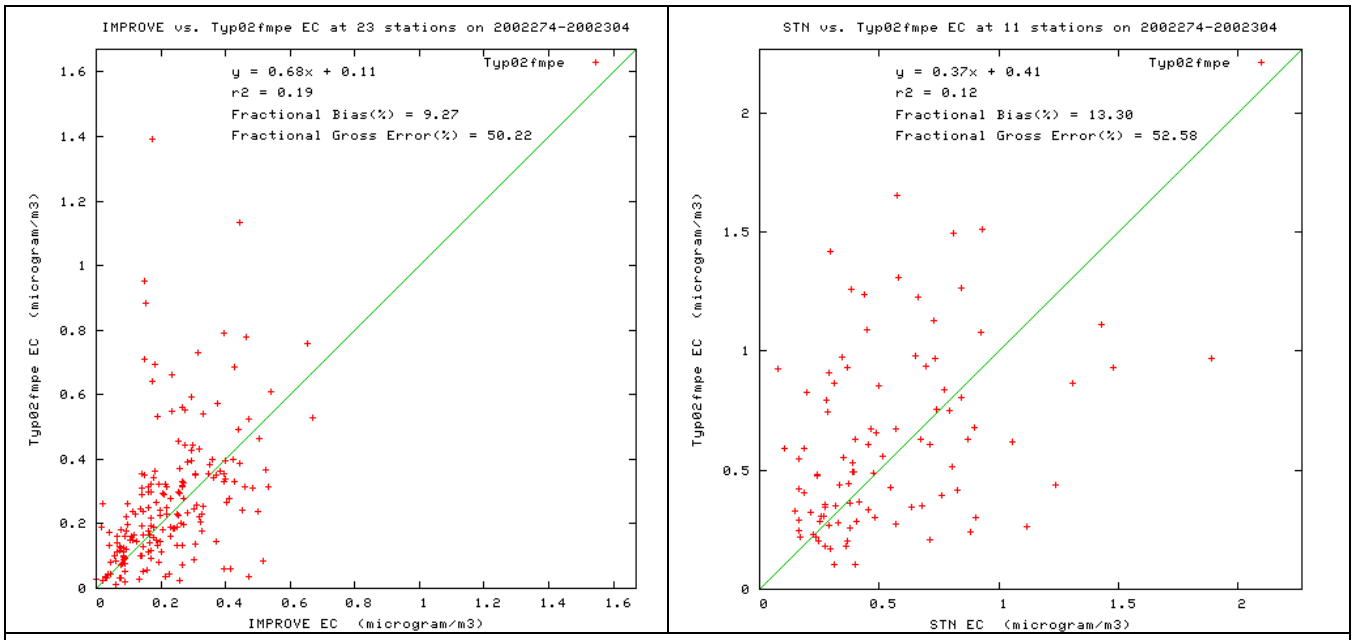
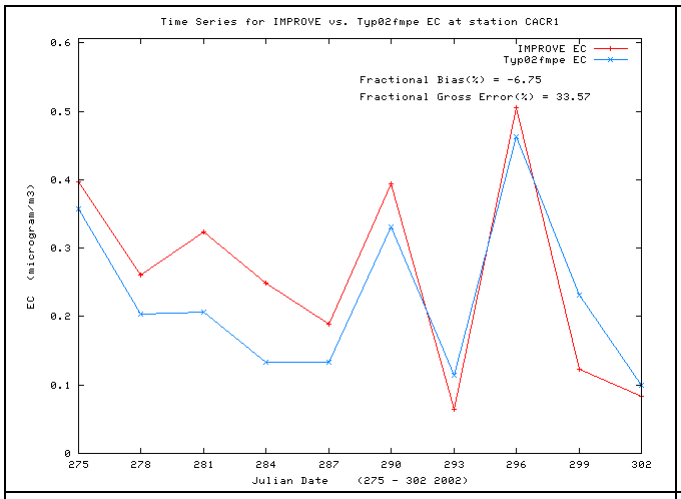
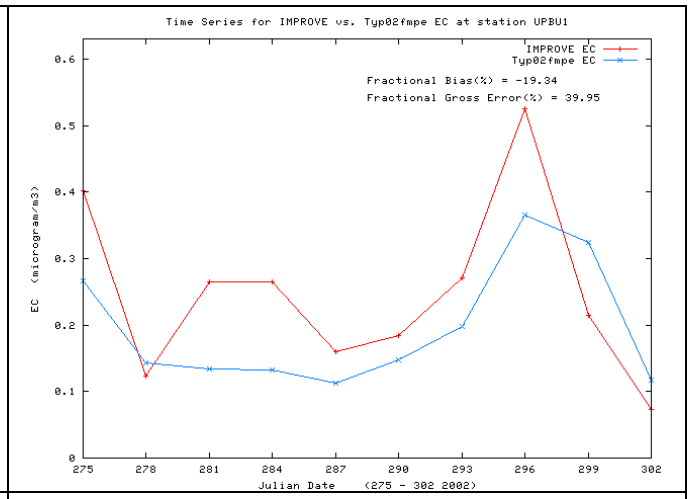
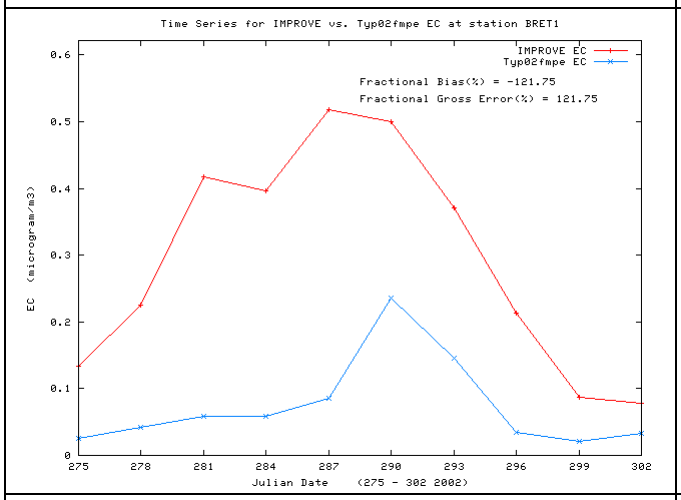
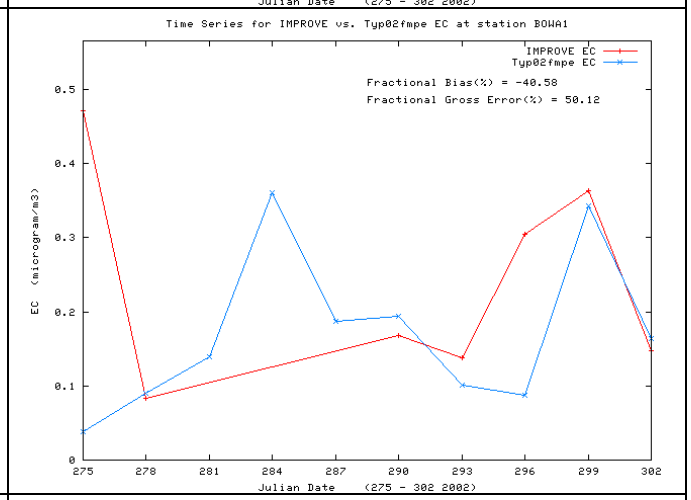


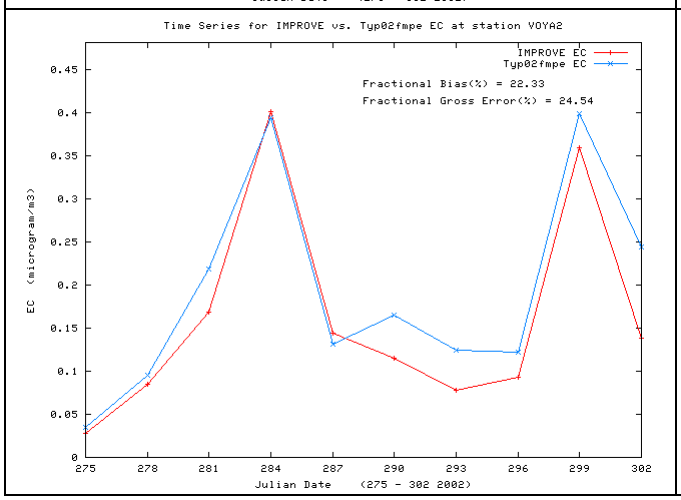
Figure C-25a. Scatter plots of predicted and observed elemental carbon (EC) concentrations for October 2002 and sites in the CENRAP region using IMPROVE (left) and STN (right) monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

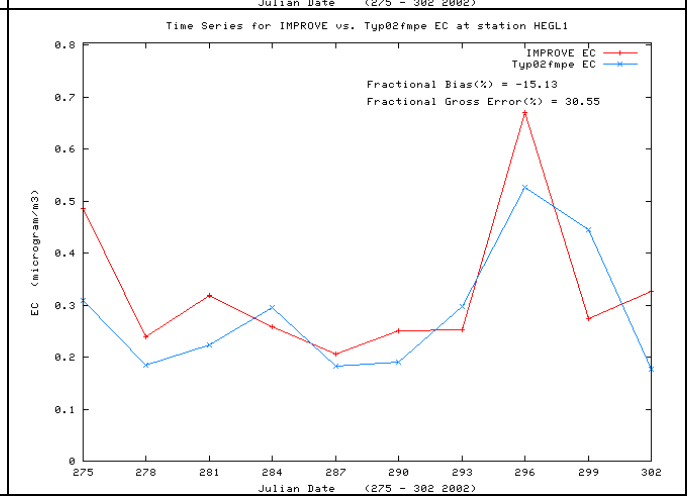

Time Series for IMPROVE vs. Typ02fmpe EC at station CACR1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -6.75
Fractional Gross Error(%) = 33.57
EC (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station UPBU1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -19.34
Fractional Gross Error(%) = 39.95
EC (microgram/m3)
Julian Date (275 - 302 2002)

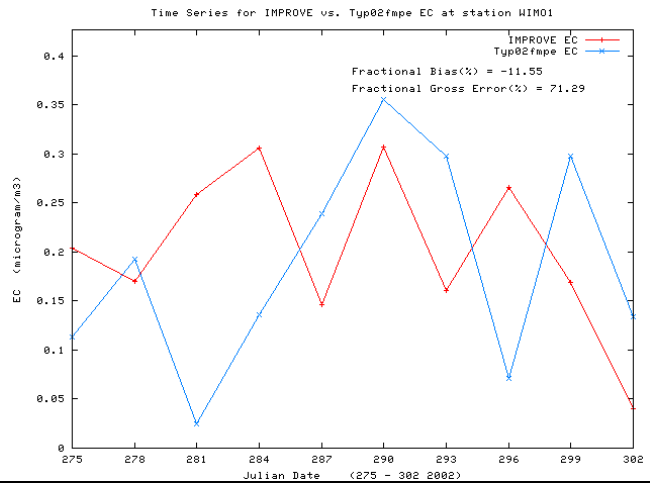

Time Series for IMPROVE vs. Typ02fmpe EC at station BRET1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -121.75
Fractional Gross Error(%) = 121.75
EC (microgram/m3)
Julian Date (275 - 302 2002)

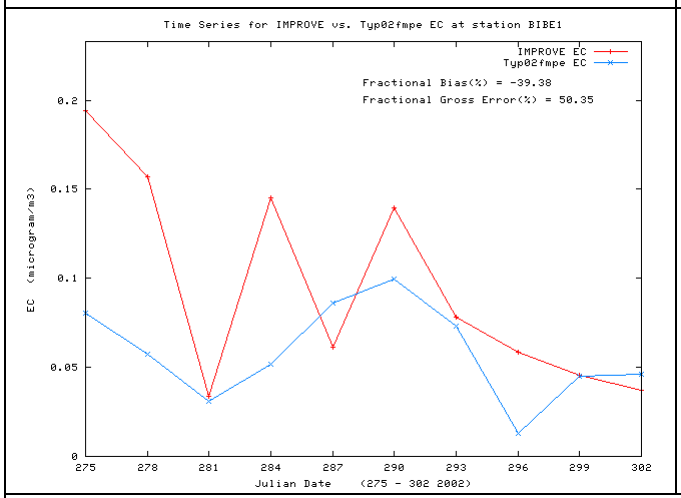

Time Series for IMPROVE vs. Typ02fmpe EC at station BOWA1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -40.58
Fractional Gross Error(%) = 50.12
EC (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station VOYA2
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = 22.33
Fractional Gross Error(%) = 24.54
EC (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe EC at station HEGL1
IMPROVE EC
Typ02fmpe EC
Fractional Bias(%) = -15.13
Fractional Gross Error(%) = 30.55
EC (microgram/m3)
Julian Date (275 - 302 2002)

No Data for Mingo (MING)





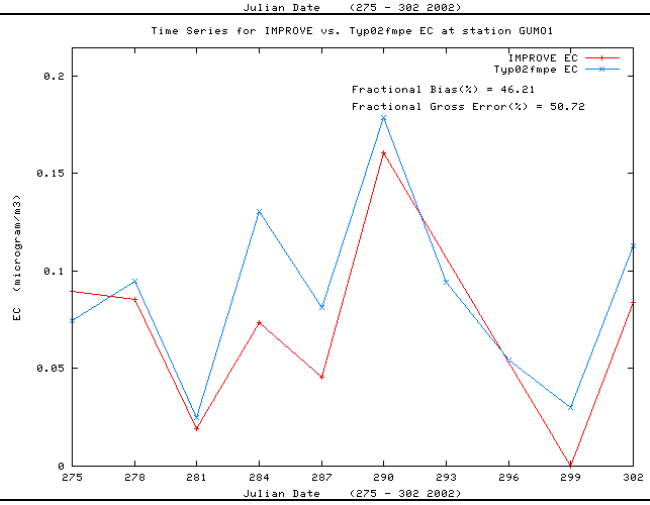


Figure C-25b. Time series of predicted and observed 24-hour elemental carbon (EC) concentrations at CENRAP IMPROVE CLASS I AREA sites in October 2002 for CMAQ 2002 36 km Base F base case simulation.

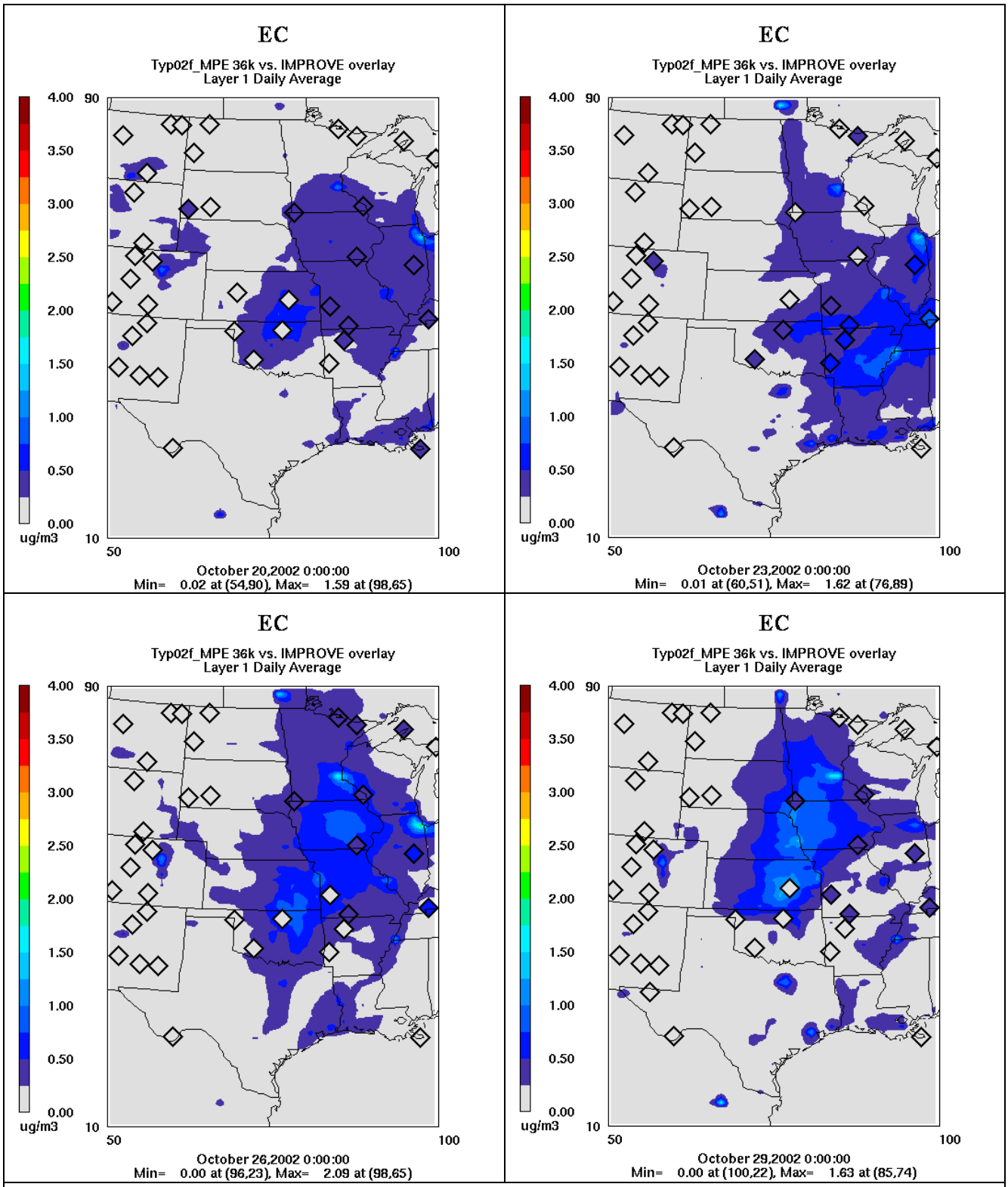


Figure C-25c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour EC concentrations for October 20, 23, 26 and 29, 2002.

C.3.4.5 EC Monthly Bias and Error

The monthly average bias and error for EC across the IMPROVE and STN monitors in the CENRAP region are shown in Figure C-26. The STN network exhibits low bias year round, whereas the IMPROVE monitoring network exhibits a large under-prediction bias in the summer months (-40% to -60%) and much lower EC bias in the winter. The errors in the IMPROVE summer EC performance are also quite high (60% to 80%), whereas during the winter the IMPROVE errors are in the 40% to 50% range which is also where the STN errors reside year round.

The Bugle Plot puts the EC performance in context (Figure C-27). The low EC concentrations put the IMPROVE EC performance in the horn of the Bugle Plot so that it achieves the proposed PM performance goal for all months of the year.

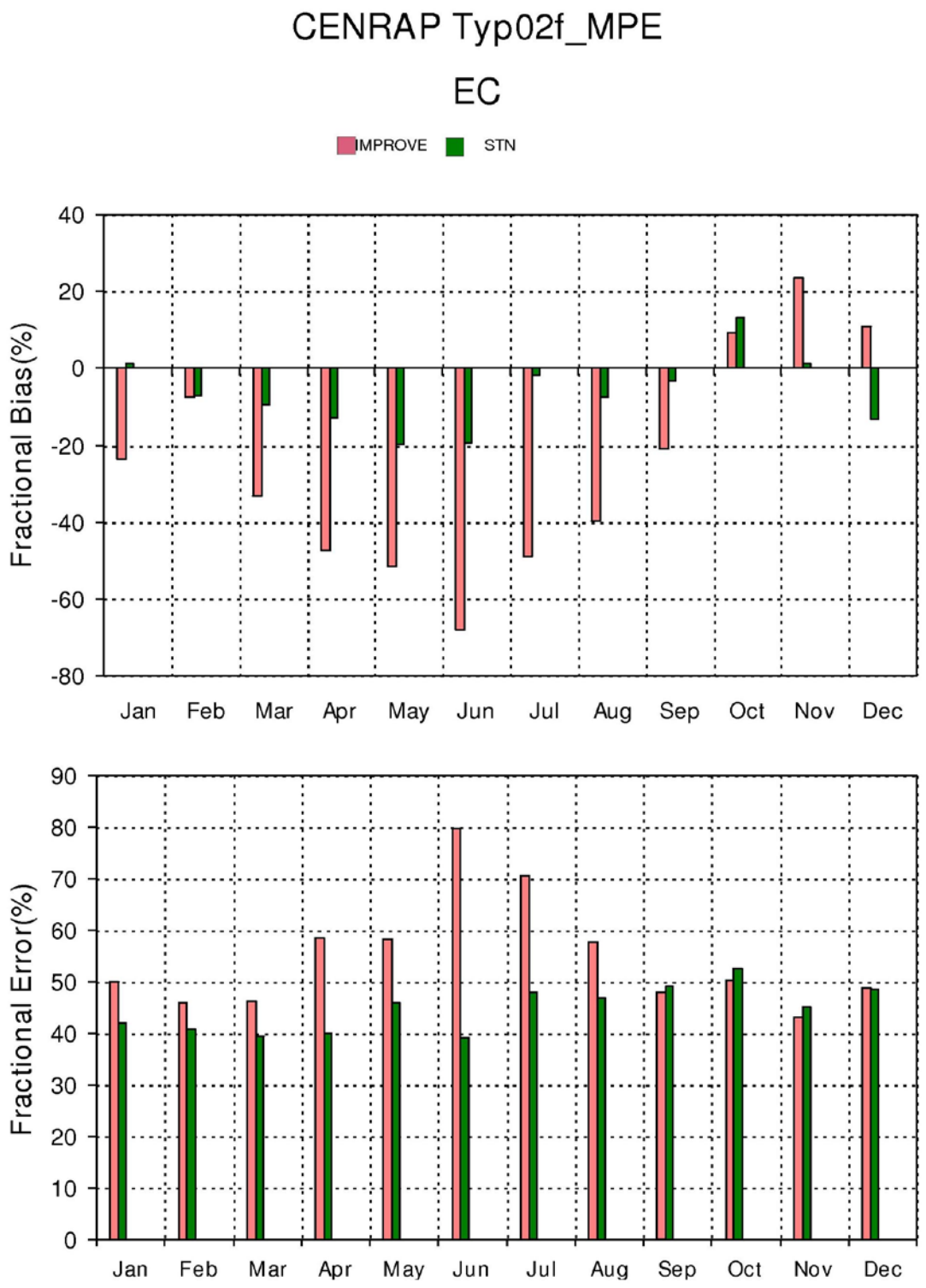


Figure C-26. Monthly EC fractional bias (top) and fractional gross error (bottom) statistical measures for IMPROVE and STN monitoring sites in the CENRAP region.

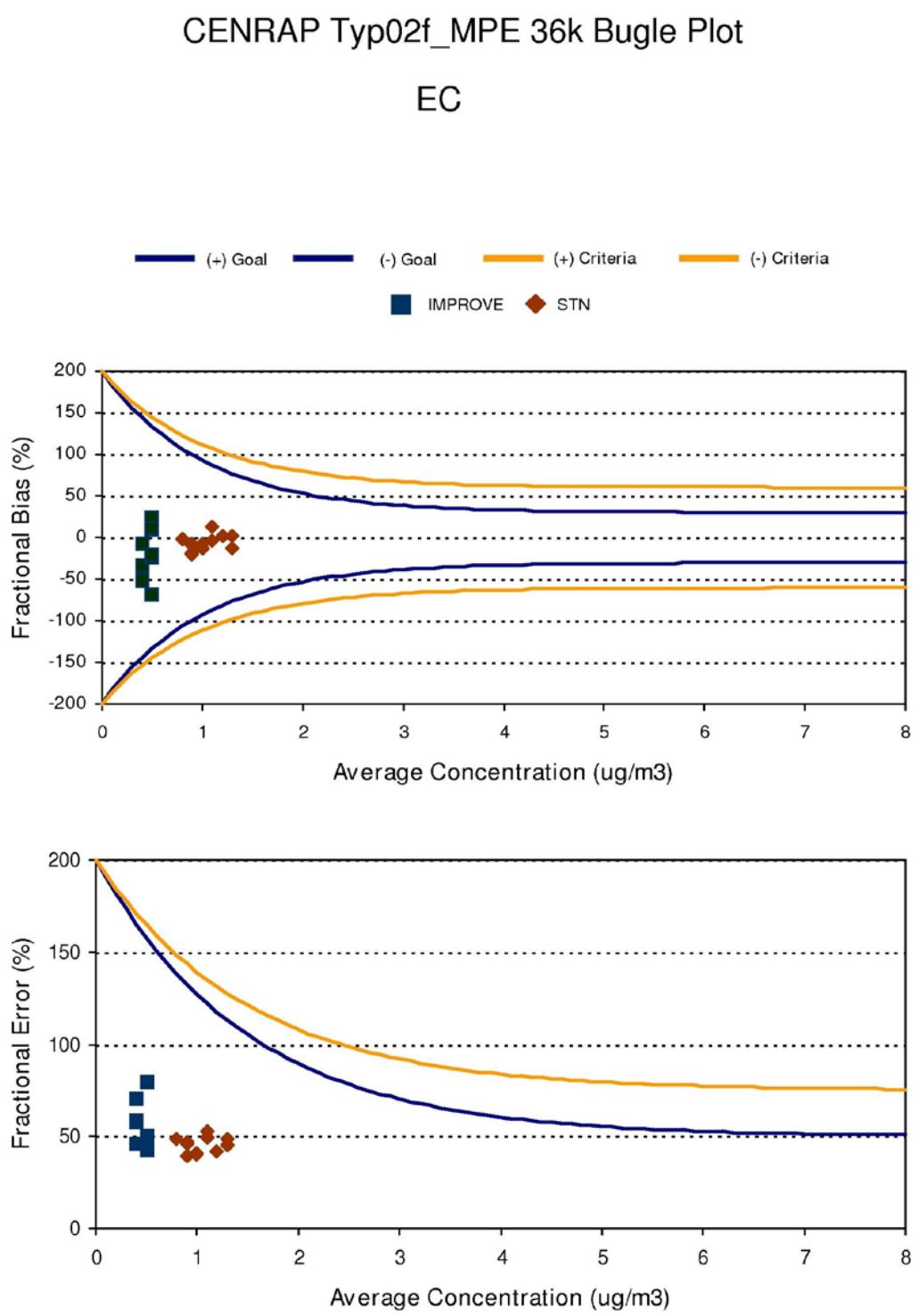


Figure C-27. Bugle Plots of monthly fractional bias (top) and fractional gross error (bottom) and comparisons with model performance goals and criteria for EC and IMPROVE and STN monitoring sites in the CENRAP region.

C.3.5 Other $PM_{2.5}$ (Soil) Monthly Model Performance

There are also model-measurement incommensurability problems with the other $PM_{2.5}$ (Soil) species. Whereas the IMPROVE Soil species is built up from measure elements, the modeled other $PM_{2.5}$ concentrations are based on emissions speciation profiles that likely include other species besides just elements. Soil is only collected at the IMPROVE monitors.

C.3.5.1 Soil in January 2002

The model greatly overestimates the Soil species at IMPORVE sites in January (Figure C-28a). The fractional bias exceeds 100% with errors of almost 130%. With the possible exception of the two Texas sites, the model Soil overestimation bias occurs across all of the CENRAP Class I areas in January (Figure C-28b). The model also does a poor job in reproducing the spatial variability of the observed Soil with a general overestimation tendency except at GUMO where it fails to reproduce the high Soil events.

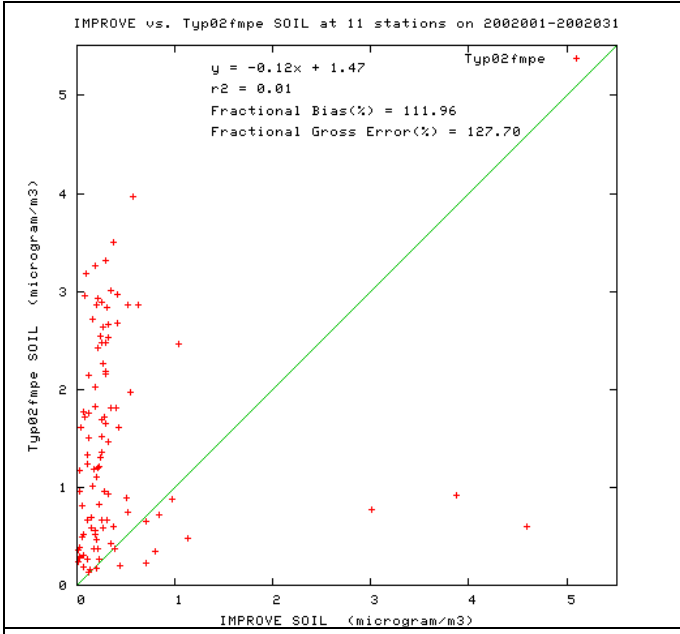
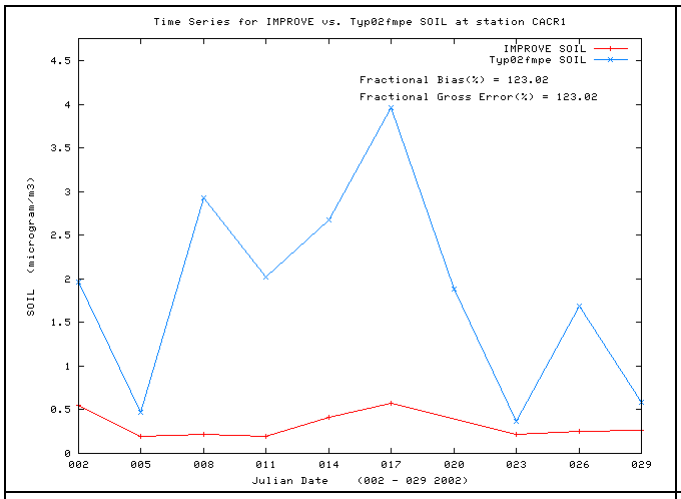
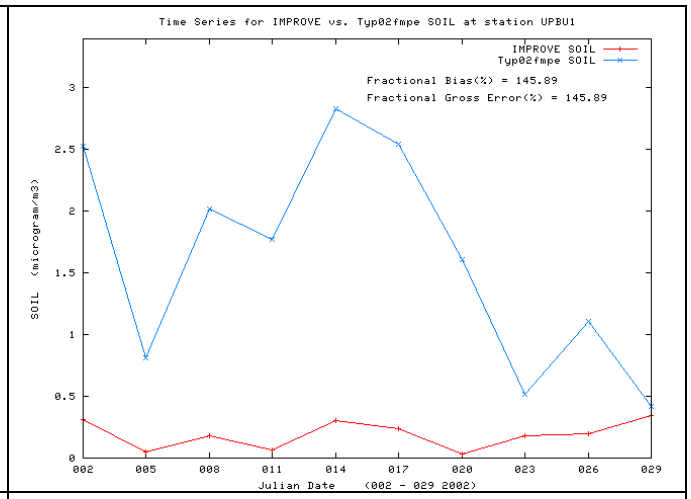
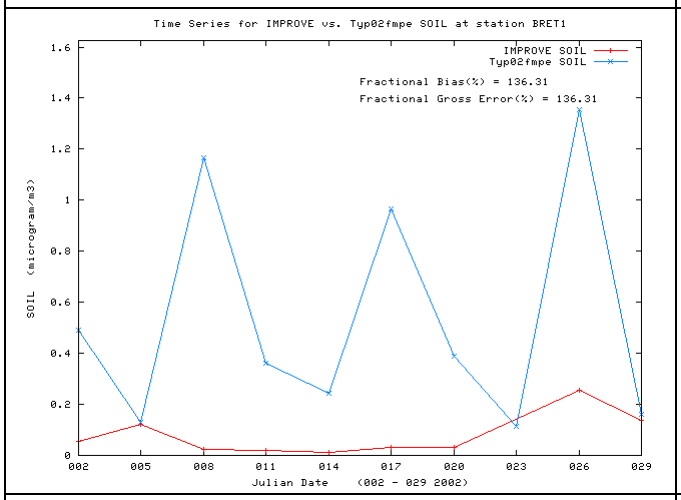
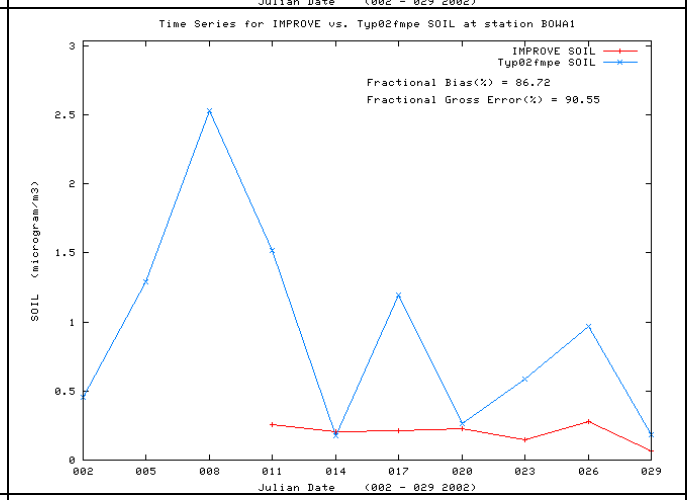


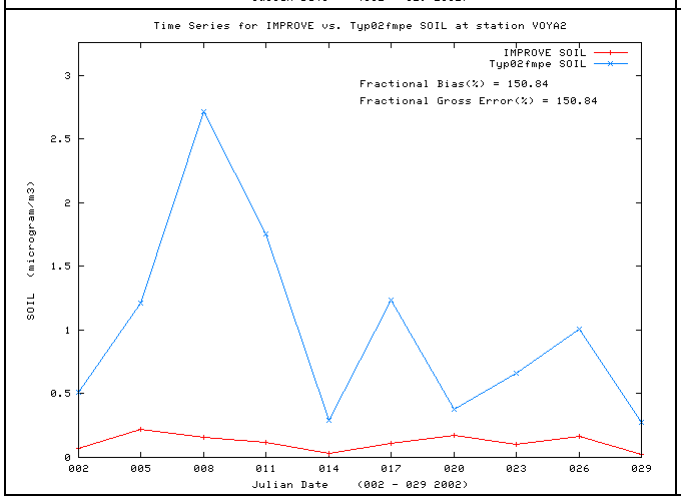
Figure C-28a. Scatter plots of predicted and observed other $PM_{2.5}$ (Soil) concentrations for January 2002 and sites in the CENRAP region using IMPROVE monitoring network and the CMAQ 2002 36 km Base F base case simulation.

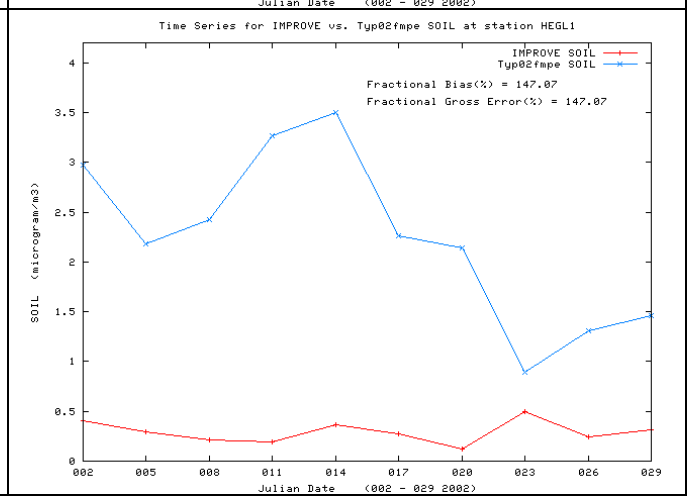

Time Series for IMPROVE vs. Typ02fmpe SOIL at station CACR1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 123.02
Fractional Gross Error(%) = 123.02
SOIL (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station UPBU1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 145.89
Fractional Gross Error(%) = 145.89
SOIL (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station BRET1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 136.31
Fractional Gross Error(%) = 136.31
SOIL (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station BOWA1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 86.72
Fractional Gross Error(%) = 90.55
SOIL (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station VOYA2
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 150.84
Fractional Gross Error(%) = 150.84
SOIL (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station HEGL1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 147.07
Fractional Gross Error(%) = 147.07
SOIL (microgram/m3)
Julian Date (002 - 029 2002)

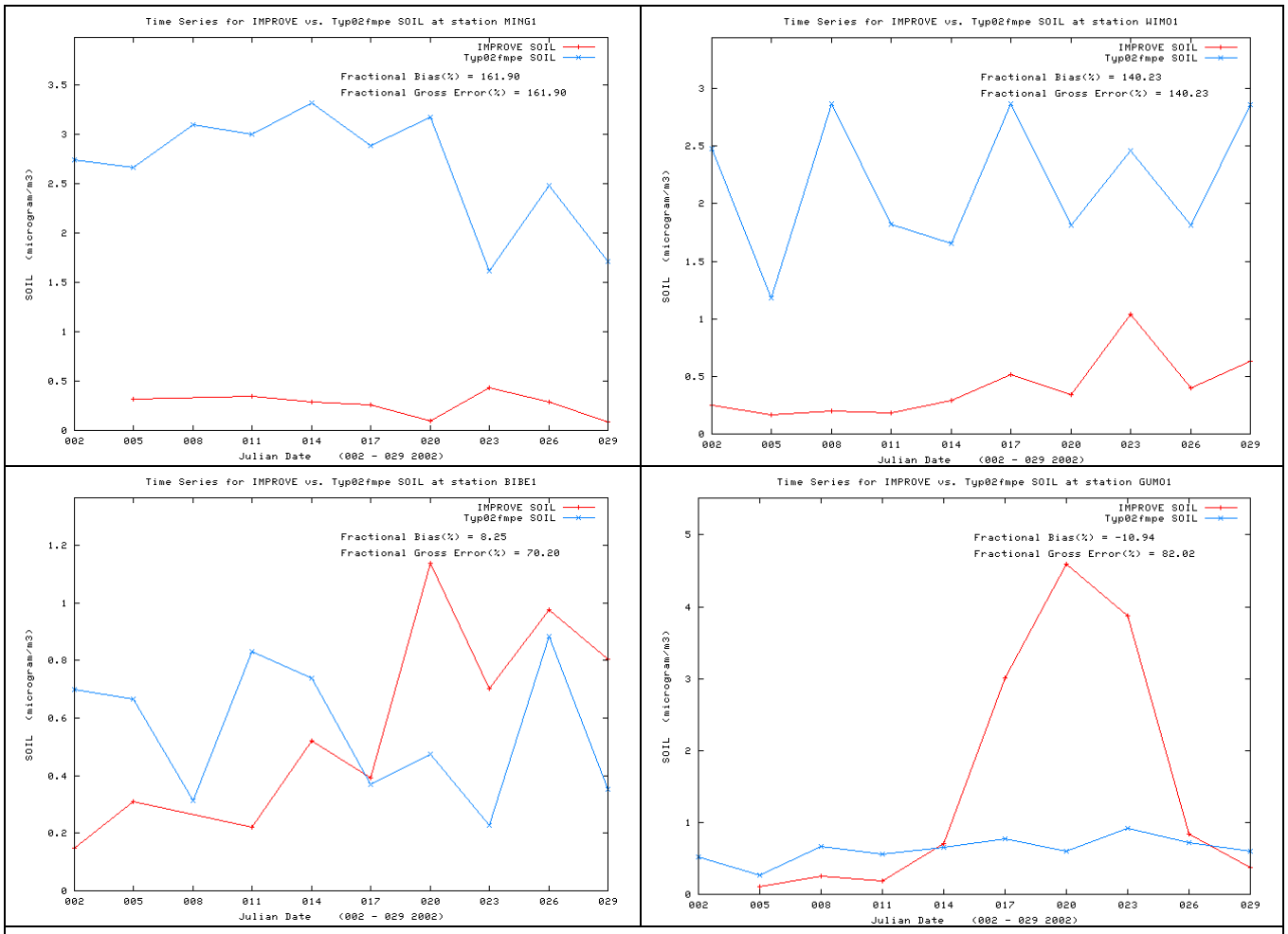


Figure C-28b. Time series of predicted and observed 24-hour other $PM_{2.5}$ (Soil) concentrations at CENRAP IMPROVE CLASS I AREA sites in January 2002 for CMAQ 2002 36 km Base F base case simulation.

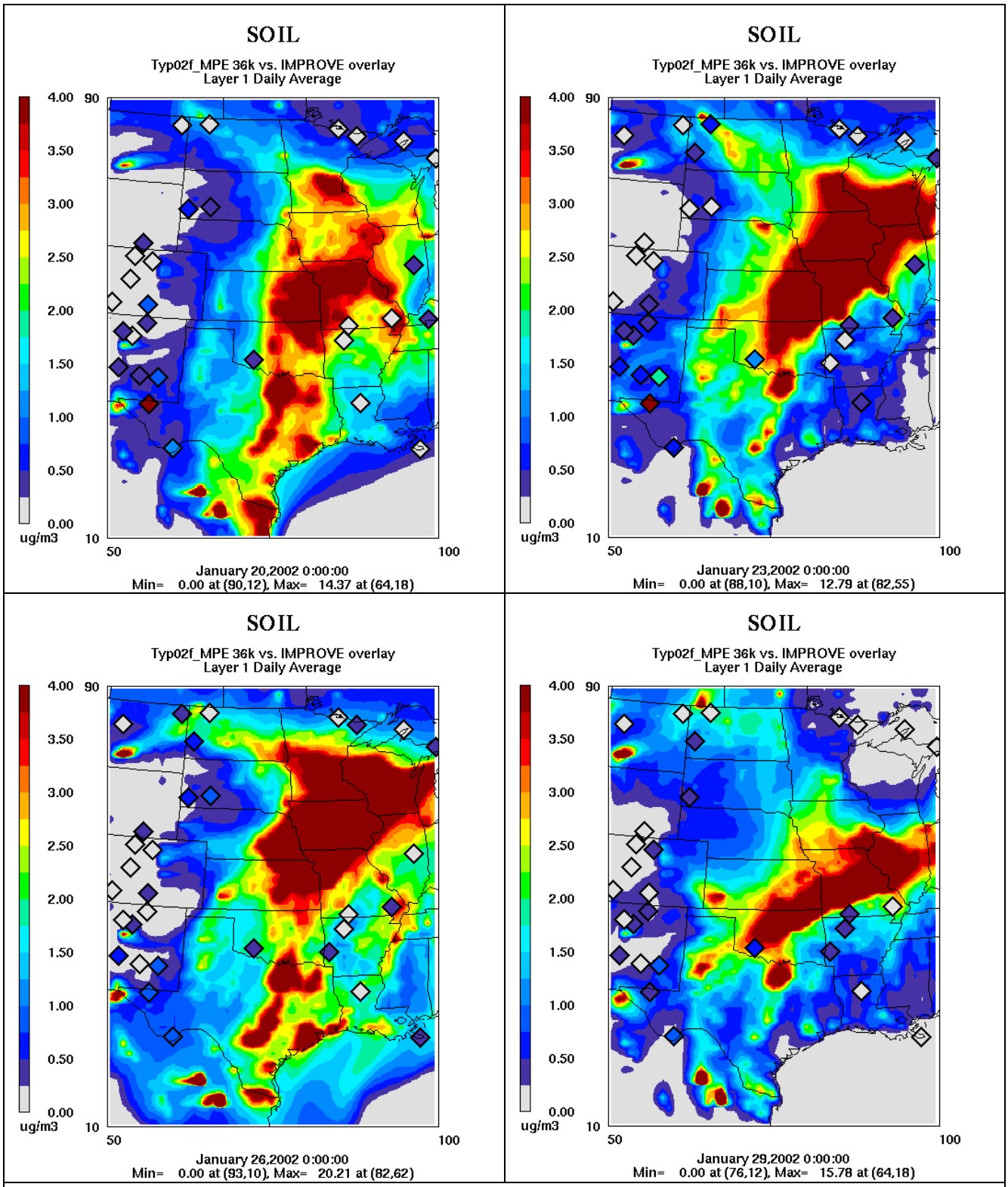


Figure C-28c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour Soil concentrations for January 20, 23, 26 and 29, 2002.

C.3.5.2 Soil in April 2002

The model does a better job in reproducing the overall magnitude of the Soil measurements in April with a bias of 13% (Figure C-29a). But it exhibits little skill with lots of scatter and an error of 81%. The model is generally exhibiting a lot more day-to-day variability than observed with the observed daily time series much flatter than the modeled values (Figure C-29b). The modeled and observed spatial variability in Soil on April 5, 8, 11 and 14 are shown in Figure C-29c. Although the model exhibits large day-to-day variability, the observations do not reflect what the model predicts.

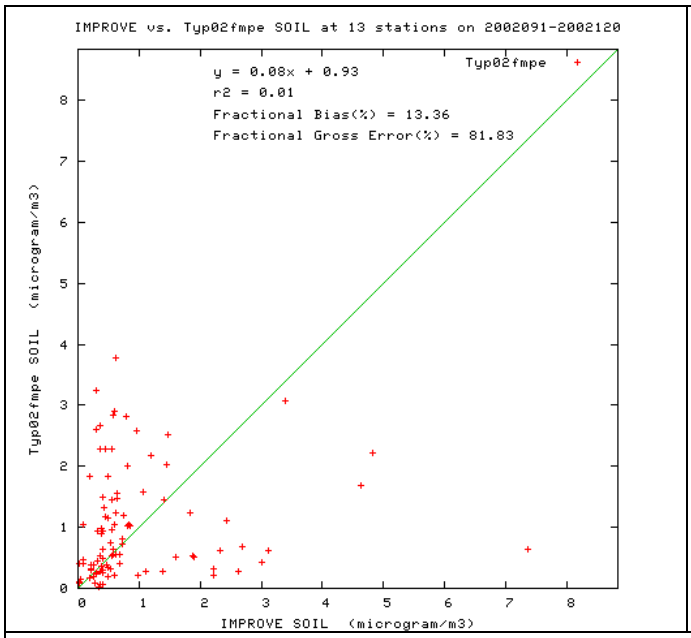
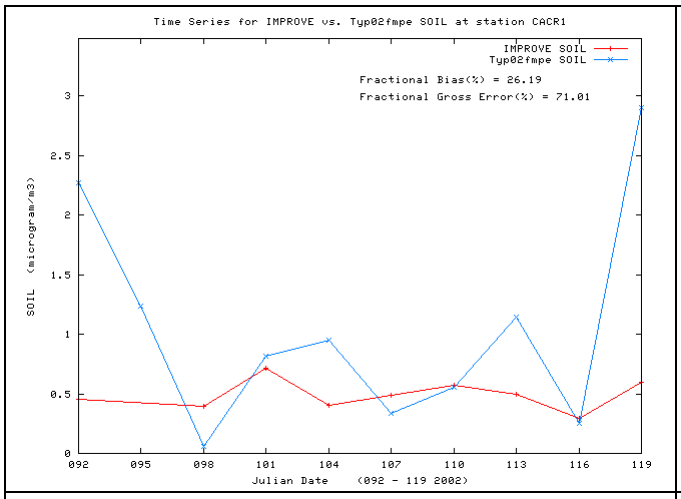
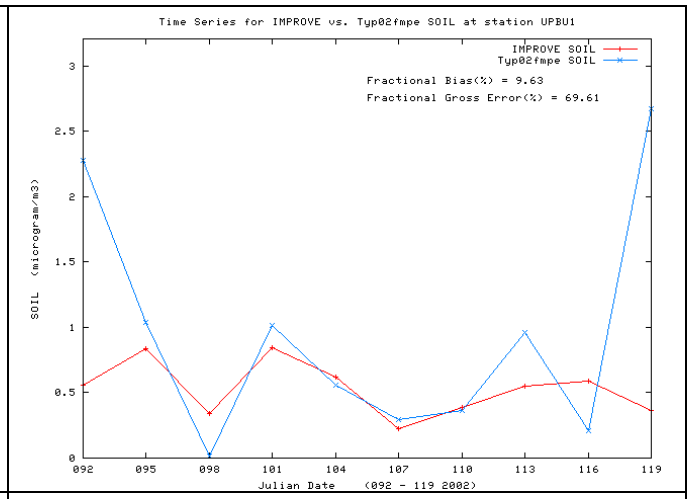
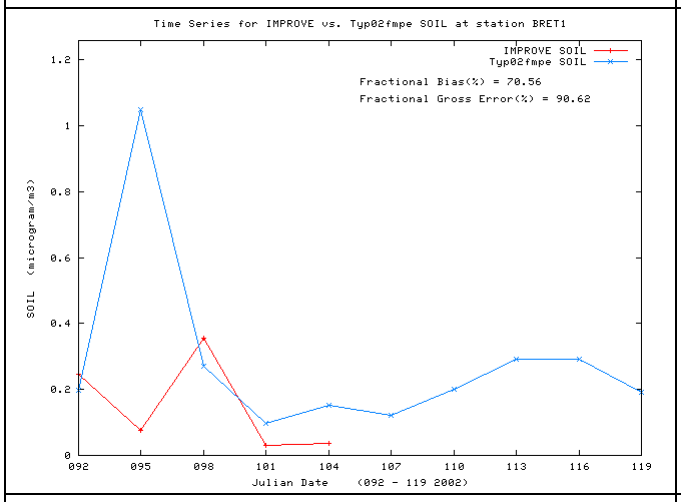
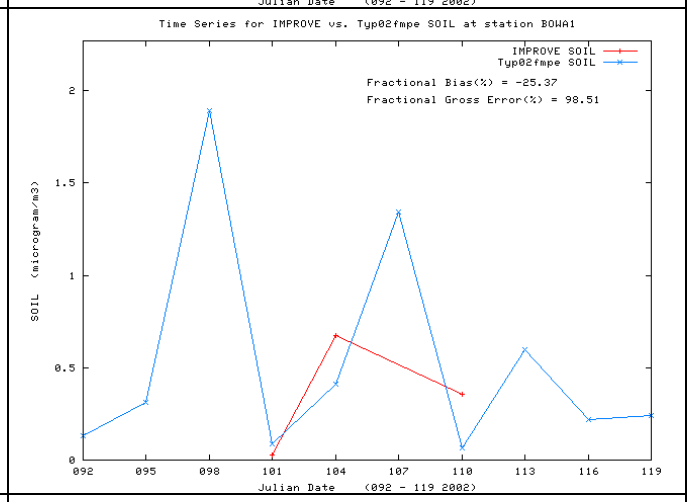


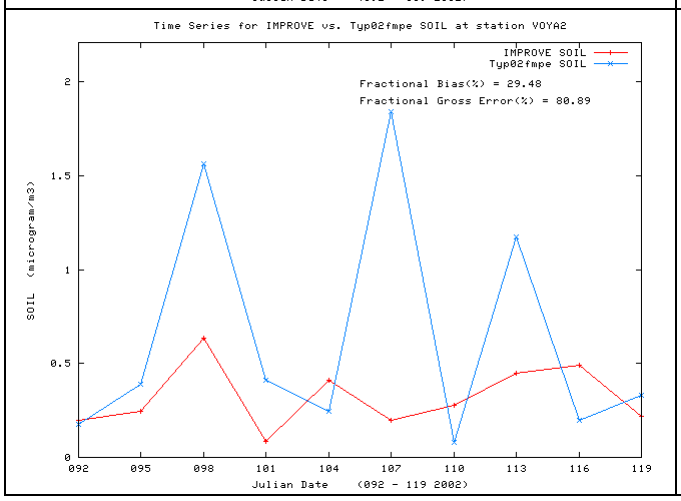
Figure C-29a. Scatter plots of predicted and observed other $PM_{2.5}$ (Soil) concentrations for April 2002 and sites in the CENRAP region using IMPROVE monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

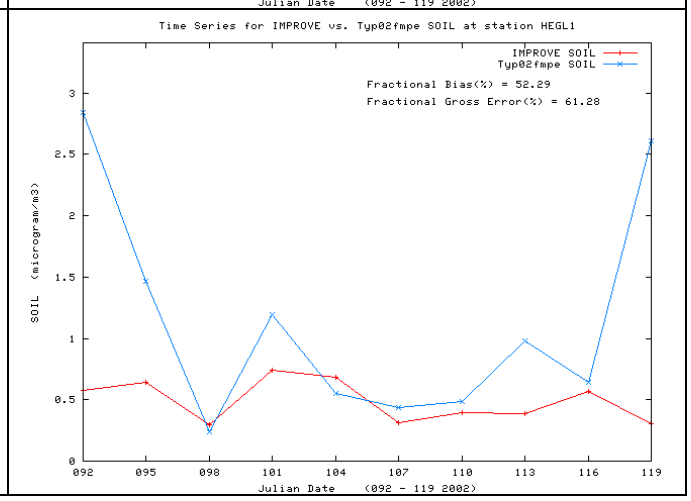

Time Series for IMPROVE vs. Typ02fmpe SOIL at station CACR1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 26.19
Fractional Gross Error(%) = 71.01
SOIL (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station UPBU1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 9.63
Fractional Gross Error(%) = 69.61
SOIL (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station BRET1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 70.56
Fractional Gross Error(%) = 90.62
SOIL (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station BOWA1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = -25.37
Fractional Gross Error(%) = 98.51
SOIL (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station VOYA2
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 29.48
Fractional Gross Error(%) = 80.89
SOIL (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station HEGL1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 52.29
Fractional Gross Error(%) = 61.28
SOIL (microgram/m3)
Julian Date (092 - 119 2002)

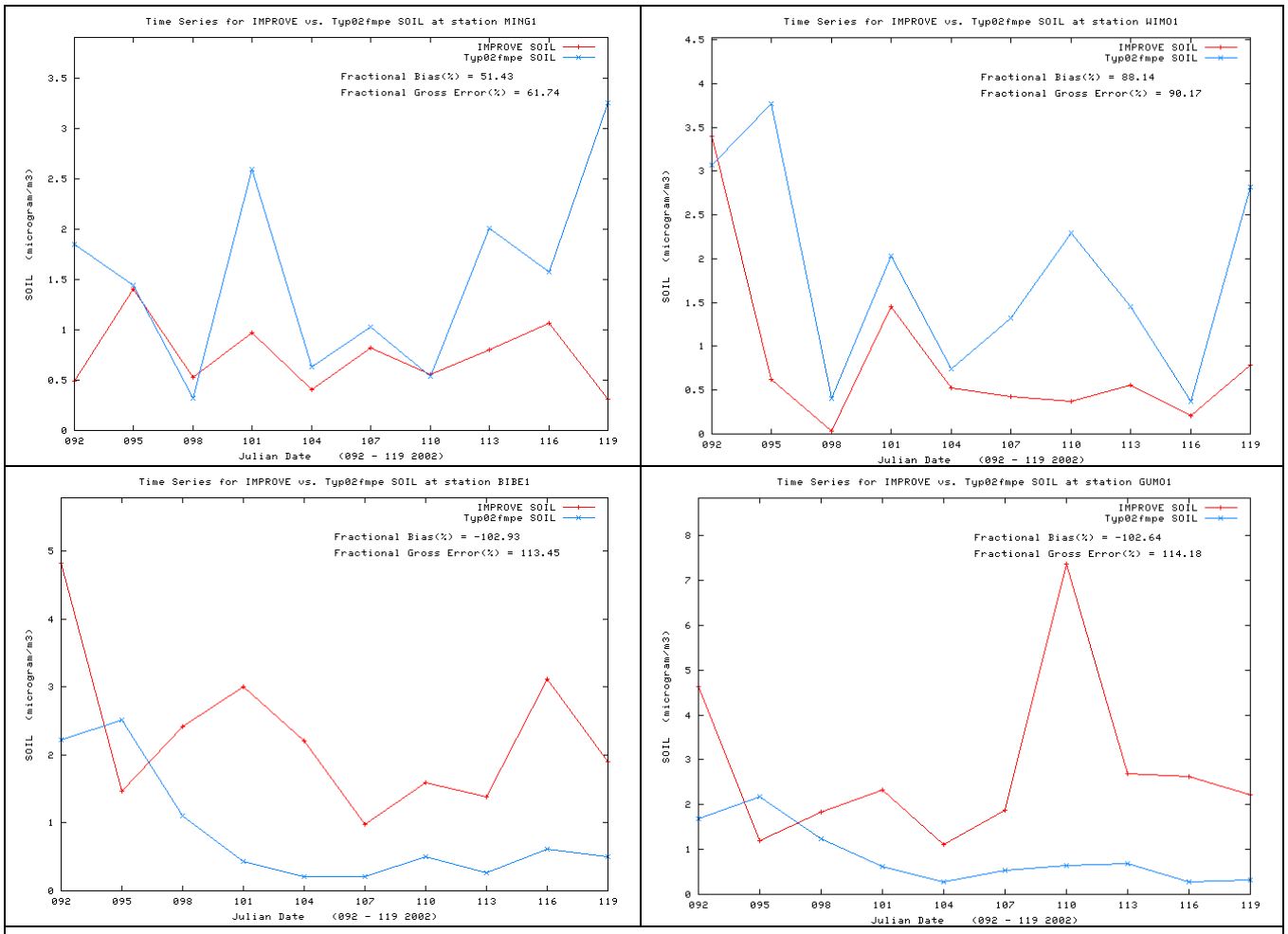


Figure C-29b. Time series of predicted and observed 24-hour other $PM_{2.5}$ (Soil) concentrations at CENRAP IMPROVE CLASS I AREA sites in April 2002 for CMAQ 2002 36 km Base F base case simulation.

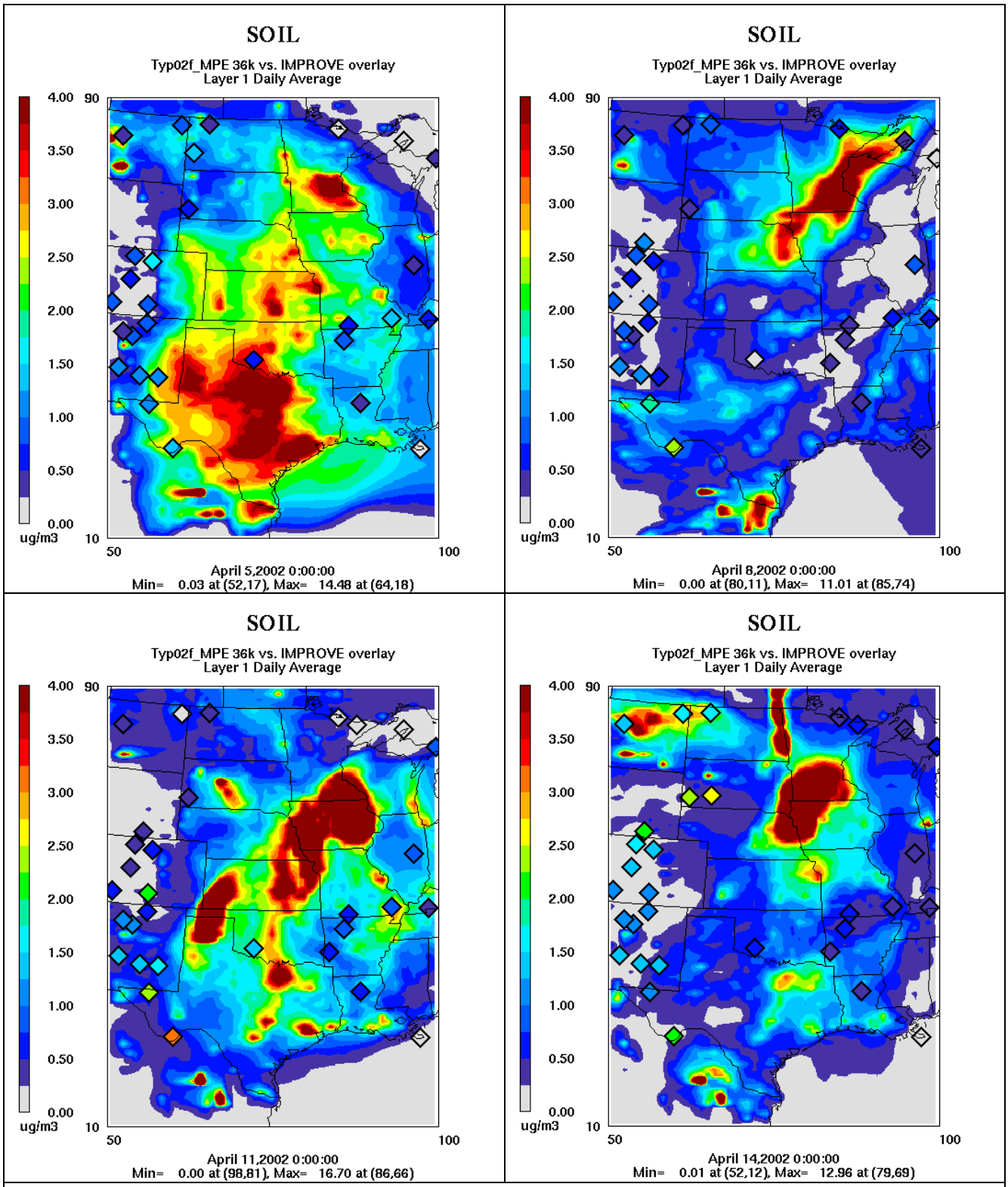


Figure C-29c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour Soil concentrations for April 5, 8, 11 and 14, 2002.

C.3.5.3 Soil in July 2002

The -50% Soil under-prediction bias seen in July appears to be driven to several high Soil measurements (Figure C-30a). An observed high Soil event took place on July 1 (Julian Day 182) across the Arkansas and Missouri Class I areas that all observed Soil values in excess of 15 μg/m^3. This event was not captured by the model. With the exception of a systematic Soil underestimation bias at the two Texas sites and missing these high Soil events, the model generally reproduces the magnitudes of the Soil observations in July.

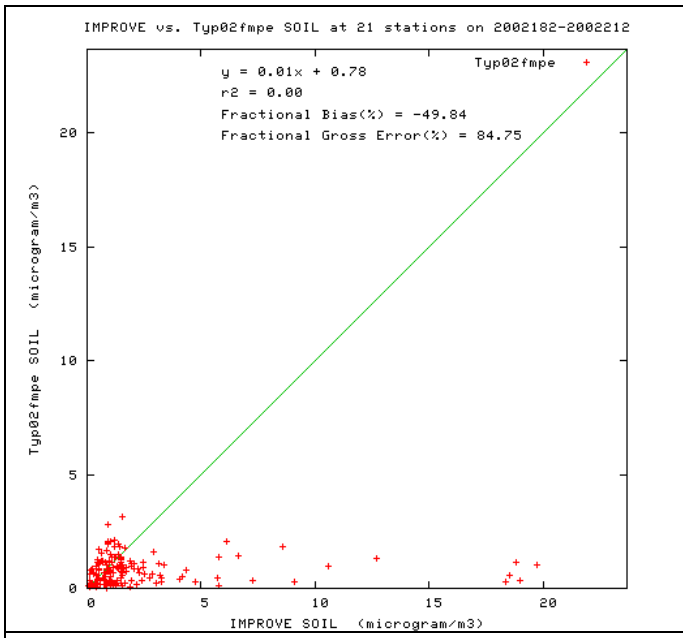
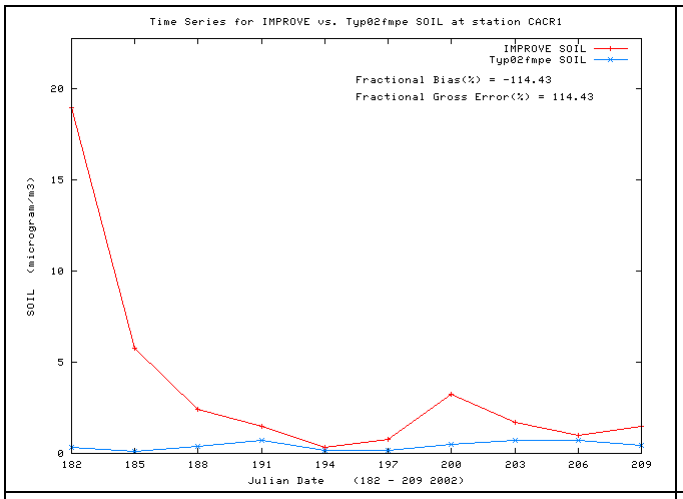
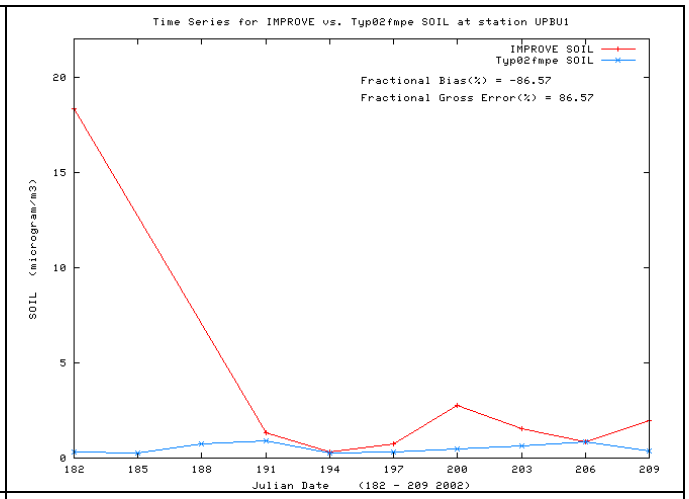
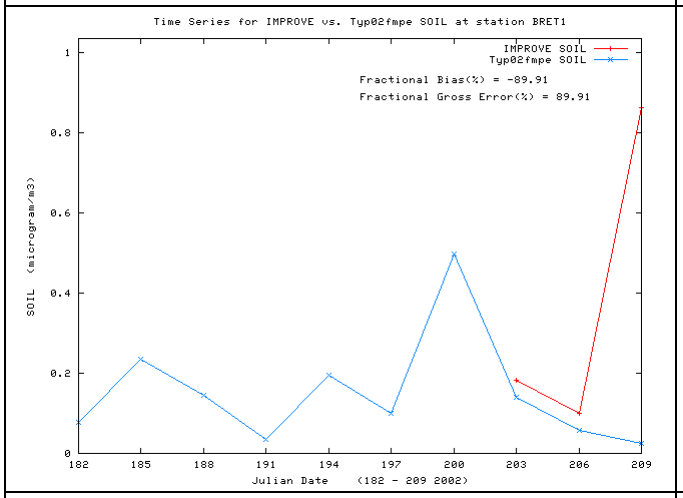
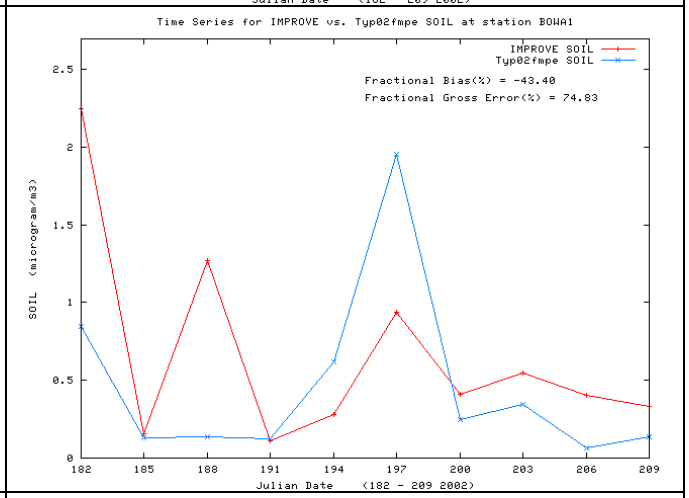


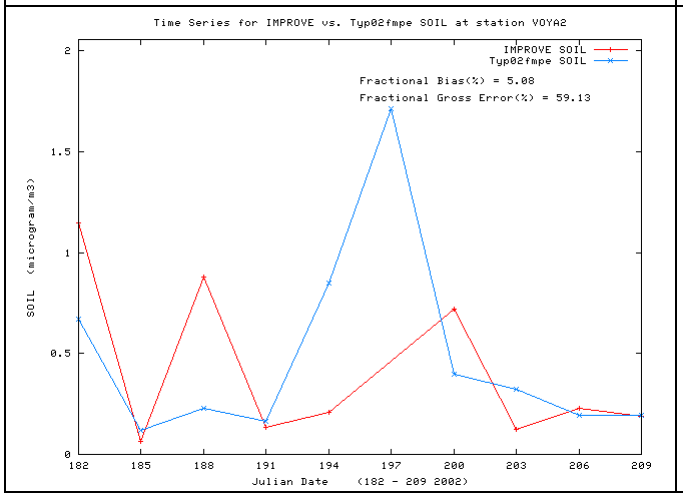
Figure C-30a. Scatter plots of predicted and observed other $PM_{2.5}$ (Soil) concentrations for July 2002 and sites in the CENRAP region using IMPROVE monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

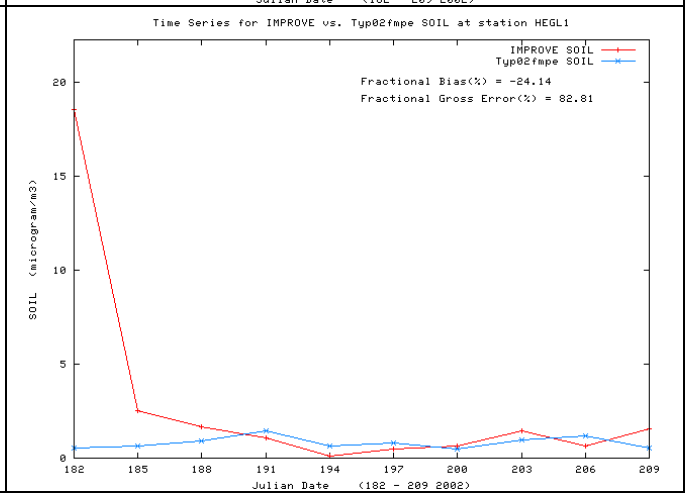

Time Series for IMPROVE vs. Typ02fmpe SOIL at station CACR1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = -114.43
Fractional Gross Error(%) = 114.43
SOIL (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station UPBU1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = -86.57
Fractional Gross Error(%) = 86.57
SOIL (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station BRET1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = -89.91
Fractional Gross Error(%) = 89.91
SOIL (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station BOWA1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = -43.40
Fractional Gross Error(%) = 74.83
SOIL (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station VOYA2
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 5.08
Fractional Gross Error(%) = 59.13
SOIL (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station HEGL1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = -24.14
Fractional Gross Error(%) = 82.81
SOIL (microgram/m3)
Julian Date (182 - 209 2002)

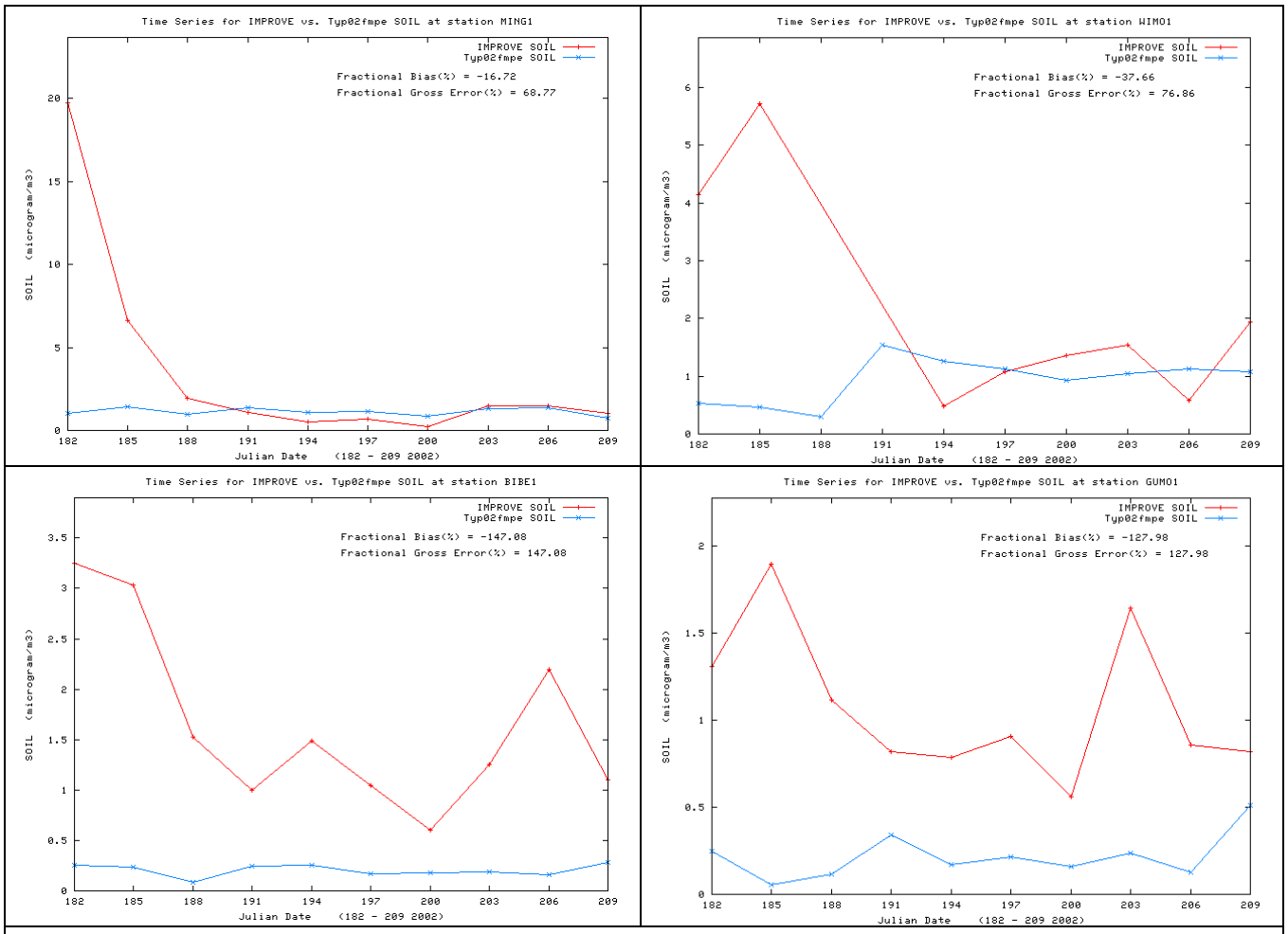


Figure C-30b. Time series of predicted and observed 24-hour other $PM_{2.5}$ (Soil) concentrations at CENRAP IMPROVE sites in July 2002 for CMAQ 2002 36 km Base F base case simulation.

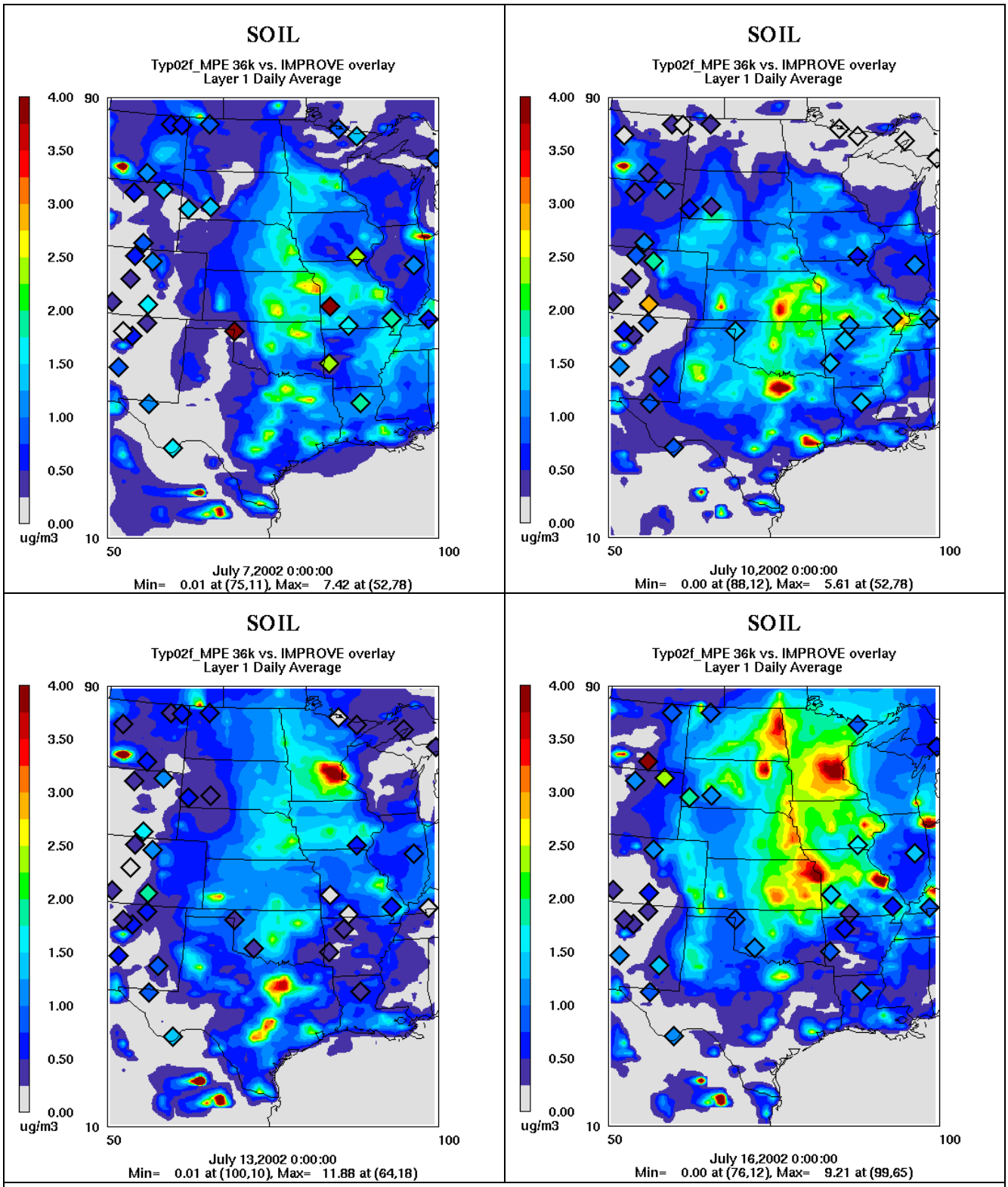


Figure C-30c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour Soil concentrations for July 7, 10, 13 and 16, 2002.

C.3.5.4 Soil in October 2002

The nearly systematic Soil over-prediction bias seen in January returns in October (Figure C-31a). Except for the two Texas sites, BRET and BOWA, the model overstates the observed Soil during all days of October at the other monitoring sites (Figure C-31b). The model is predicting elevated Soil concentrations in the OK-KS-MO-IA area that is not reflected in the measurements (Figure C-31c).

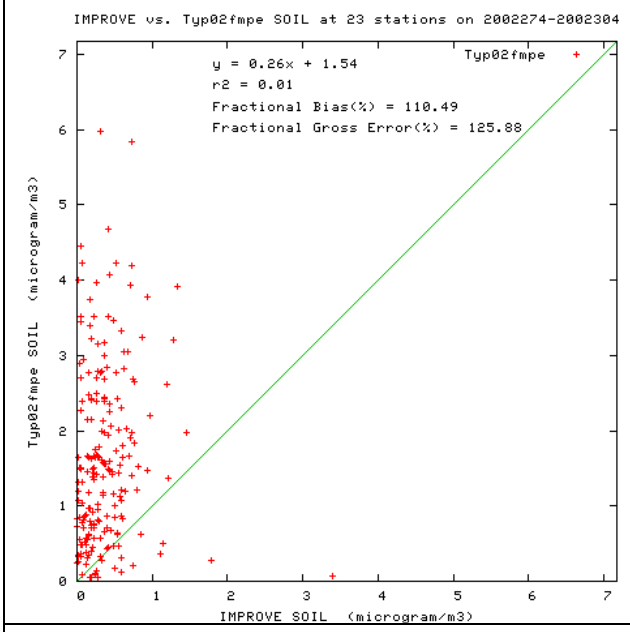
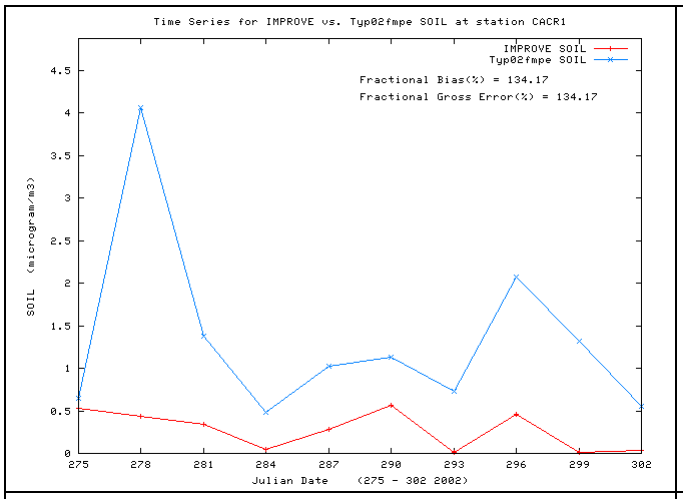
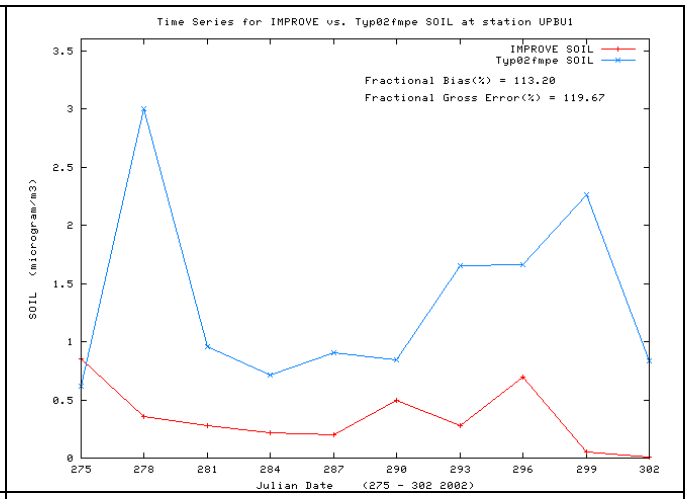
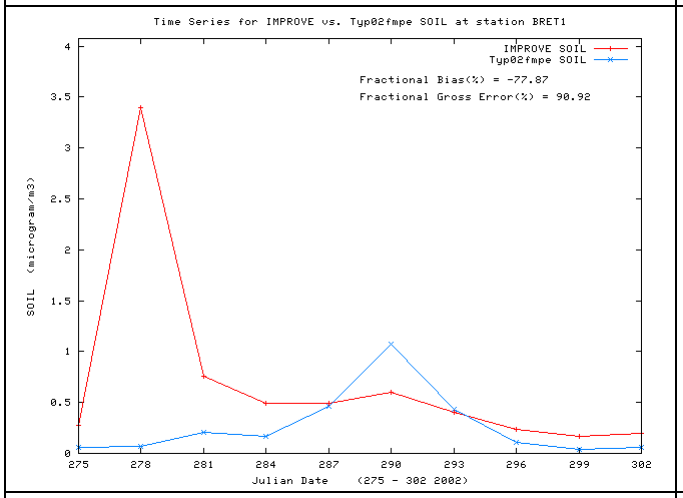
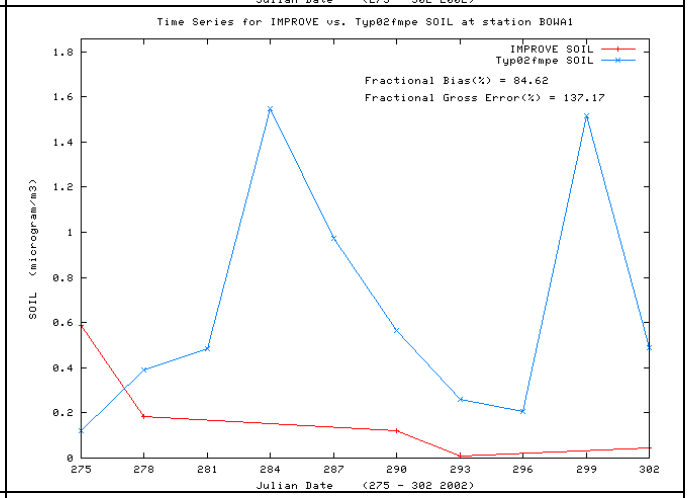


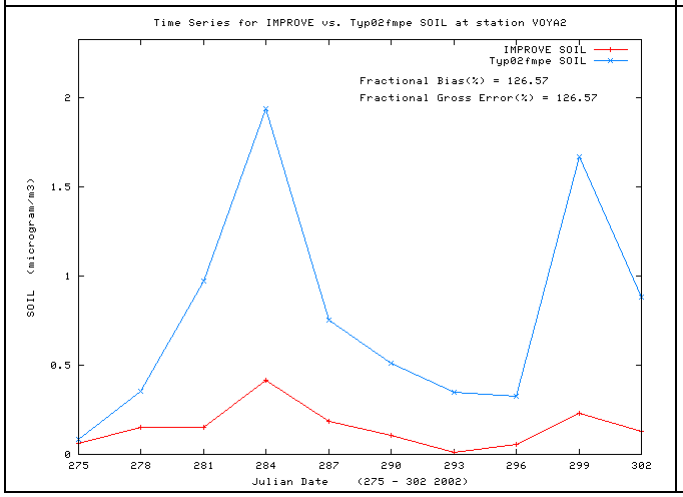
Figure C-31a. Scatter plots of predicted and observed other $PM_{2.5}$ (Soil) concentrations for October 2002 and sites in the CENRAP region using IMPROVE monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

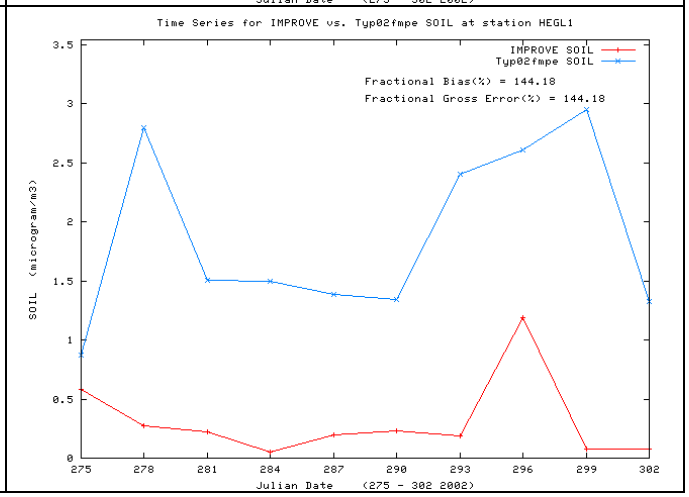

Time Series for IMPROVE vs. Typ02fmpe SOIL at station CACR1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 134.17
Fractional Gross Error(%) = 134.17
SOIL (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station UPBU1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 113.20
Fractional Gross Error(%) = 119.67
SOIL (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station BRET1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = -77.87
Fractional Gross Error(%) = 90.92
SOIL (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station BOWA1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 84.62
Fractional Gross Error(%) = 137.17
SOIL (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station VOYA2
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 126.57
Fractional Gross Error(%) = 126.57
SOIL (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe SOIL at station HEGL1
IMPROVE SOIL
Typ02fmpe SOIL
Fractional Bias(%) = 144.18
Fractional Gross Error(%) = 144.18
SOIL (microgram/m3)
Julian Date (275 - 302 2002)

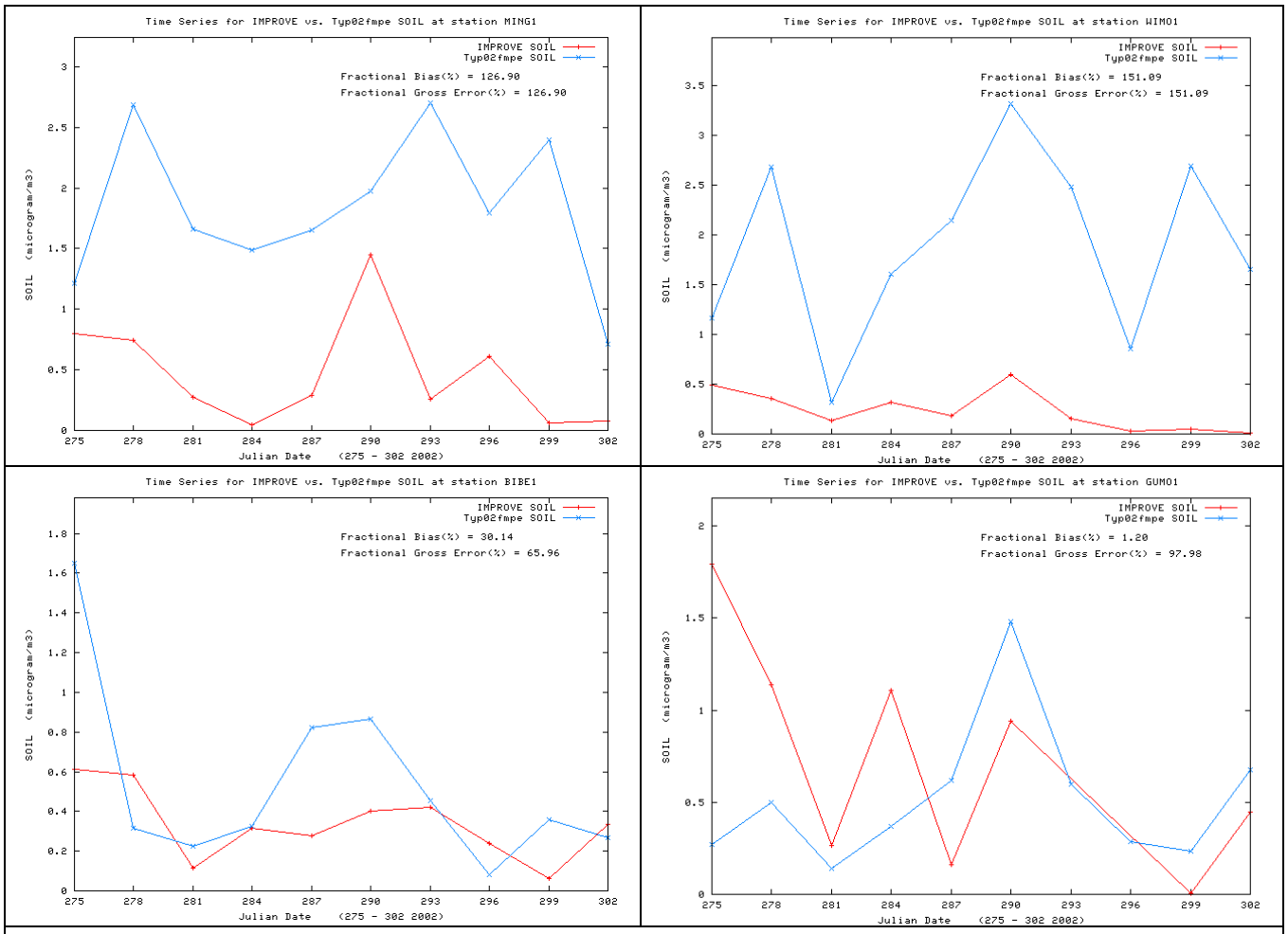


Figure C-31b. Time series of predicted and observed 24-hour other $PM_{2.5}$ (Soil) concentrations at CENRAP IMPROVE CLASS I AREA sites in October 2002 for CMAQ 2002 36 km Base F base case simulation.

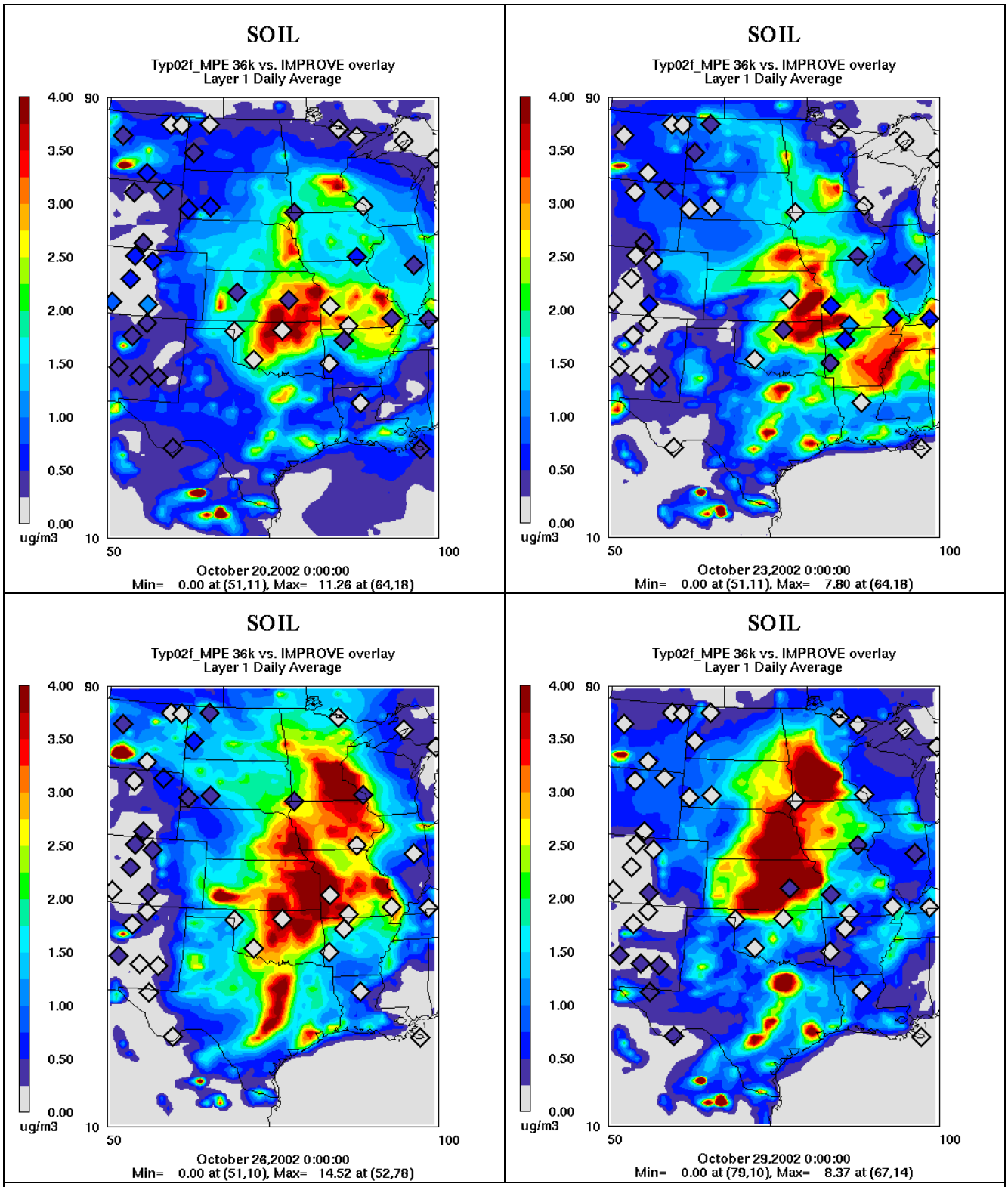


Figure C-31c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour Soil concentrations for October 20, 23, 26 and 29, 2002.

C.3.5.5 Soil Monthly Bias and Error

Figure C-32 displays the monthly variation in the Soil bias and error. During the winter months the model exhibits a very large (> 100%) overestimation bias with large errors as well. With the exception of July, in the summer the model bias is a slight over-prediction but generally less than 20% with errors of 60% to 80%. The Bugle Plot indicates that the summer Soil performance achieves the PM performance goal, a few months in the Spring/Fall period fall between the performance goal and criteria and the winter Soil performance exceeds the model performance criteria by a far margin. Thus, the Soil performance is a cause for concern.

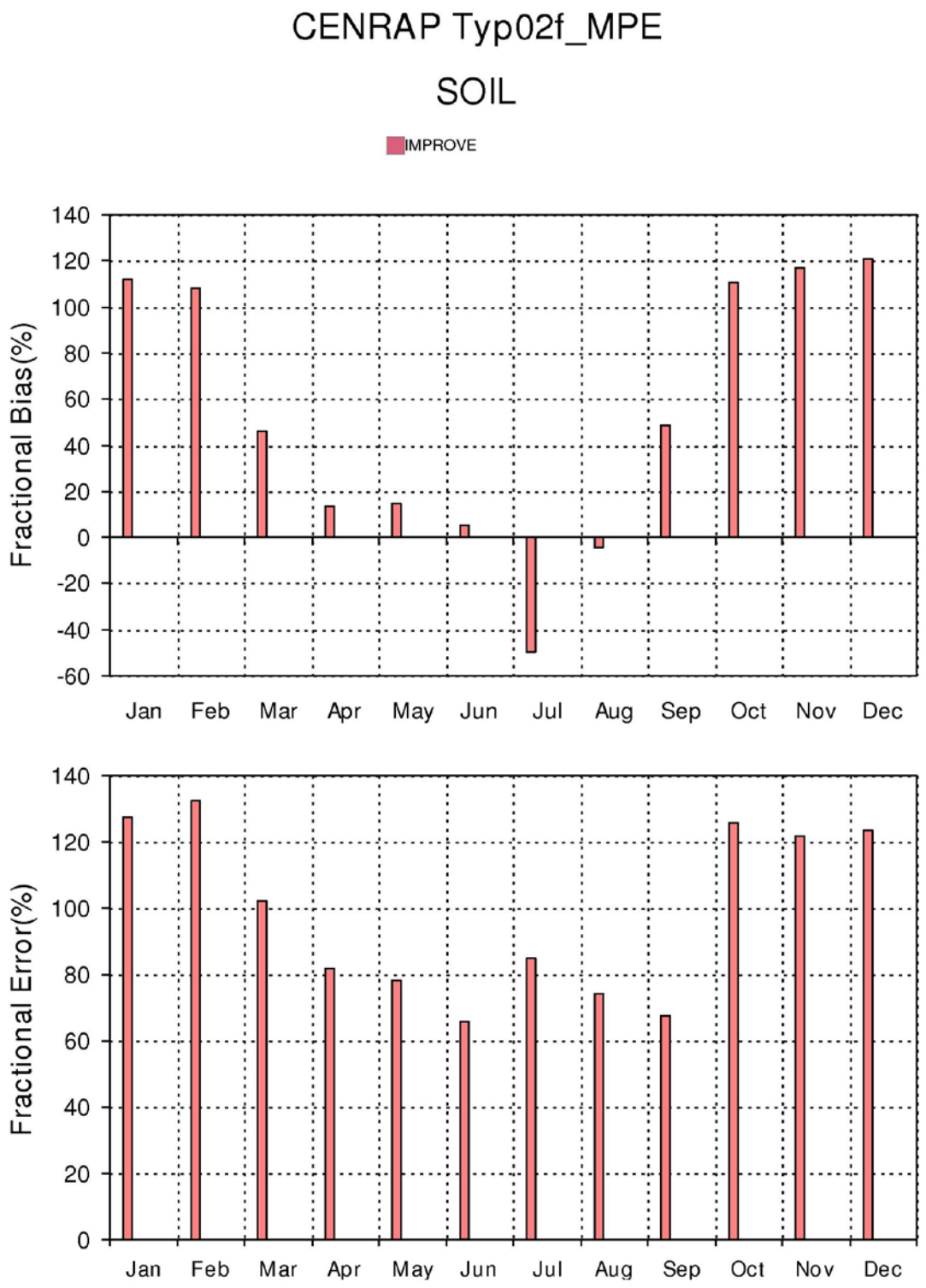


Figure C-32. Monthly Soil fractional bias (top) and fractional gross error (bottom) statistical measures for IMPROVE, STN and CASTNet monitoring sites in the CENRAP region.

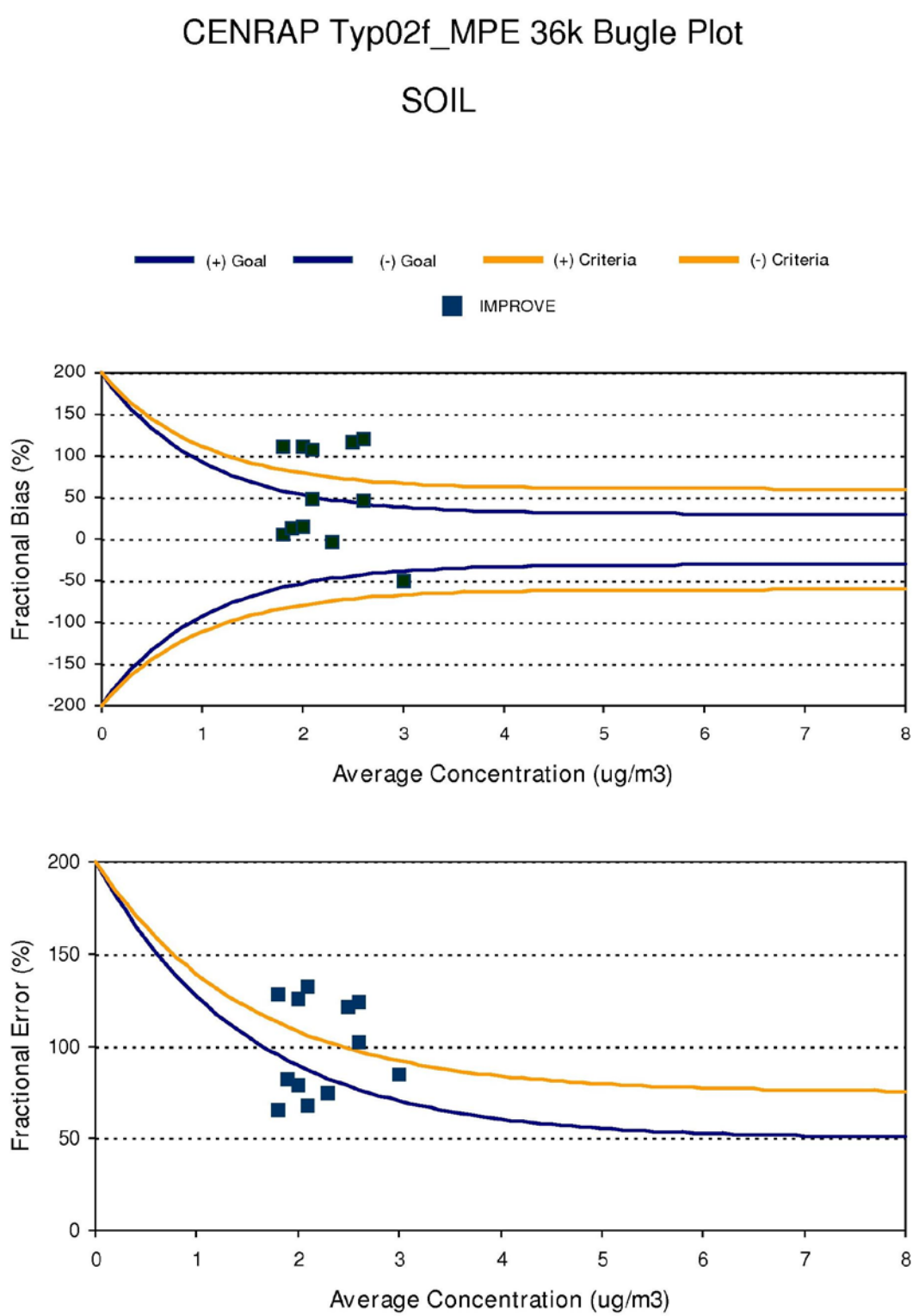


Figure C-33. Bugle Plots of monthly fractional bias (top) and fractional gross error (bottom) and comparisons with model performance goals and criteria for Soil and IMPROVE monitoring sites in the CENRAP region.

C.3.6 Coarse Mass (CM) Monthly Model Performance

The IMPROVE coarse mass (CM) measurement is taken as the difference between the PM_{10} and $PM_{2.5}$ mass measurement. Any SO4 or NO3 in the coarse mode will be in the CM measurement. The model, on the other hand, only includes primary CM. Any coarse SO4 or NO3 will be in the SO4 and NO3 modeled species.

C.3.6.1 CM in January 2002

The model underestimates the observed CM in January with a fractional bias of -83% (Figure C-34a). Although the model appears to reproduce CM at some sites (e.g., VOYA) at the two Texas sites the bias is approximately -150% (Figure C-34b). The observed spatial distribution of CM in January is not reproduced by the model at all (Figure C-34c). Whereas the observations indicate high CM concentrations in the west Texas-New Mexico area, the model estimates elevated CM in northeast Texas, through Oklahoma, Kansas, Iowa and into southern Minnesota. Although the CM measurements at WIMO in this area are also elevated, the rest of the high modeled CM values fall in between the IMPROVE monitors so can not be verified or refuted by the measurements.

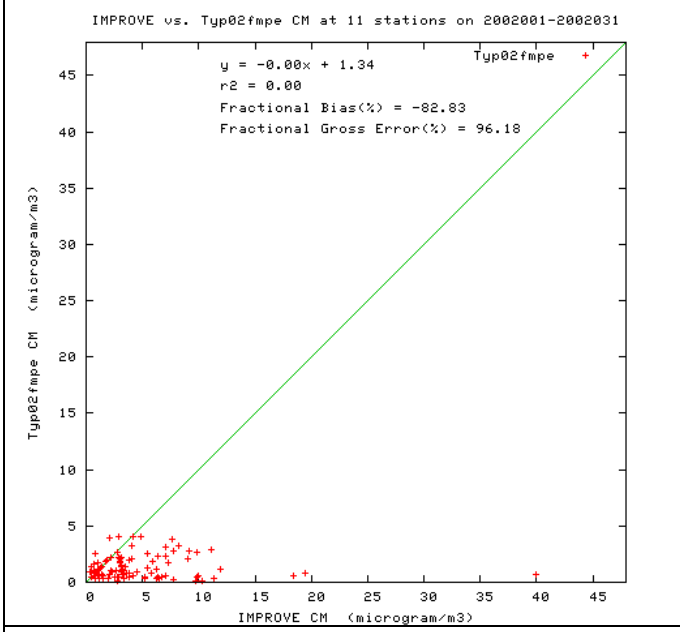
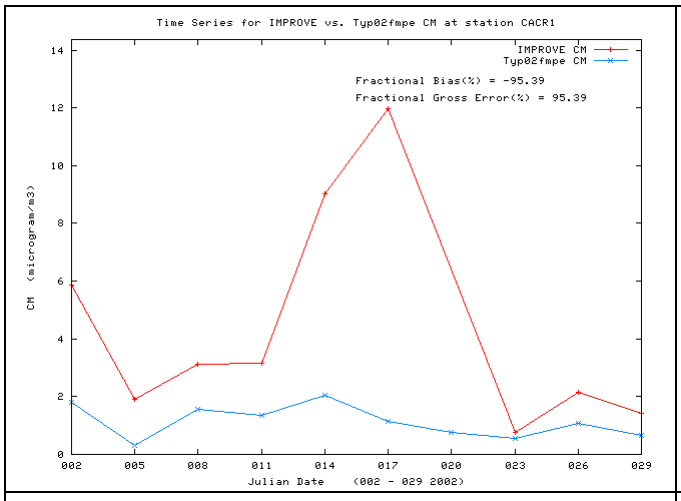
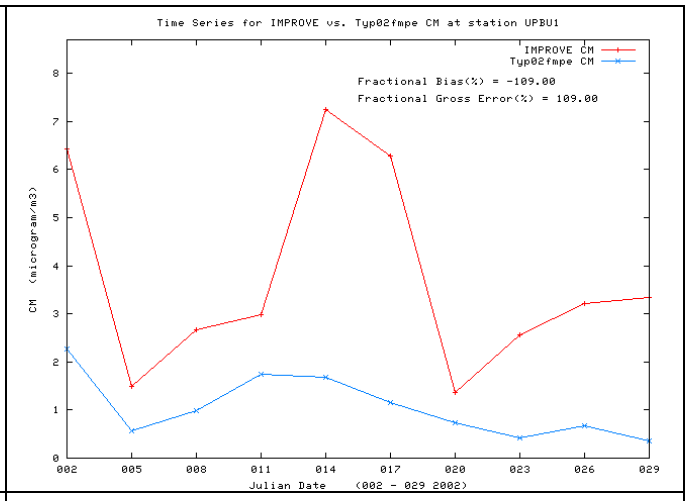
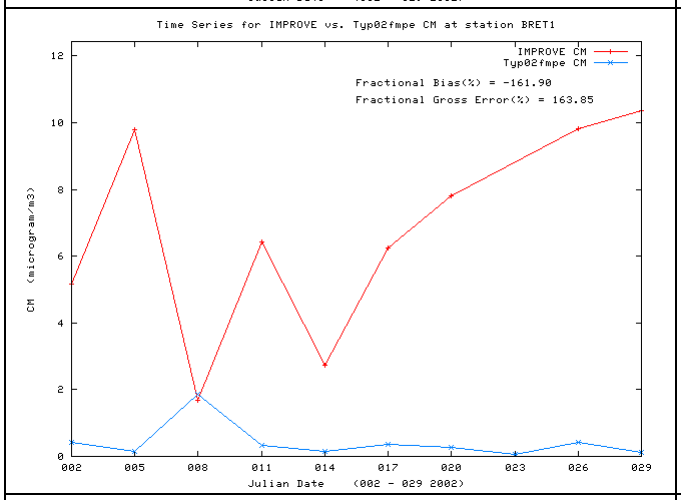
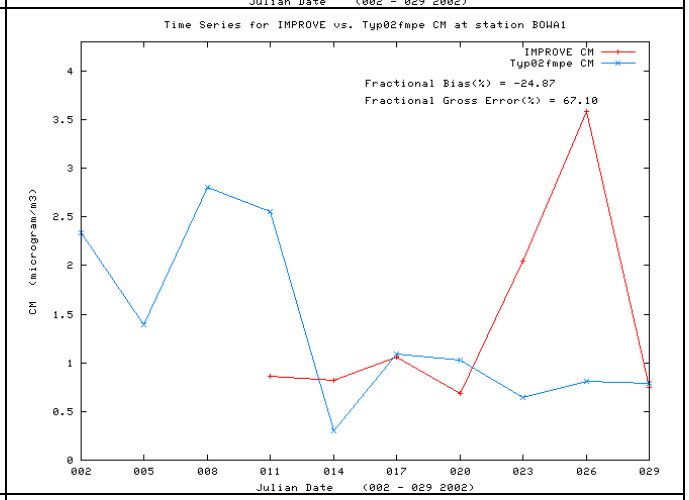


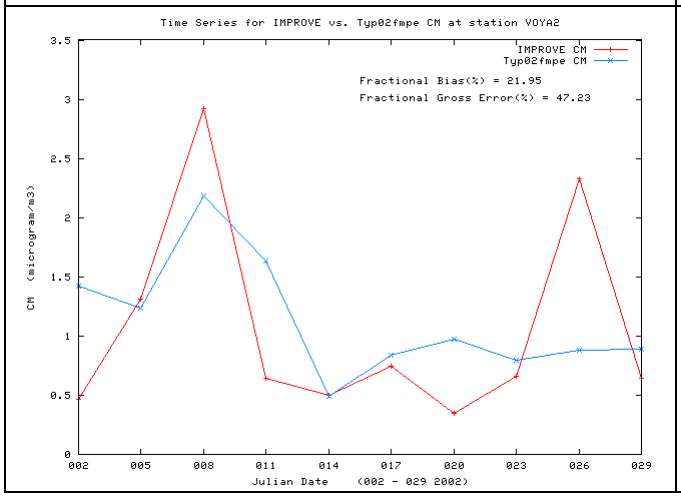
Figure C-34a. Scatter plots of predicted and observed coarse mass (CM) concentrations for January 2002 and sites in the CENRAP region using IMPROVE monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

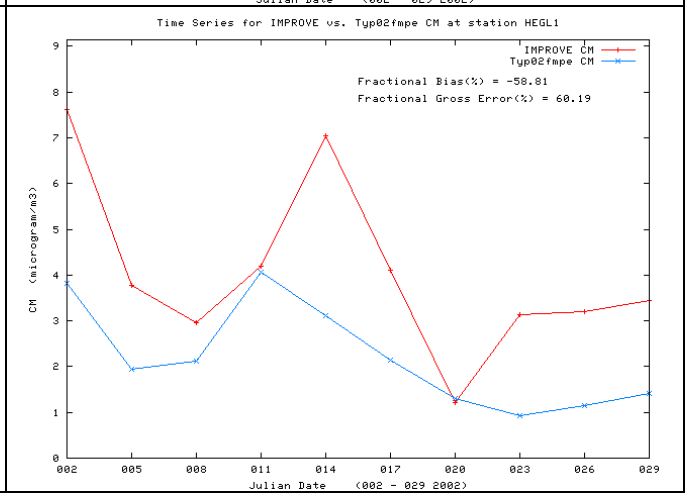

Time Series for IMPROVE vs. Typ02fmpe CM at station CACR1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -95.39
Fractional Gross Error(%) = 95.39
CM (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station UPBU1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -109.00
Fractional Gross Error(%) = 109.00
CM (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station BRET1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -161.90
Fractional Gross Error(%) = 163.85
CM (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station BOWA1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -24.87
Fractional Gross Error(%) = 67.10
CM (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station VOYA2
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = 21.95
Fractional Gross Error(%) = 47.23
CM (microgram/m3)
Julian Date (002 - 029 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station HEGL1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -58.81
Fractional Gross Error(%) = 60.19
CM (microgram/m3)
Julian Date (002 - 029 2002)

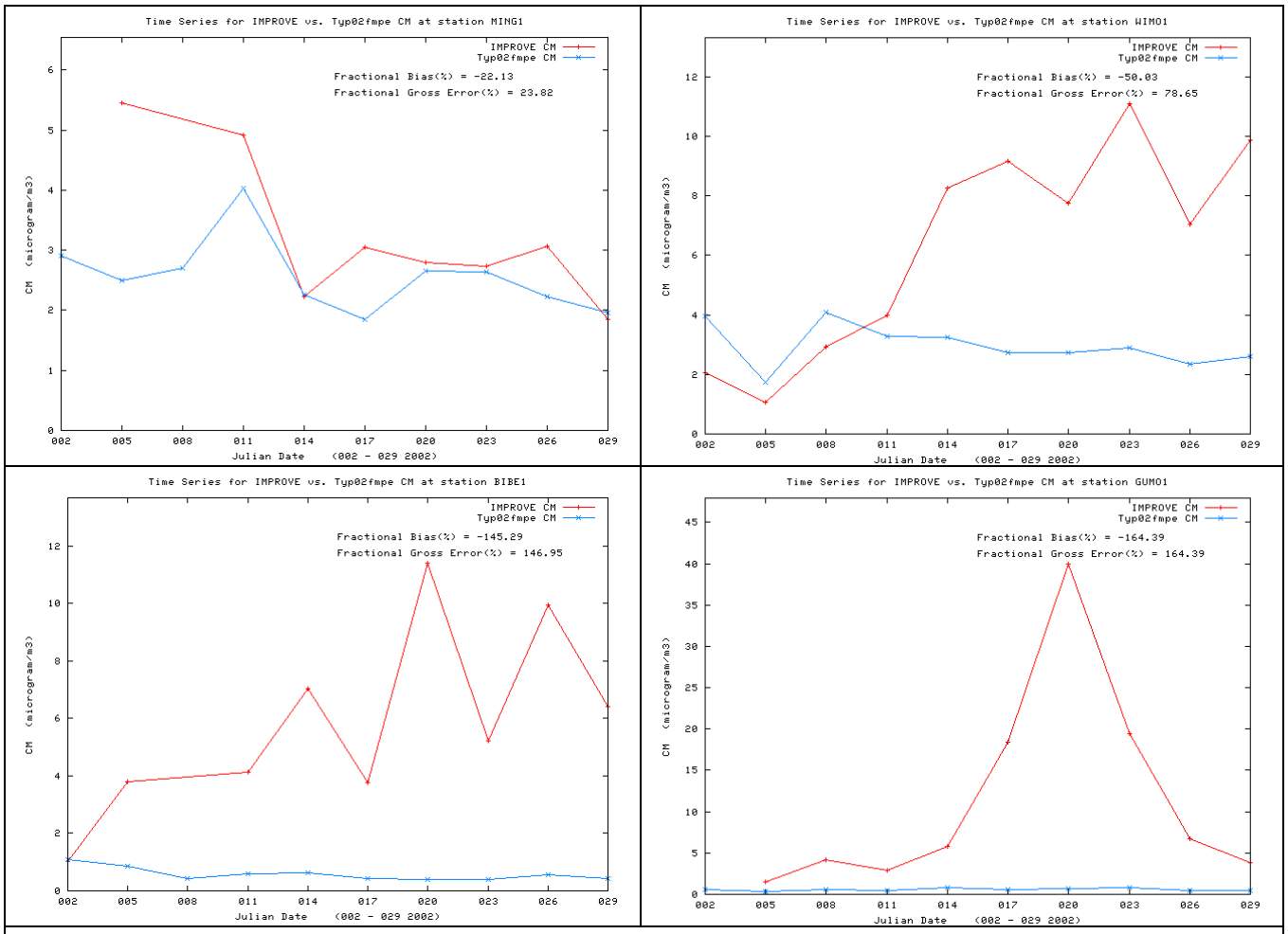


Figure C-34b. Time series of predicted and observed 24-hour coarse mass (CM) concentrations at CENRAP IMPROVE CLASS I AREA sites in January 2002 for CMAQ 2002 36 km Base F base case simulation.

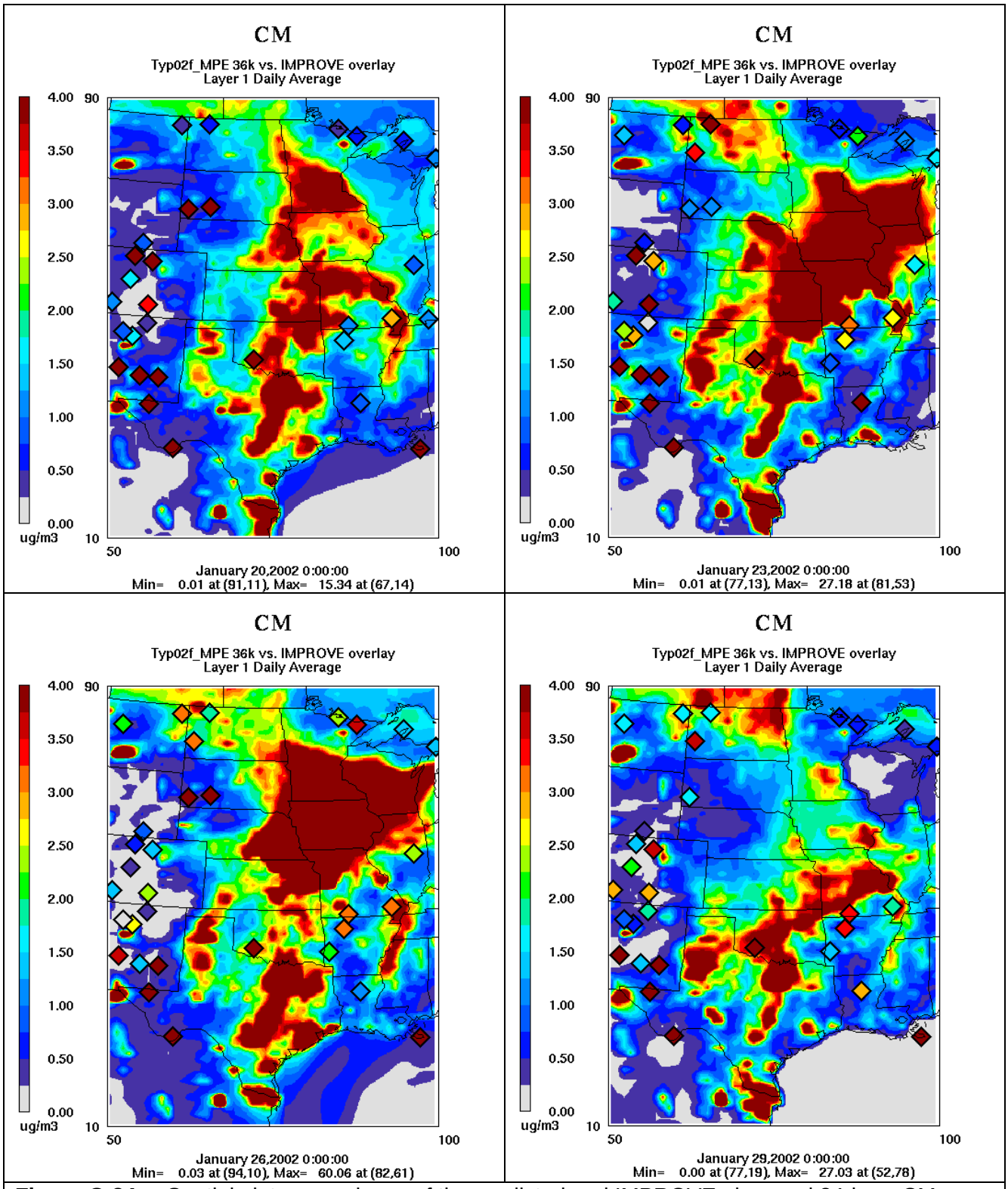


Figure C-34c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour CM concentrations for January 20, 23, 26 and 29, 2002.

C.3.6.2 CM in April 2002

The CM underestimation bias is even greater in April (-137%) and occurs at all IMPROVE sites (Figure C-35).

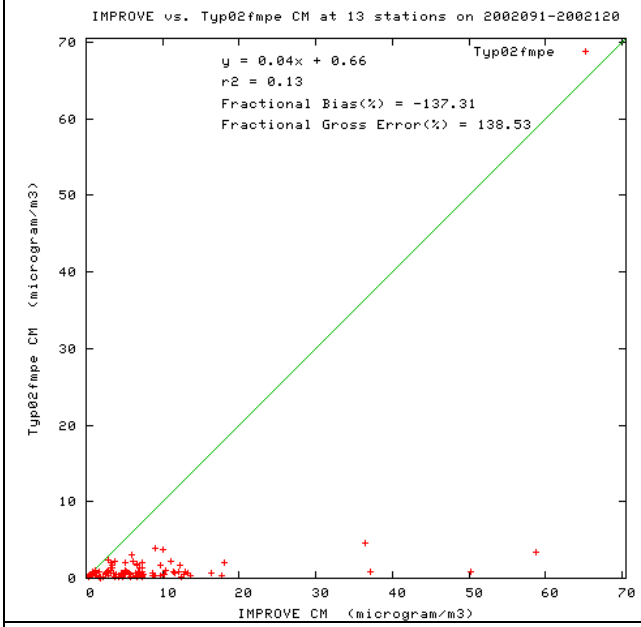
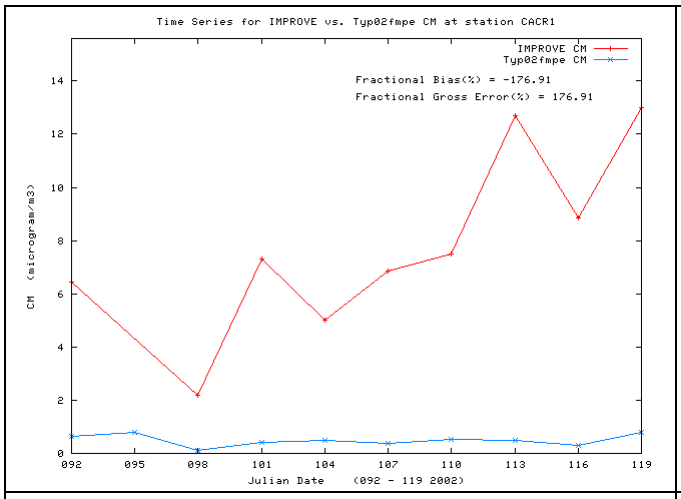
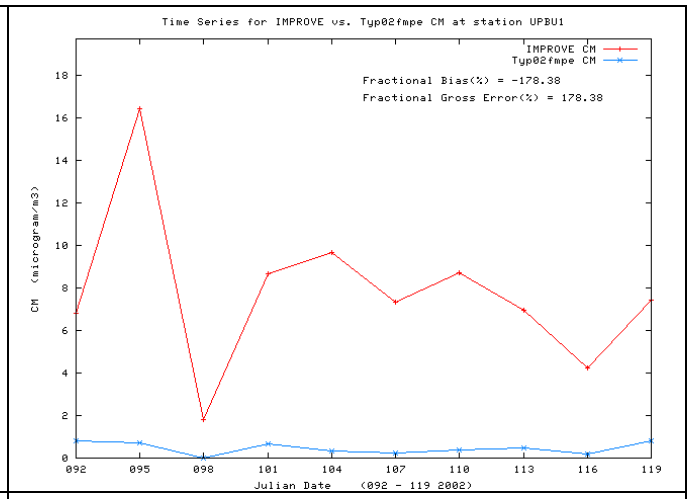
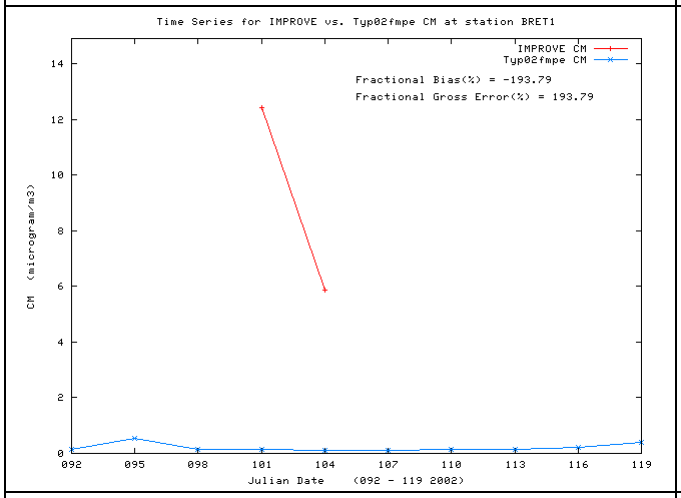
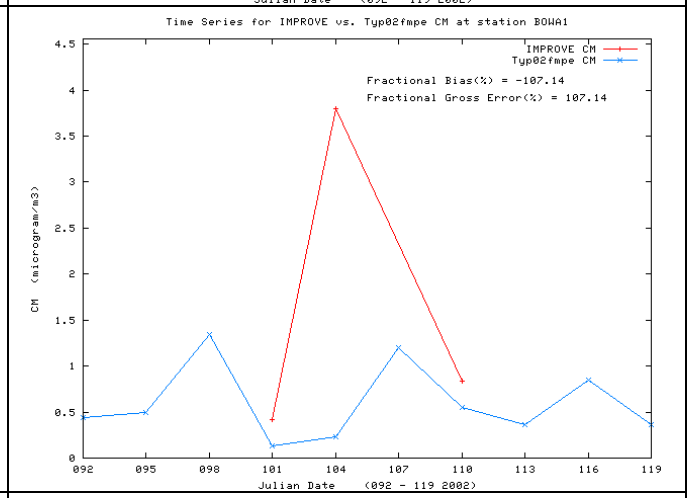


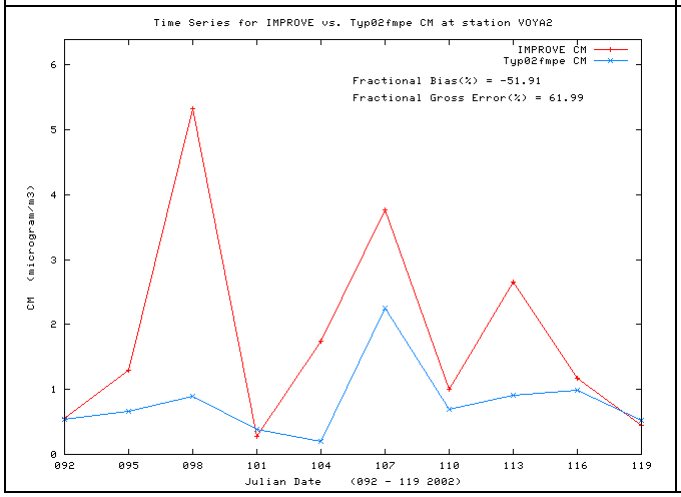
Figure C-35a. Scatter plots of predicted and observed coarse mass (CM) concentrations for April 2002 and sites in the CENRAP region using IMPROVE monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

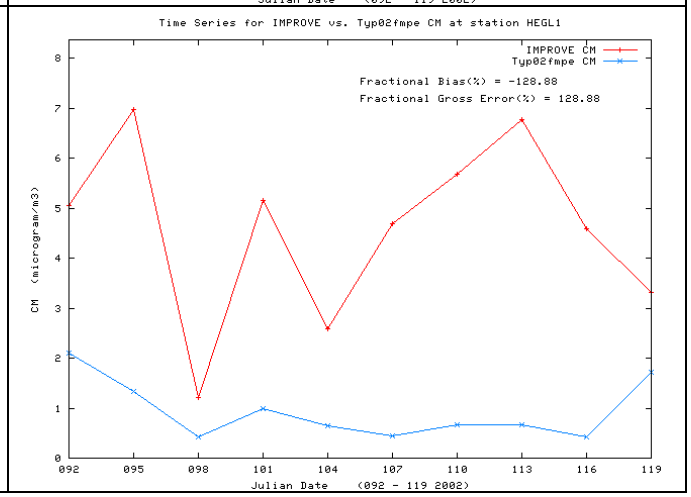

Time Series for IMPROVE vs. Typ02fmpe CM at station CACR1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -176.91
Fractional Gross Error(%) = 176.91
CM (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station UPBU1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -178.38
Fractional Gross Error(%) = 178.38
CM (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station BRET1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -193.79
Fractional Gross Error(%) = 193.79
CM (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station BOWA1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -107.14
Fractional Gross Error(%) = 107.14
CM (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station VOYA2
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -51.91
Fractional Gross Error(%) = 61.99
CM (microgram/m3)
Julian Date (092 - 119 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station HEGL1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -128.88
Fractional Gross Error(%) = 128.88
CM (microgram/m3)
Julian Date (092 - 119 2002)

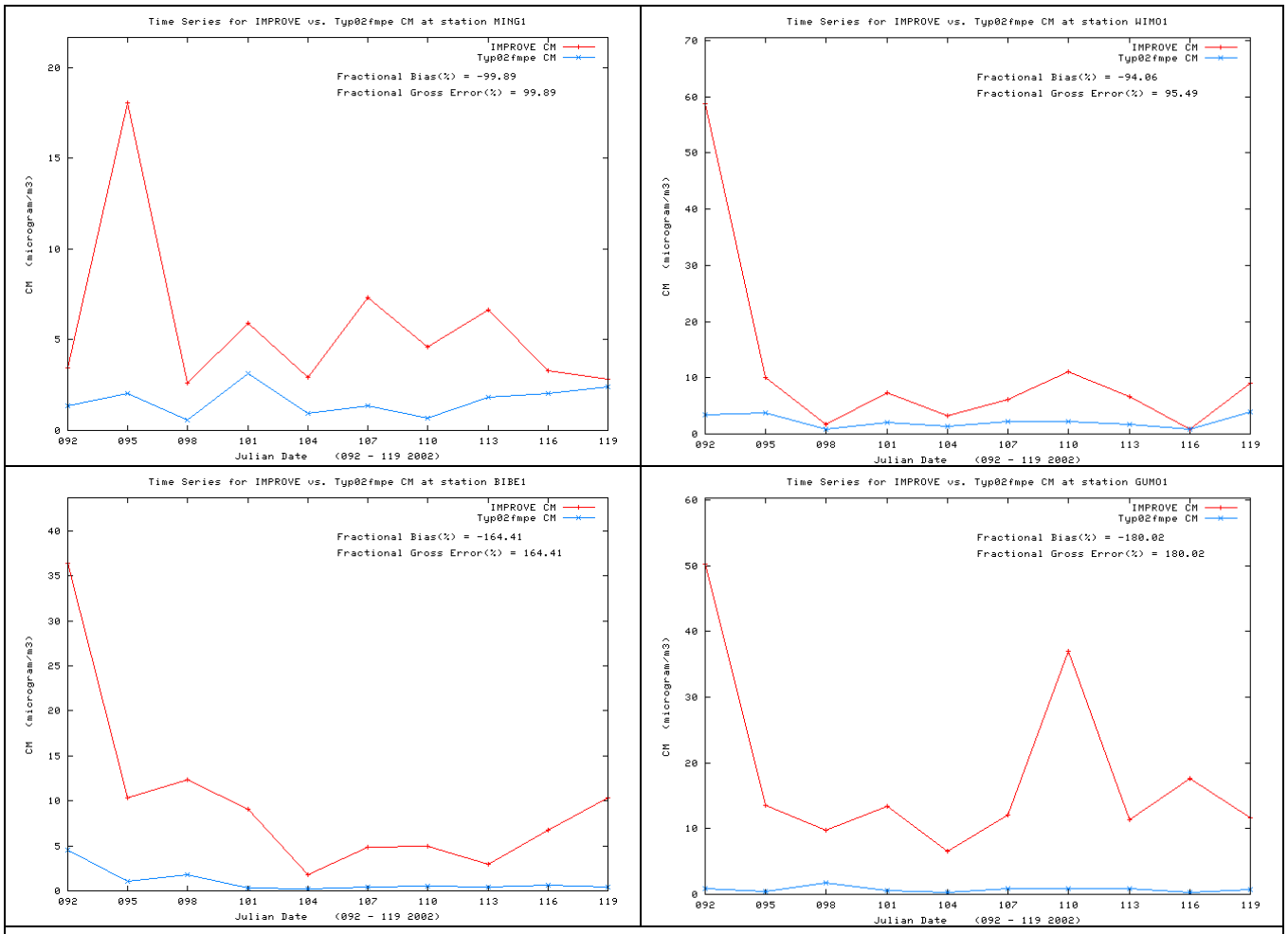


Figure C-35b. Time series of predicted and observed 24-hour coarse mass (CM) concentrations at CENRAP IMPROVE CLASS I AREA sites in April 2002 for CMAQ 2002 36 km Base F base case simulation.

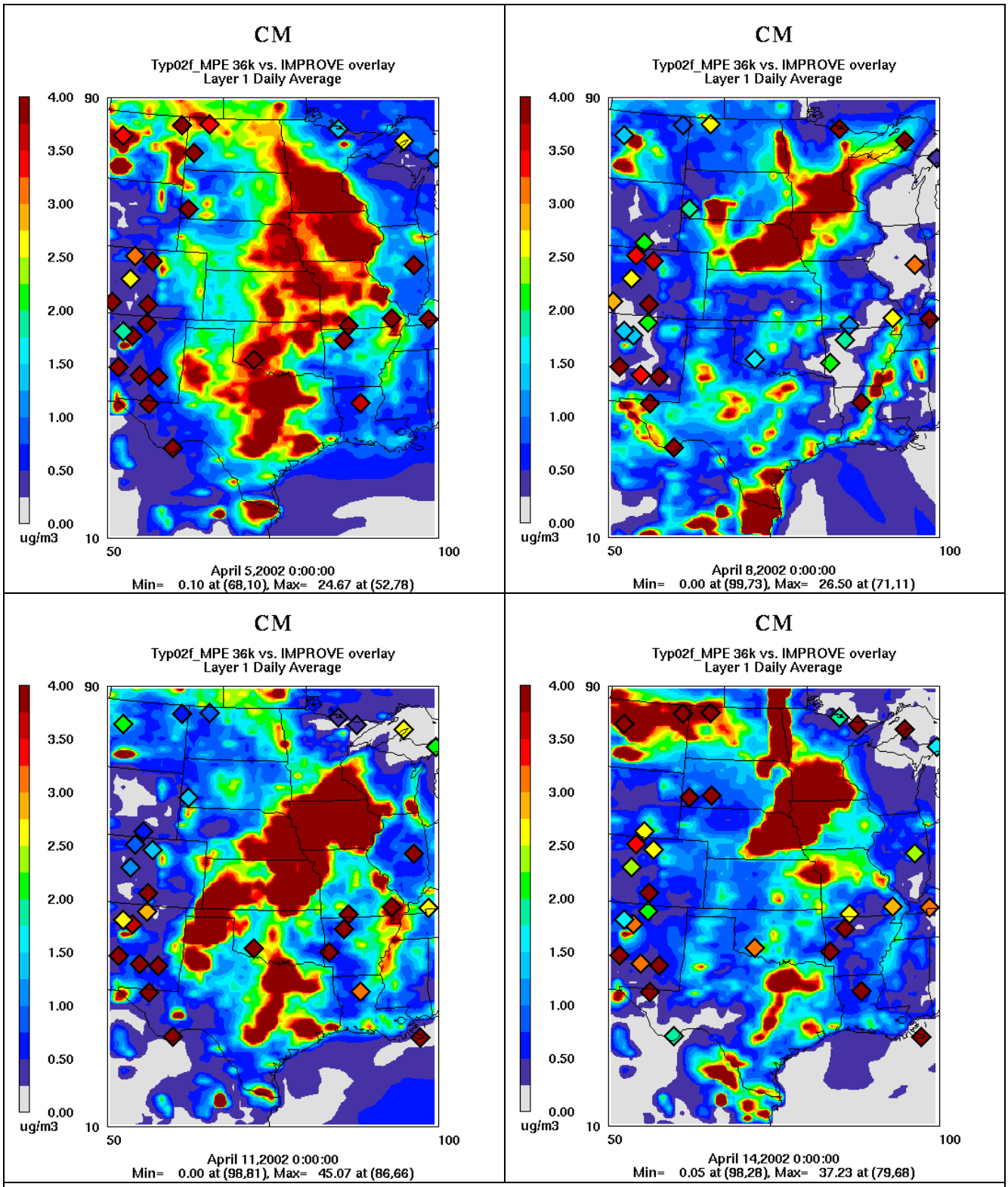


Figure C-35c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour CM concentrations for April 5, 8, 11 and 14, 2002.

C.3.6.3 CM in July 2002

CM performance in July is also very poor with a fractional bias value of -160% (Figure C-36).

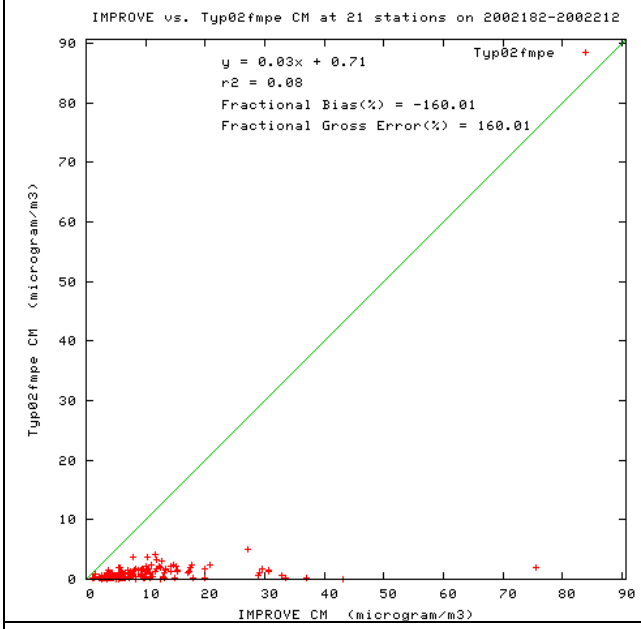
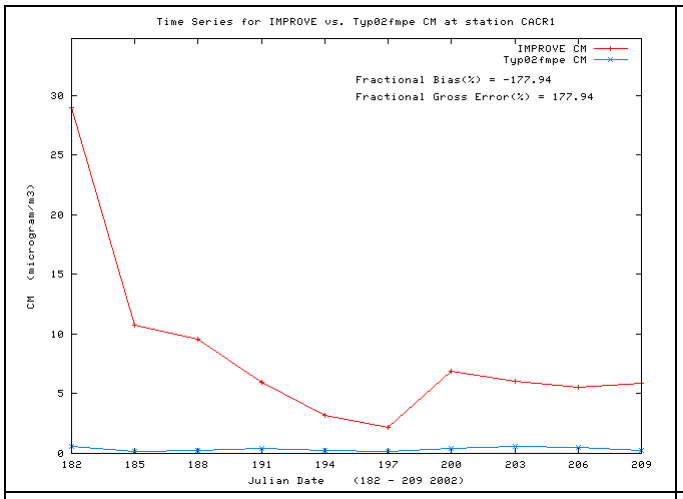
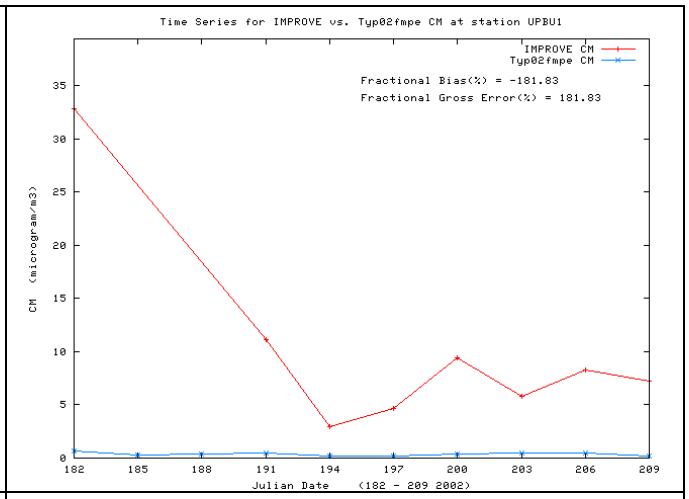
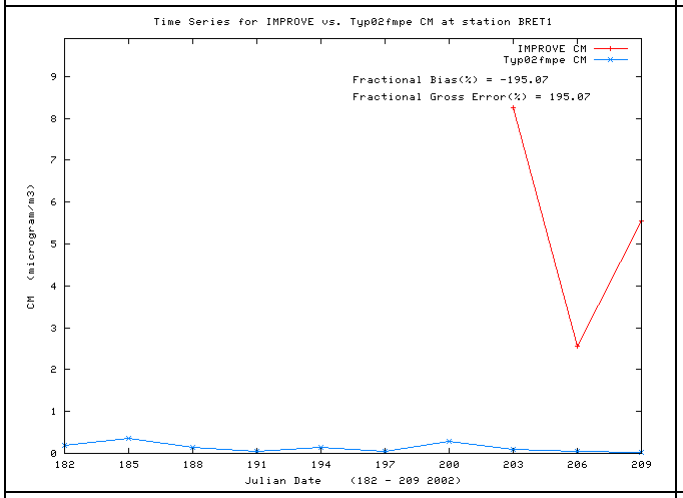
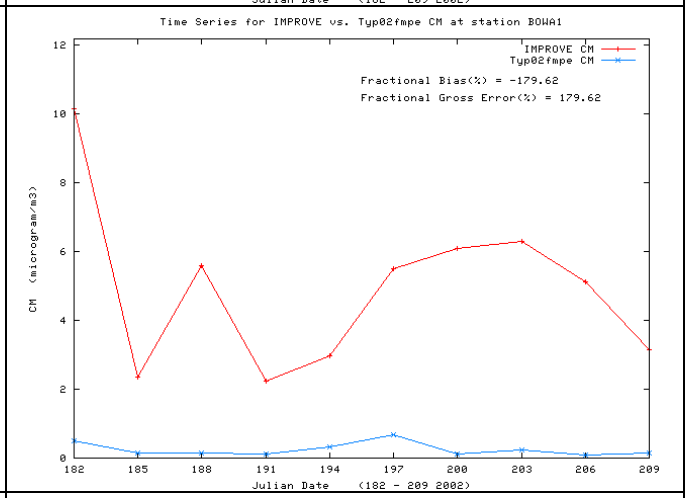


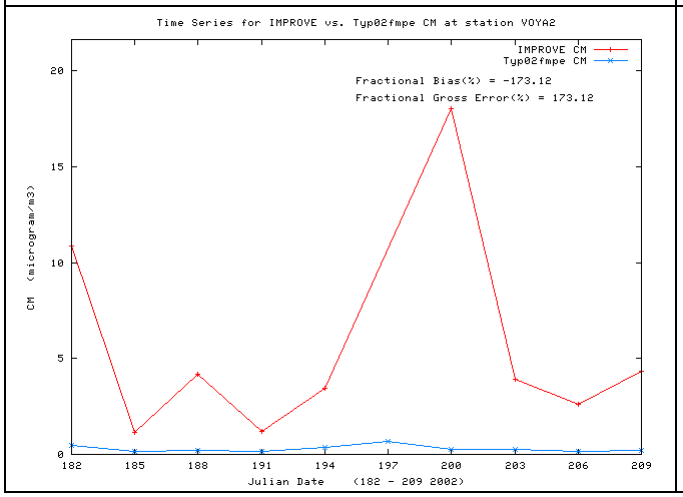
Figure C-36a. Scatter plots of predicted and observed coarse mass (CM) concentrations for July 2002 and sites in the CENRAP region using IMPROVE monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

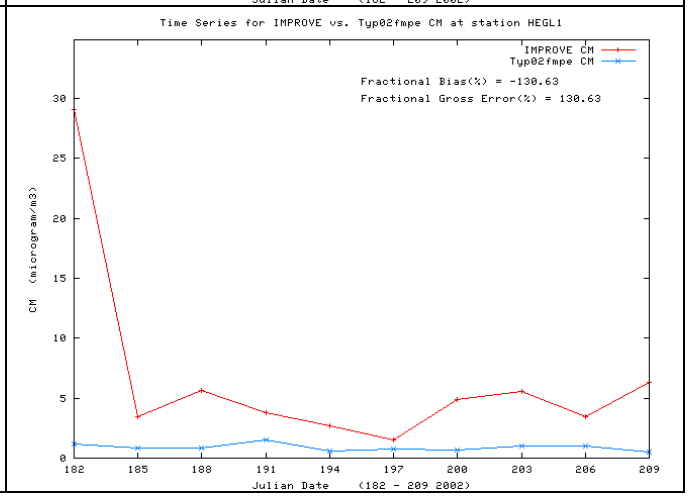

Time Series for IMPROVE vs. Typ02fmpe CM at station CACR1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -177.94
Fractional Gross Error(%) = 177.94
CM (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station UPBU1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -181.83
Fractional Gross Error(%) = 181.83
CM (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station BRET1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -195.07
Fractional Gross Error(%) = 195.07
CM (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station BOWA1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -179.62
Fractional Gross Error(%) = 179.62
CM (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station VOYA2
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -173.12
Fractional Gross Error(%) = 173.12
CM (microgram/m3)
Julian Date (182 - 209 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station HEGL1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -130.63
Fractional Gross Error(%) = 130.63
CM (microgram/m3)
Julian Date (182 - 209 2002)

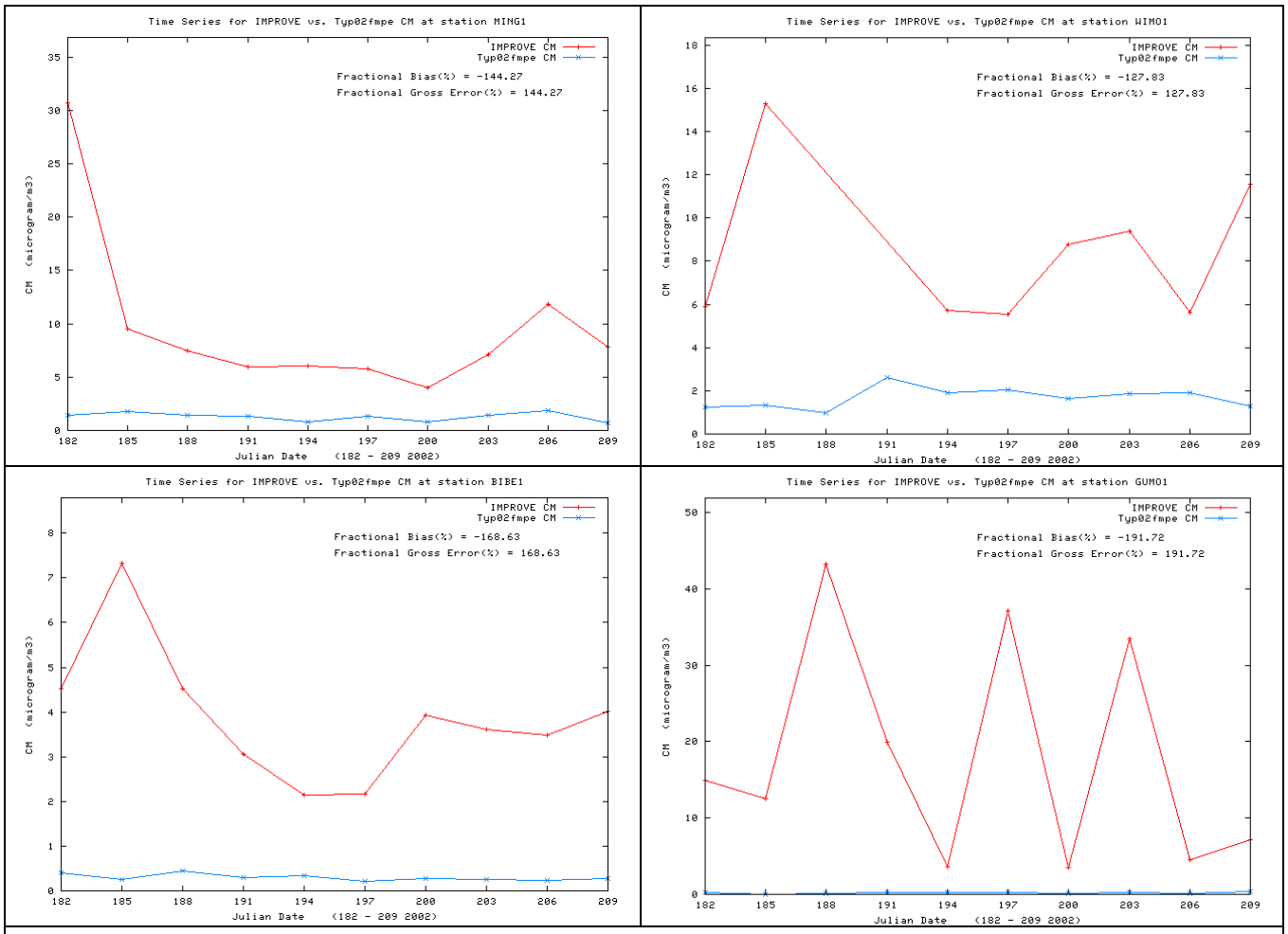


Figure C-36b. Time series of predicted and observed 24-hour coarse mass (CM) concentrations at CENRAP IMPROVE CLASS I AREA sites in July 2002 for CMAQ 2002 36 km Base F base case simulation.

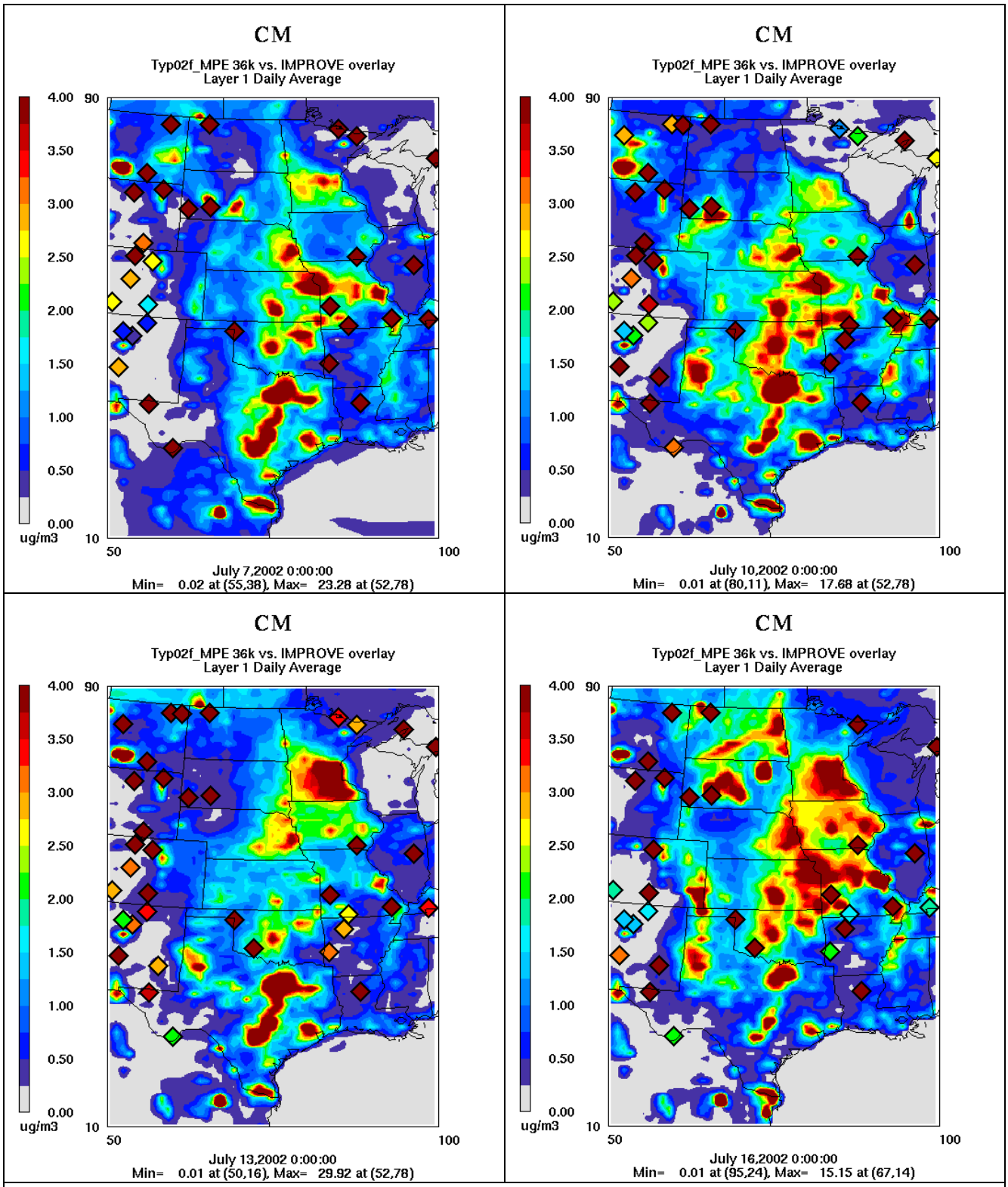


Figure C-36c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour CM concentrations for July 7, 10, 13 and 16, 2002.

C.3.6.4 CM in October 2002

CM is also underestimated in October, although the overestimation bias (-72%) is not as great as seen in July (Figure C-37).

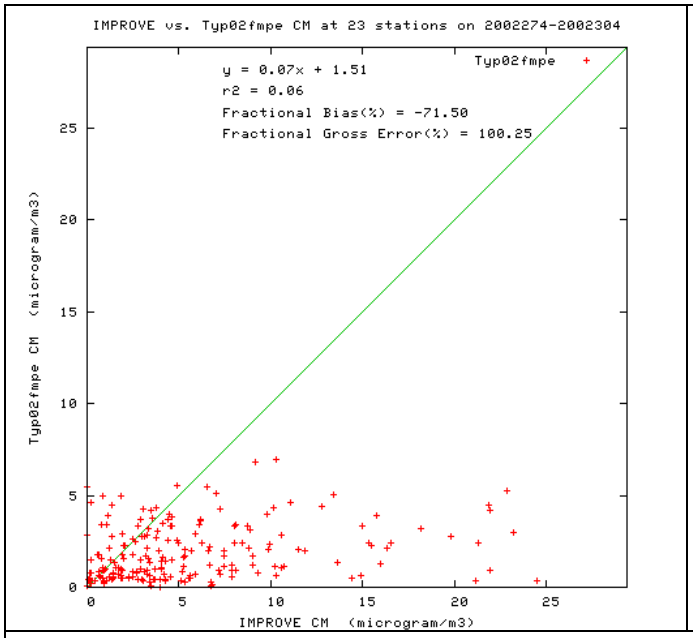
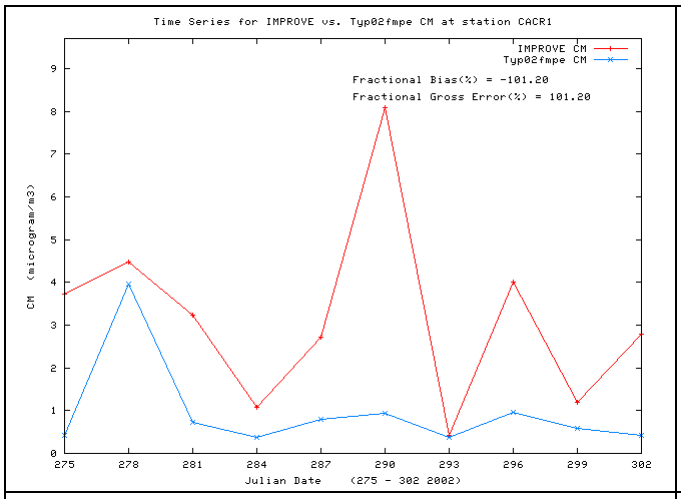
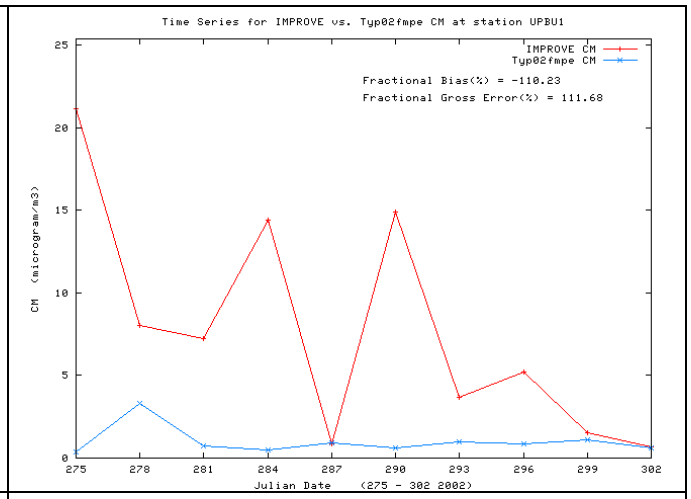
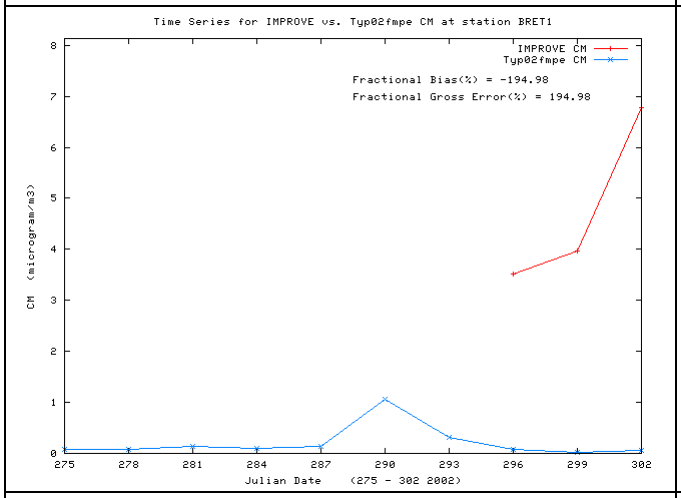
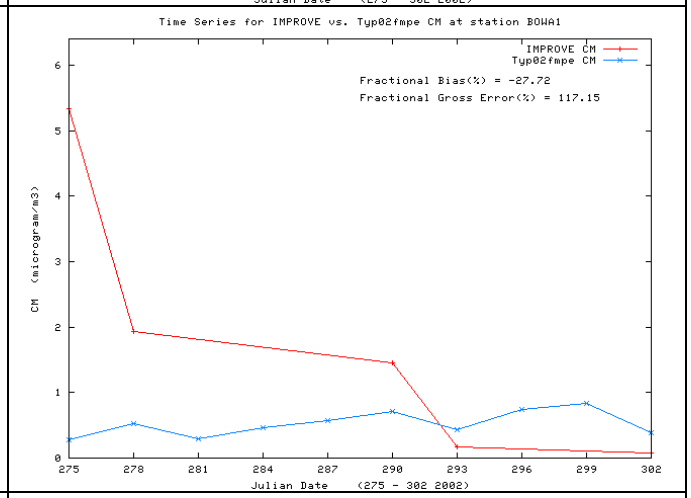


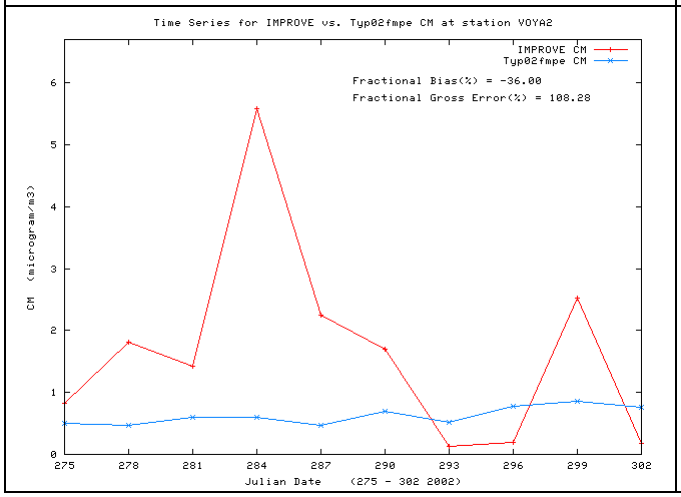
Figure C-37a. Scatter plots of predicted and observed coarse mass (CM) concentrations for October 2002 and sites in the CENRAP region using IMPROVE monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

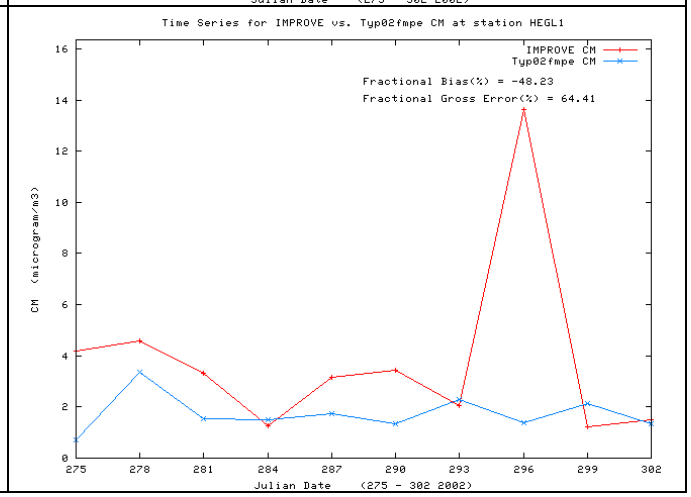

Time Series for IMPROVE vs. Typ02fmpe CM at station CACR1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -101.20
Fractional Gross Error(%) = 101.20
CM (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station UPBU1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -110.23
Fractional Gross Error(%) = 111.68
CM (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station BRET1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -194.98
Fractional Gross Error(%) = 194.98
CM (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station BOWA1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -27.72
Fractional Gross Error(%) = 117.15
CM (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station VOYA2
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -36.00
Fractional Gross Error(%) = 108.28
CM (microgram/m3)
Julian Date (275 - 302 2002)


Time Series for IMPROVE vs. Typ02fmpe CM at station HEGL1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -48.23
Fractional Gross Error(%) = 64.41
CM (microgram/m3)
Julian Date (275 - 302 2002)

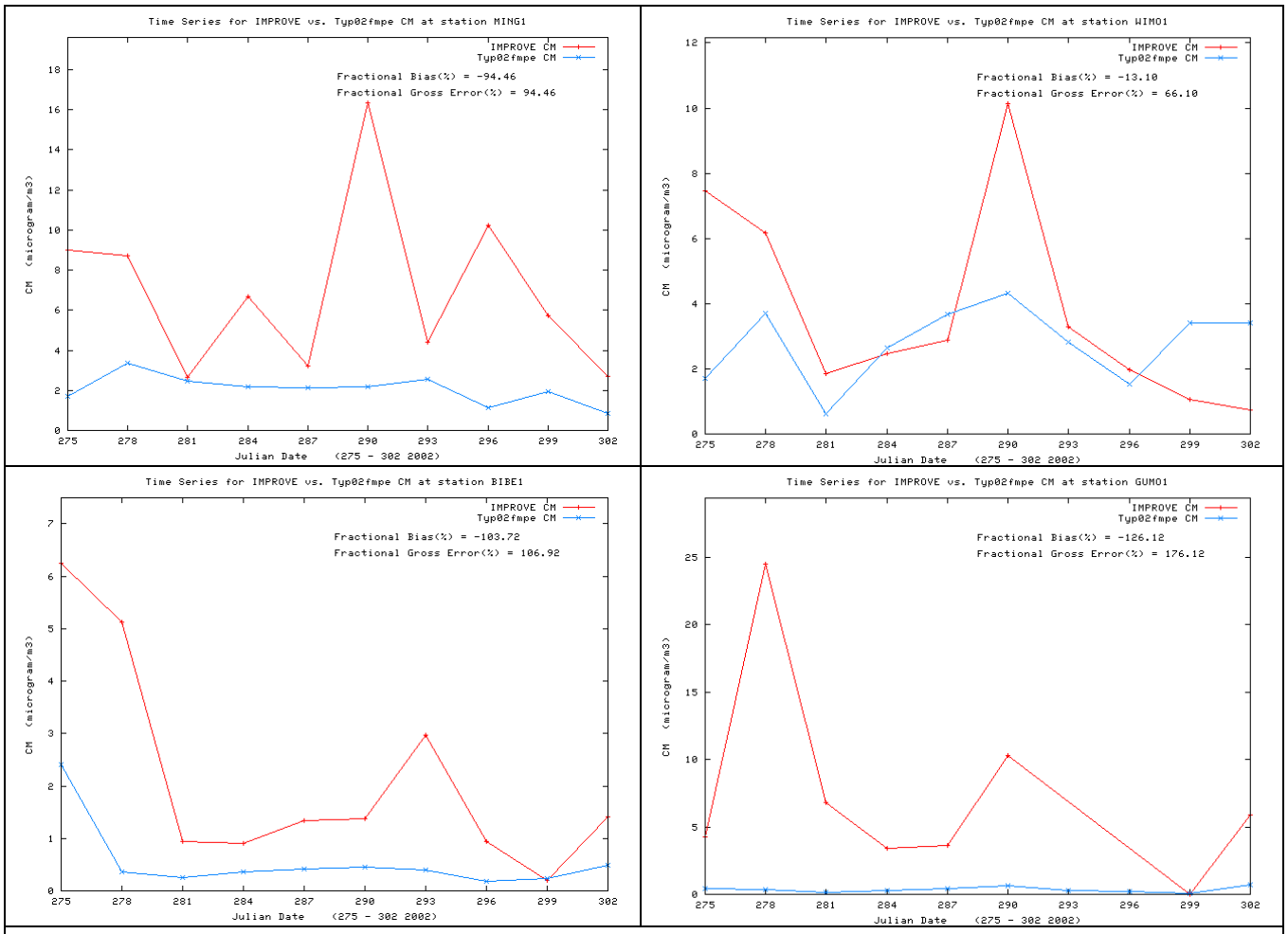


Figure C-37b. Time series of predicted and observed 24-hour coarse mass (CM) concentrations at CENRAP IMPROVE CLASS I AREA sites in October 2002 for CMAQ 2002 36 km Base F base case simulation.

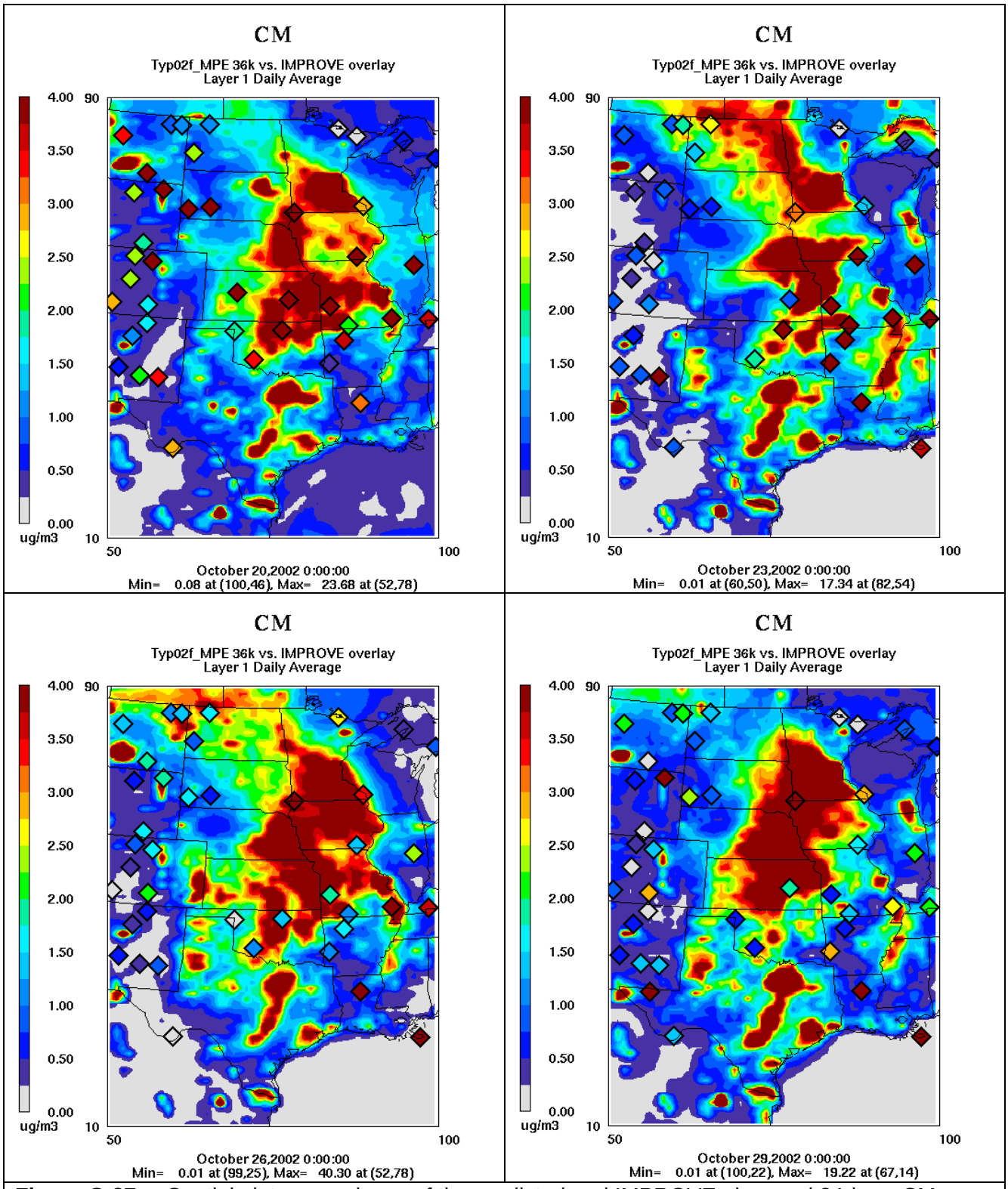


Figure C-37c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour CM concentrations for October 20, 23, 26 and 29, 2002.

C.3.6.5 CM Monthly Bias and Error

The monthly average fractional bias and error values for CM are shown in Figure C-38. In the winter the under-prediction bias is typically in the -60% to -80% range. In the late Spring and Summer the under-prediction bias ranges from -120% to -160%. As this under-prediction bias is nearly systematic, then the errors are the same magnitude as the bias.

The Bugle Plots clearly show that the CM model performance is a problem. The monthly bias exceeds both the performance goal and criteria for almost every month of the year. The error criteria are also exceeded for all months of the year.

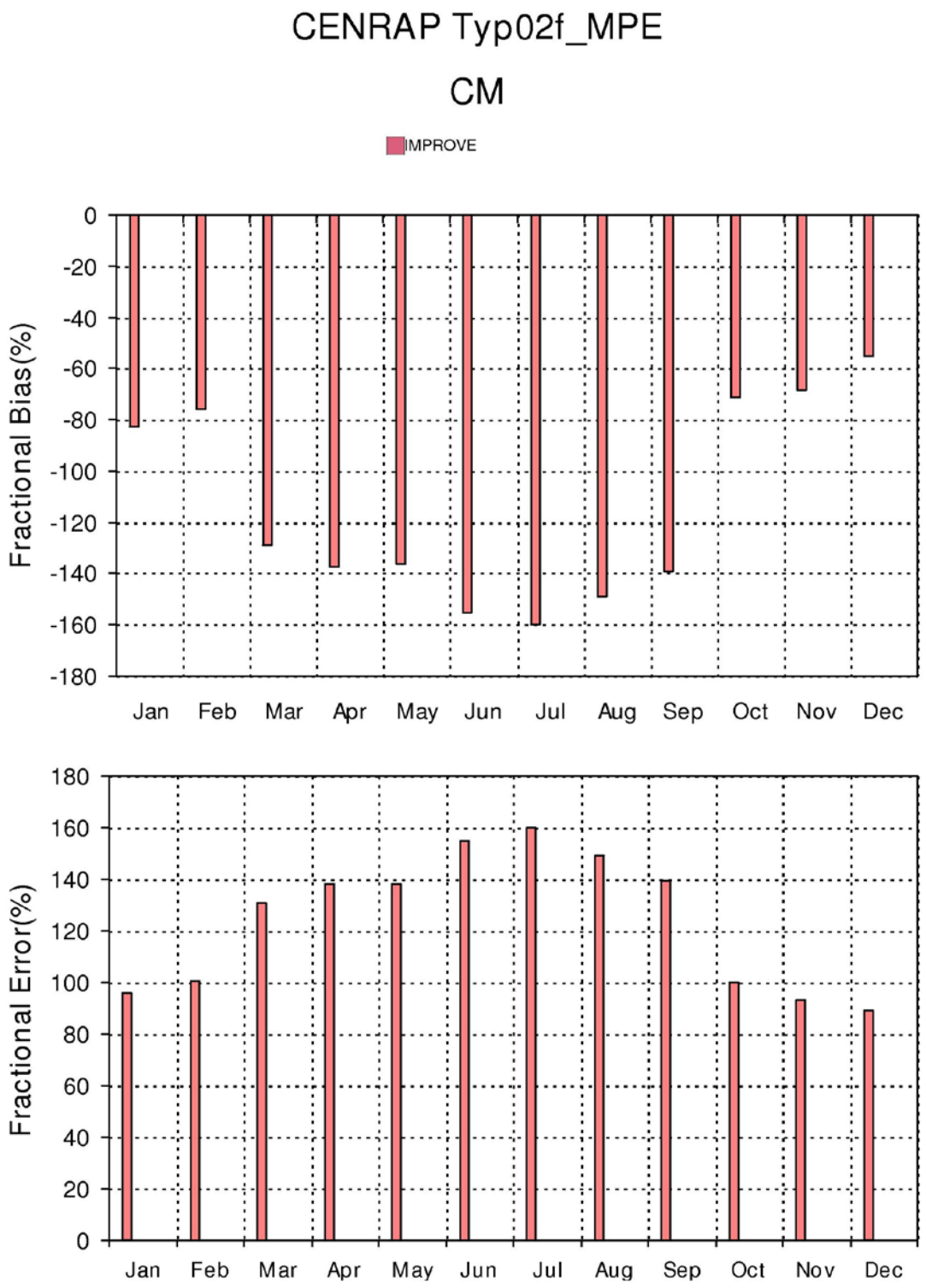


Figure C-38. Monthly CM fractional bias (top) and fractional gross error (bottom) statistical measures for IMPROVE monitoring sites in the CENRAP region.

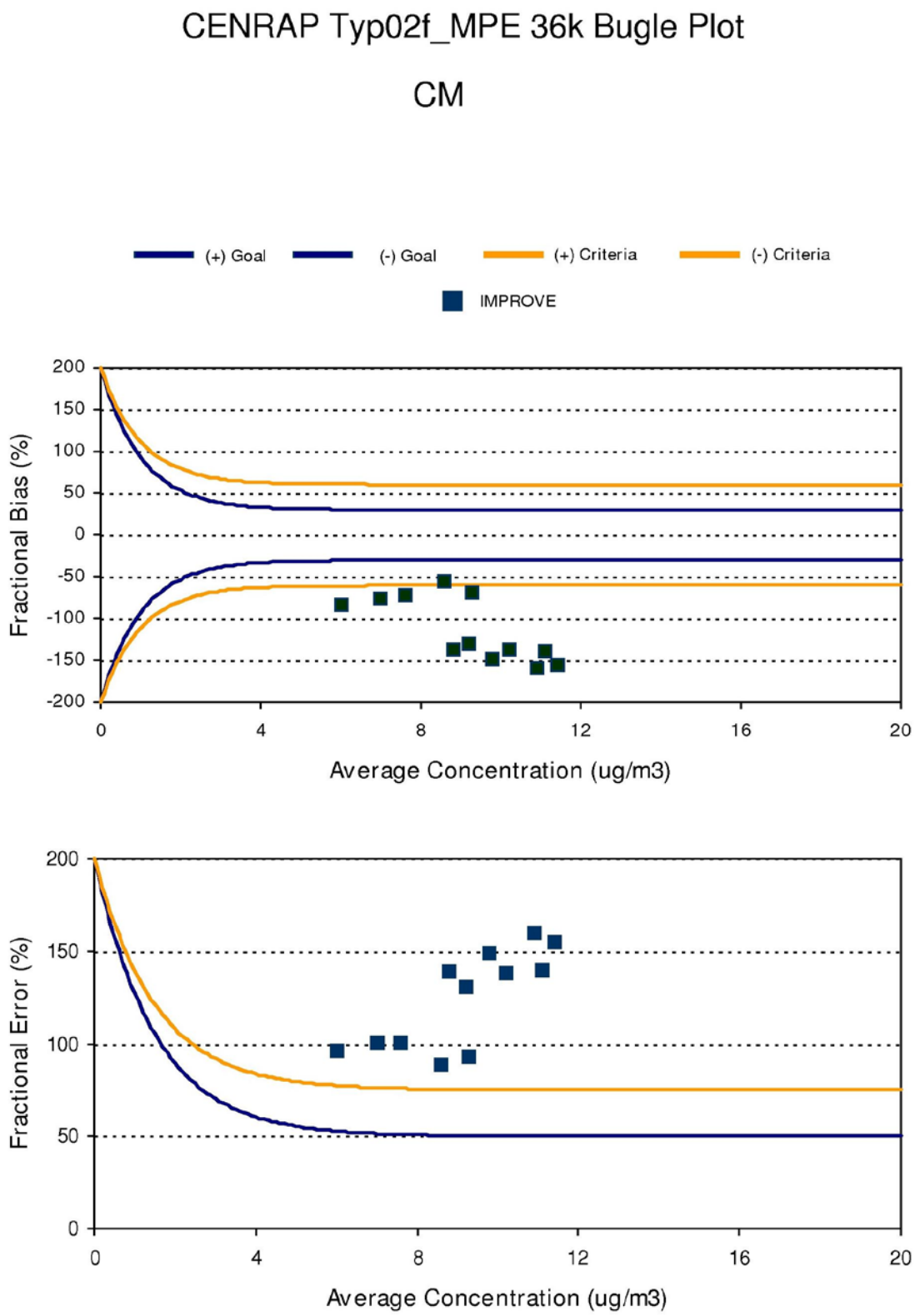


Figure C-39. Bugle Plots of monthly fractional bias (top) and fractional gross error (bottom) and comparisons with model performance goals and criteria for CM and IMPROVE monitoring sites in the CENRAP region.

C.4 Diagnostic Model Evaluation for Gas-Phase and Precursor Species

The CASTNet and AQS networks also measure gas-phase species that are PM precursor or related species. The diagnostic evaluation of the 2002 36 km Base F CMAQ base case simulation for these compounds and the four seasonal months presented previously is provided below.

The CASTNet network measures weekly average samples of SO2, SO4, NO2, HNO3, NO3 and NH4. The AQS network collects hourly measurements of SO2, NO2, O3 and CO. A comparison of the SO2 and SO4 performance provides insight into whether the SO4 formation rate may be too slow or fast. For example, if SO4 is underestimated and SO2 is overestimated that may indicate too slow chemical conversion rate. Analyzing the performance for SO4, HNO3, NO3, Total NO3 and NH4 provides insight into the equilibrium of these species. For example, if Total NO3 performs well but HNO3 and NO3 do not, then there may be issues associated with the partitioning between the gaseous and particle phases of nitrate.

C.4.1 Diagnostic Model Performance in January 2002

In January, SO2 is overstated across both the CASTNet and AQS sites with fractional bias values of 38% (Figure C-40) and 31% (Figure C-41), respectively. SO4 is understated by -34% across the CASTNet monitors (Figure C-40) and -12% and -13% for the IMPROVE and STN networks (Figure C-4a). As noted previously, wet SO4 deposition is also overstated in January (+40%, Figure C-4a). Given that SO2 emissions are well characterized, these results suggest that the January SO4 underestimation may be partly due to understated transformation rates of So2 to SO4 and overstated wet SO4 deposition.

Total NO3 is overestimated by 35% on average across the CASTNet sites in the CENRAP region in January (Figure C-40). HNO3 is underestimated (-34%) and particle NO3 is overestimated (+61%) suggesting there are gas/particle equilibrium issues. An analysis of the time series of the four CASTNet stations reveals that NO3, HNO3 and NH4 performance is actually very reasonable at the west Texas and the HNO3 underestimation and NO3 overestimation bias is coming from the east Kansas, central Arkansas and northern Minnesota CASTNet sites. One potential contributor for this performance problem is overstated NH3 emissions. However the overstated Total NO3 suggests that the model estimated NOx oxidation rate may be too high in January.

The SO2, NO2, O3 and CO performance across the AQS sites in January is shown in Figure C-41. The AQS monitoring network is primarily an urban-oriented network so it is not surprising that the model is underestimating concentrations of primary emissions like NO2 (-5%) and particularly CO (-67%) when a 36 km grid is used. Ozone is also underestimated on average, especially the maximum values above 60 ppb.

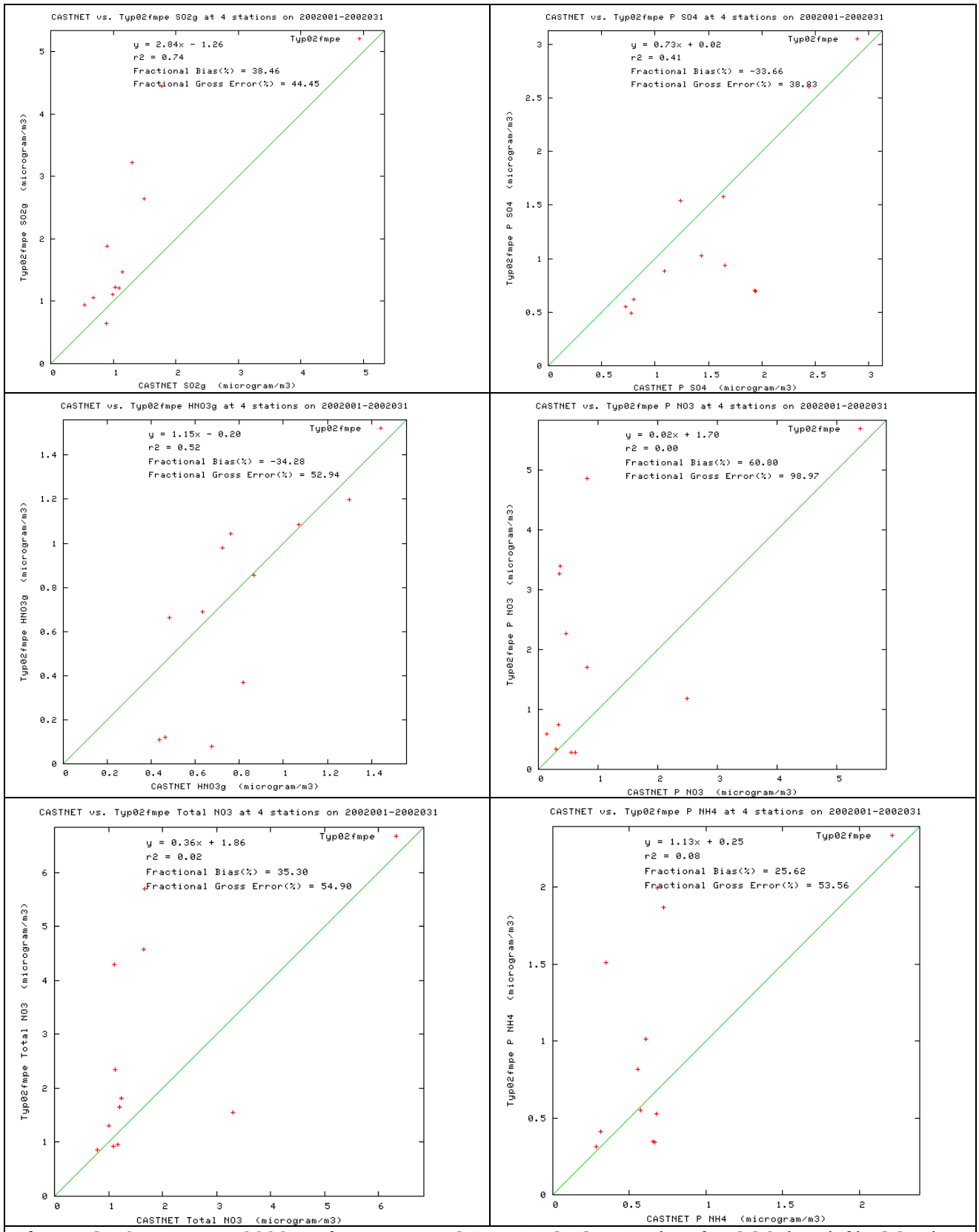


Figure C-40. January 2002 performance at CENRAP CASTNet sites for SO2 (top left), SO4 (top right), HNO3 (middle left), NO3 (middle right), Ttoal NO3 (bottom left) and NH4 (bottom right).

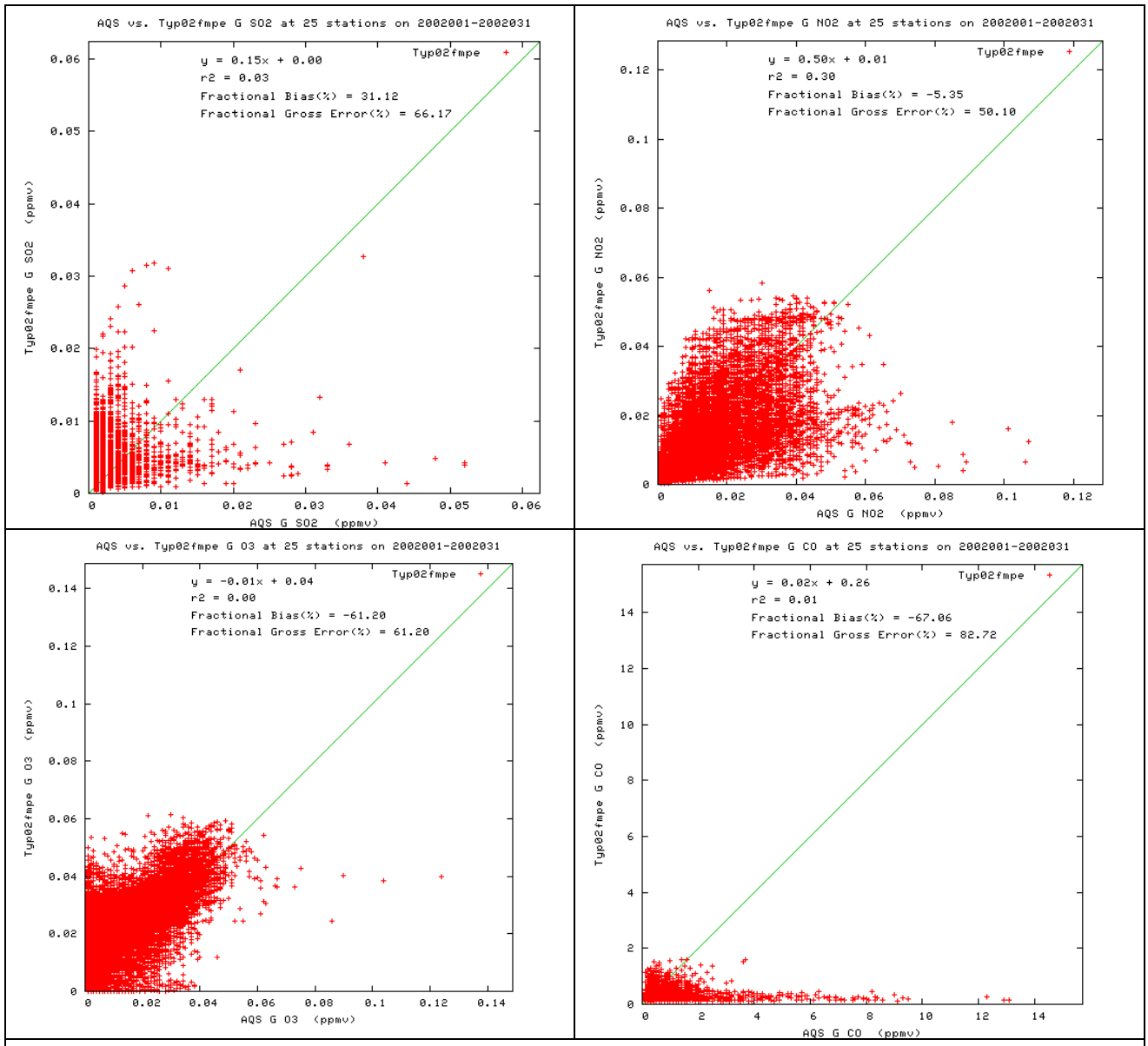


Figure C-41. January 2002 performance at CENRAP AQS sites for SO2 (top left), NO2 (top right), O3 (bottom left) and CO (bottom right).

C.4.2 Diagnostic Model Performance In April

In April there is an average SO2 overestimation bias across the CASTNet (+15%) and underestimation bias across the AQS (-10%) networks (Figures C-42 and C-43). SO4 is underestimated across all networks by -30% to -58% (Figure C-5a). The wet SO4 deposition bias is near zero. Both SO2 and SO4 are underestimated at the west Texas CASTNet monitor in April suggesting SO2 emissions in Mexico are likely understated.

The HNO3 performance in April is interesting with almost perfect agreement except for 5 modeled-observed comparisons that drives the average under-prediction bias of -29%. On Julian Day 102 there is high HNO3 at the MN, KS and OK CASTNet sites that is not captured by the model. Given that HNO3, NO3 and Total NO3 are all underestimated by about the same amount (-30%), then part of the underestimation bias is likely due to too slow oxidation of NOx.

There is a lot of scatter in the NO2 and O3 performance that is more or less centered on the 1:1 line of perfect agreement with bias values of -8% and -21%, respectively (Figure C-43). CO is underestimated by -72% with the model unable to predict CO concentrations above 1 $\mu g/m^3$ due to the use of the coarse 36 km grid spacing. Mobile sources produce a vast majority of the CO emissions so AQS monitors for CO compliance are located near roadways, which are not simulated well using a 36 km grid.

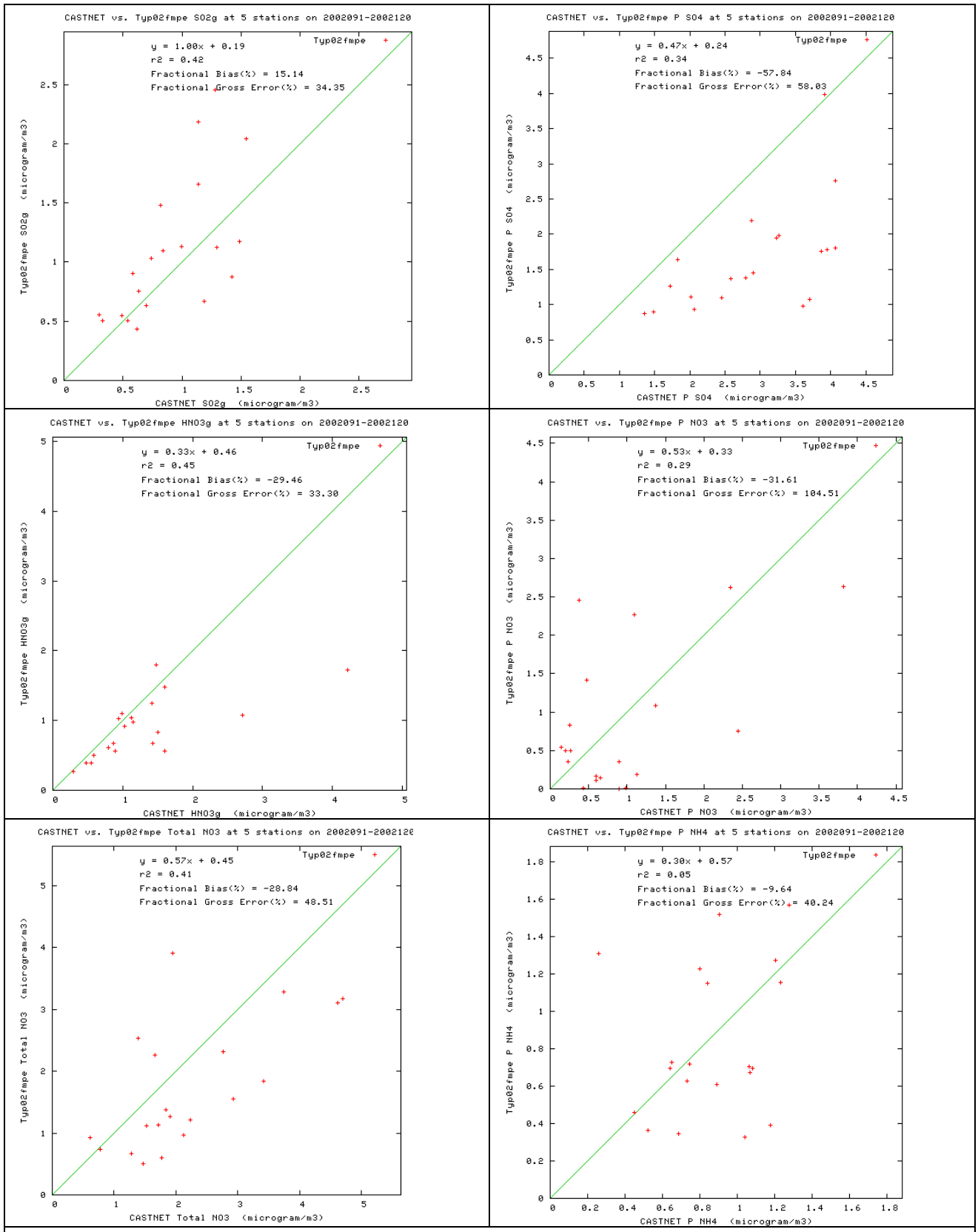


Figure C-42 April 2002 performance at CENRAP CASTNet sites for SO2 (top left), SO4 (top right), HNO3 (middle left), NO3 (middle right), Total NO3 (bottom left) and NH4 (bottom right).

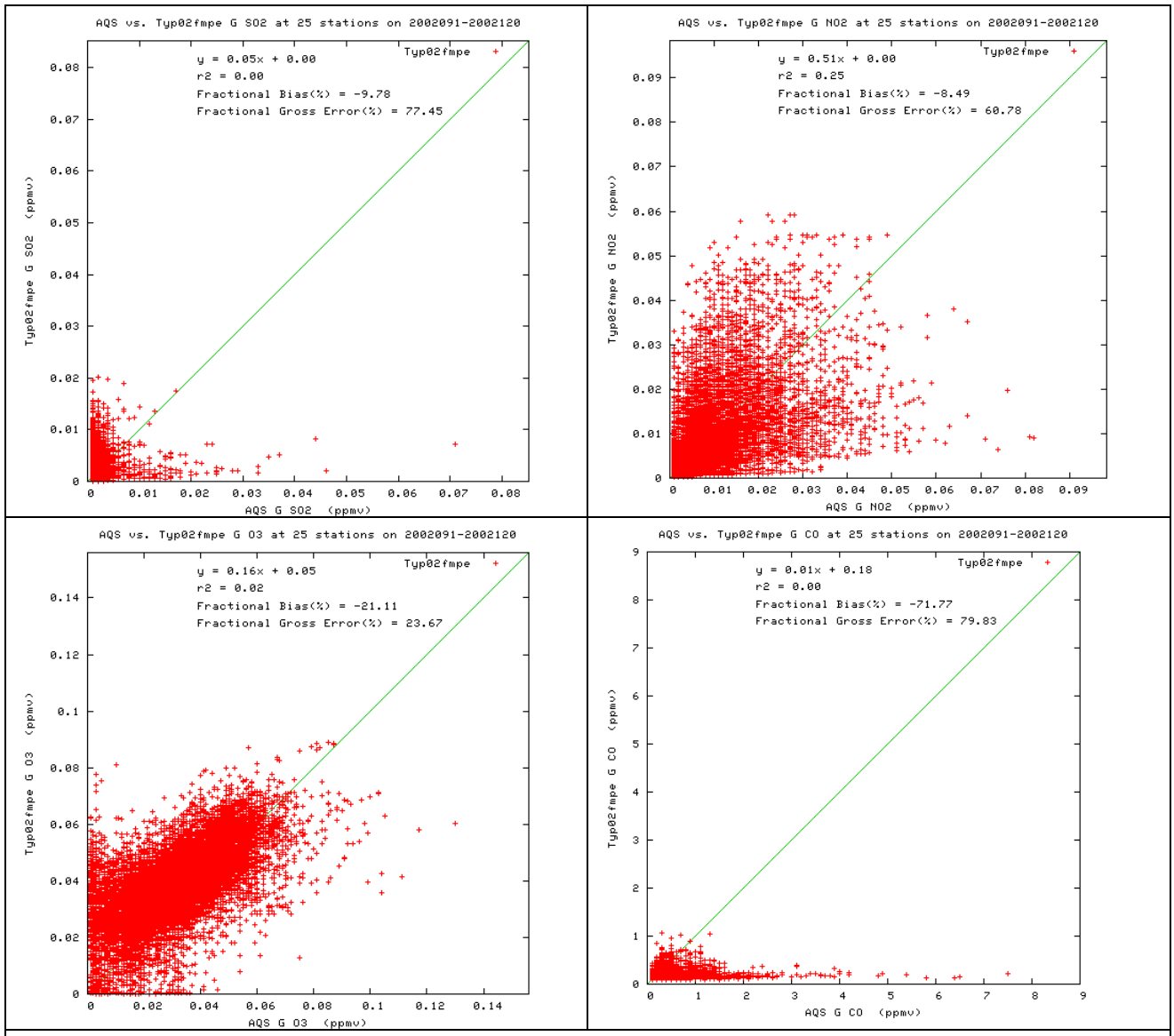


Figure C-43 April 2002 performance at CENRAP AQS sites for SO2 (top left), NO2 (top right), O3 (bottom left) and CO (bottom right).

C.4.3 Diagnostic Model Performance In July

In July SO2 is slightly underestimated across the CASTNet (-5%) and AQS (-12%) networks (Figures C-44 and C-45) and SO4 is more significantly underestimated across all networks (-22% to -53%, Figure C-6a). Since wet SO4 is also underestimated it is unclear the reasons for why all sulfur species are underestimated.

The nitrate species are also all underestimated with the Total NO3 bias (-56%) being between the HNO3 bias (-35%) and NO3 bias (-115%). The modeled NO3 values are all near zero with little correlation with the observations, whereas the observed HNO3 and Total NO3 is tracked well with correlation coefficients of 0.74 and 0.76. These results suggest that the July NO3 model performance problem is partly due to insufficient formation of Total NO3 and mainly due to too little incorrect partitioning of the Total NO3 into the particle NO3.

Again there is lots of scatter in the AQS NO2 scatter plot for July (Figure C-45) resulting in a low bias (0%) but high error (65%). Ozone performance also exhibits a low bias (-15%) and error (20%), but the model is incapable of simulating ozone above 100 ppb. Although CO performance in July is better than the previous months, it still has a large underestimation bias (-82%).

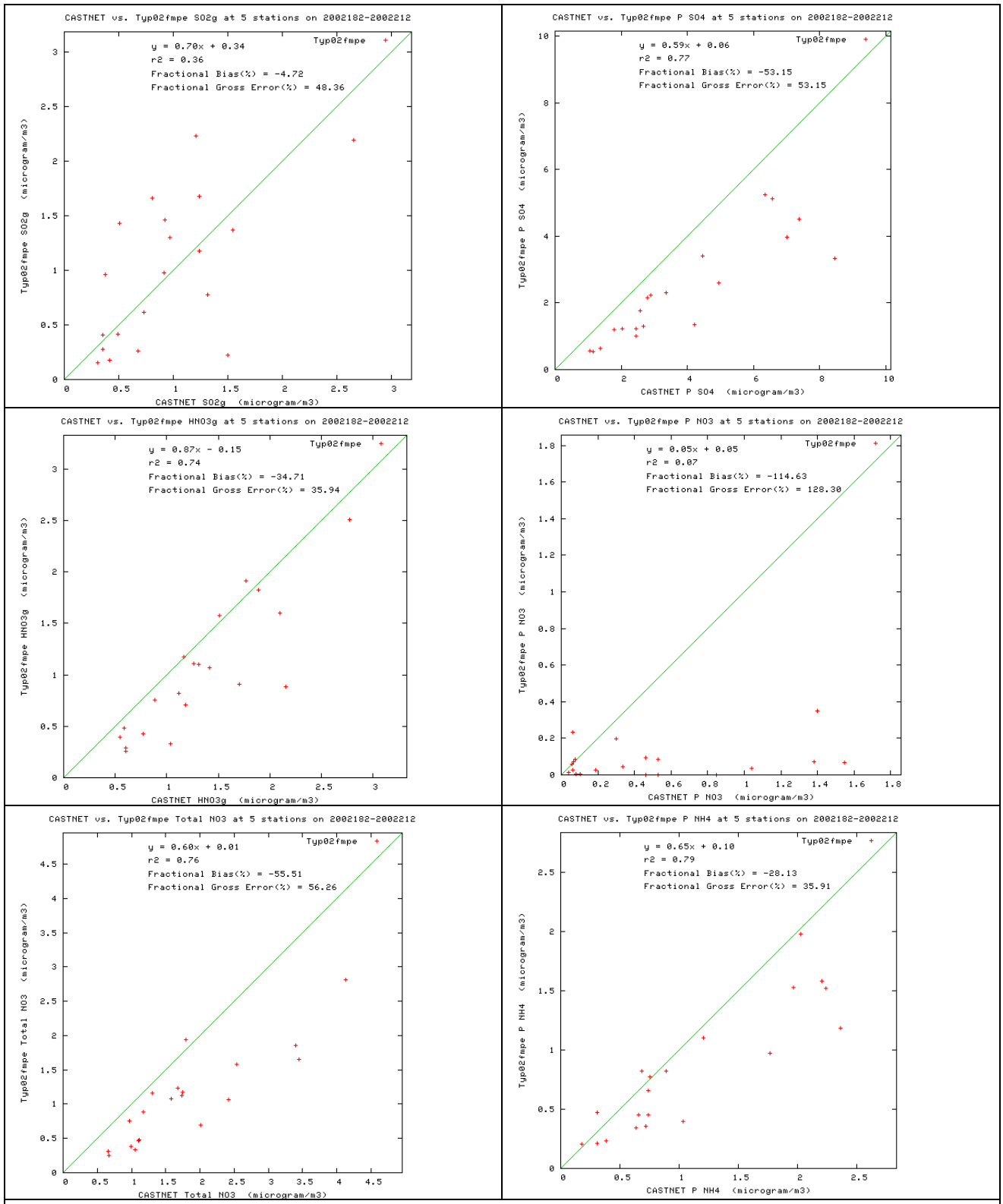


Figure C-44 July 2002 performance at CENRAP CASTNet sites for SO2 (top left), SO4 (top right), HNO3 (middle left), NO3 (middle right), Total NO3 (bottom left) and NH4 (bottom right).

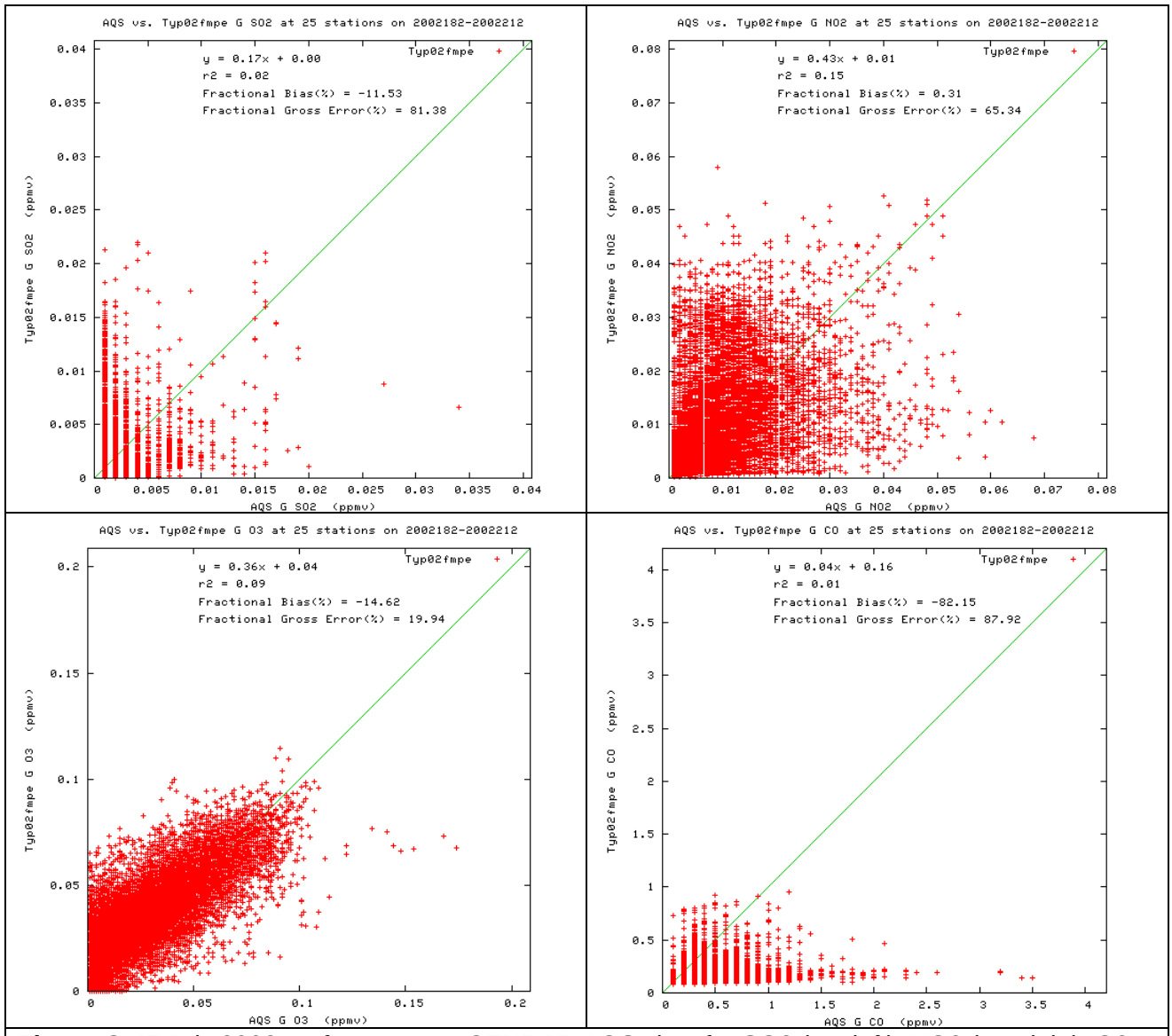


Figure C-45 July 2002 performance at CENRAP AQS sites for SO2 (top left), NO2 (top right), O3 (bottom left) and CO (bottom right).

C.4.4 Diagnostic Model Performance In October

SO2 is overstated in October across the CASTNet (+28%) and AQS (+33%) sites (Figures C-46 and C-47). Although SO4 is understated across the CASTNet sites (-24%), the bias across the IMPROVE (-6%) and STN (0%) sites are near zero (Figure C-7a).

Performance for HNO3 is fairly good with a low bias (+12%) and error (30%). But NO3 is overstated (+34%) leading to an overstatement of Total NO3 (+37%). The overstatement of NO3 leads to an overstatement of NH4 as well (Figure C-46)

As seen in the other months, NO2 exhibits a lot of scatter resulting in a low correlation (0.22) and high error (61%) but low bias (12%). The model tends to under-predict the high and over-predict the low O3 observations resulting in a -29% bias and low correlation coefficient. CO is also under-predicted (-76%) for the reasons discussed previously.

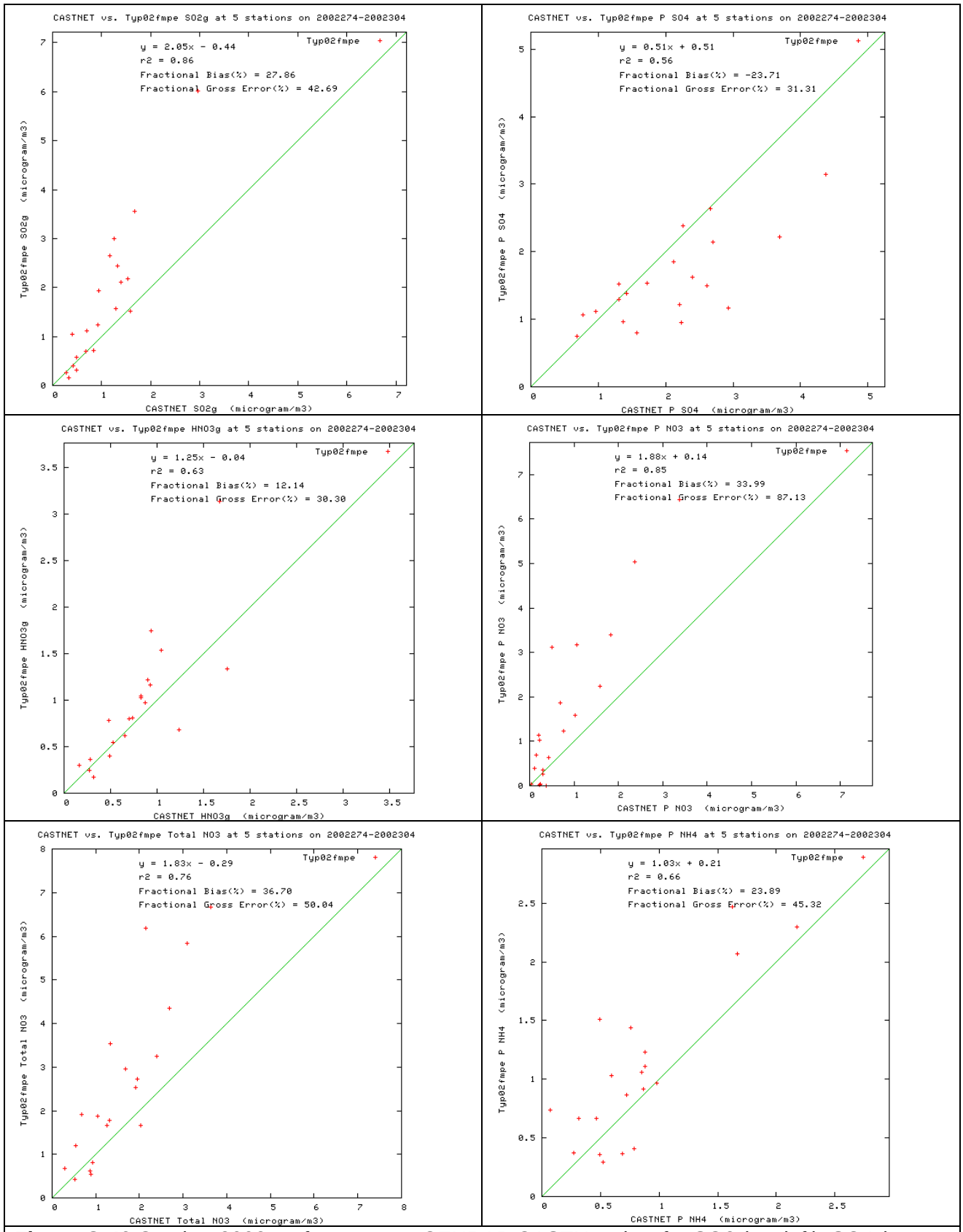


Figure C-46 October 2002 performance at CENRAP CASTNet sites for SO2 (top left), SO4 (top right), HNO3 (middle left), NO3 (middle right), Total NO3 (bottom left) and NH4 (bottom right).

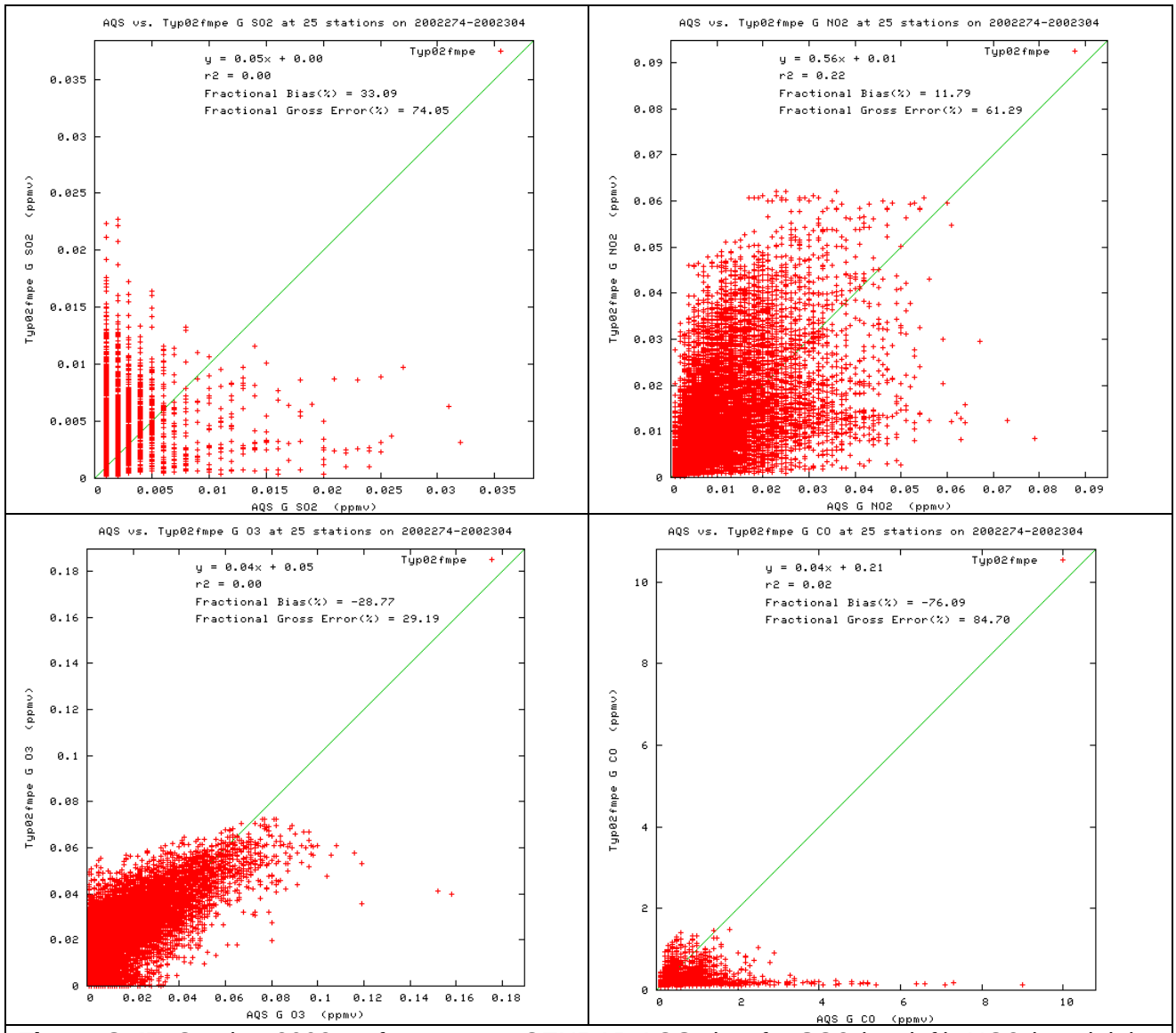


Figure C-47 October 2002 performance at CENRAP AQS sites for SO2 (top left), NO2 (top right), O3 (bottom left) and CO (bottom right).

C.5 Evaluation at Class I Areas for the Worst and Best 20 Percent Days

In this section, and in section C.5 of Appendix C, we present the results of the model performance evaluation at each of the CENRAP Class I areas for the worst and best 20 percent days. Performance on these days is critical since they are the days used in the 2018 visibility projections discussed in Chapter 4. For each Class I area we compared the predicted and observed total extinction (these figures are in Chapter 3) and PM species-specific extinction for the worst and best 20 percent days in 2002.

C.5.1 Caney Creek (CACR) Arkansas

The ability of the CMAQ model to estimate visibility extinction at the CACR Class I area on the 2002 worst and best 20 percent days is provide in Figures 3-9 and C-48. On most of the worst 20 percent days at CACR total extinction is dominated by SO4 extinction with some extinction due to OMC. On four of the worst 20 percent days extinction is dominated by NO3. The average extinction across the worst 20 percent days is underestimated by -33% (Figure 3-9), which is primarily due to a -51% underestimation of SO4 extinction combined with a 6% overestimation of NO3 extinction (Figure C-48). Performance for OMC extinction at CACR on the worst 20 percent days is pretty good with a -20% bias and 36% error, EC extinction is systematically underestimated, Soil extinction has low bias (-19%) buts lots of scatter and high error (74%), while CM extinction is greatly underestimated (bias of -153%).

On the best 20 percent days at CACR the observed extinction ranges from 20 to 40 Mm^{-1}, whereas then modeled extinction has a much larger range from 15 to 120 Mm^{-1}. Much of the modeled overestimation of total extinction on the best 20% days (+44% bias) is due to NO3 overestimation (+94% bias).

C.5.2 Upper Buffalo (UOBU) Arkansas

Model performance at the UPBU Class I area for the worst and best 20 percent days is shown in Figures 3-10 and C-49. On most of the worst 20 percent days at UPBU visibility impairment is dominated by SO4, although there are also two high NO3 days. The model underestimates the average of the total extinction on the worst 20 percent days at UPBU by -40% (Figure 3-10), which is due to an underestimation of extinction due to SO4, OMC and CM by, respectively,

-46%, -33% and -179%.

On the best 20 percent days at UPBU, the model performs reasonably well with a low bias (2%) and error (42%). But again the model has a much wider range in extinction values across the best 20 percent days (15 to 120 Mm^{-1}) than observed (20 to 45 Mm^{-1}). There are five days in which the modeled NO3 over-prediction is quite severe and when those days are removed the range in the modeled and observed extinction on the best 20 percent days is quite similar, although the model gets much cleaner on the very cleanest modeled days.

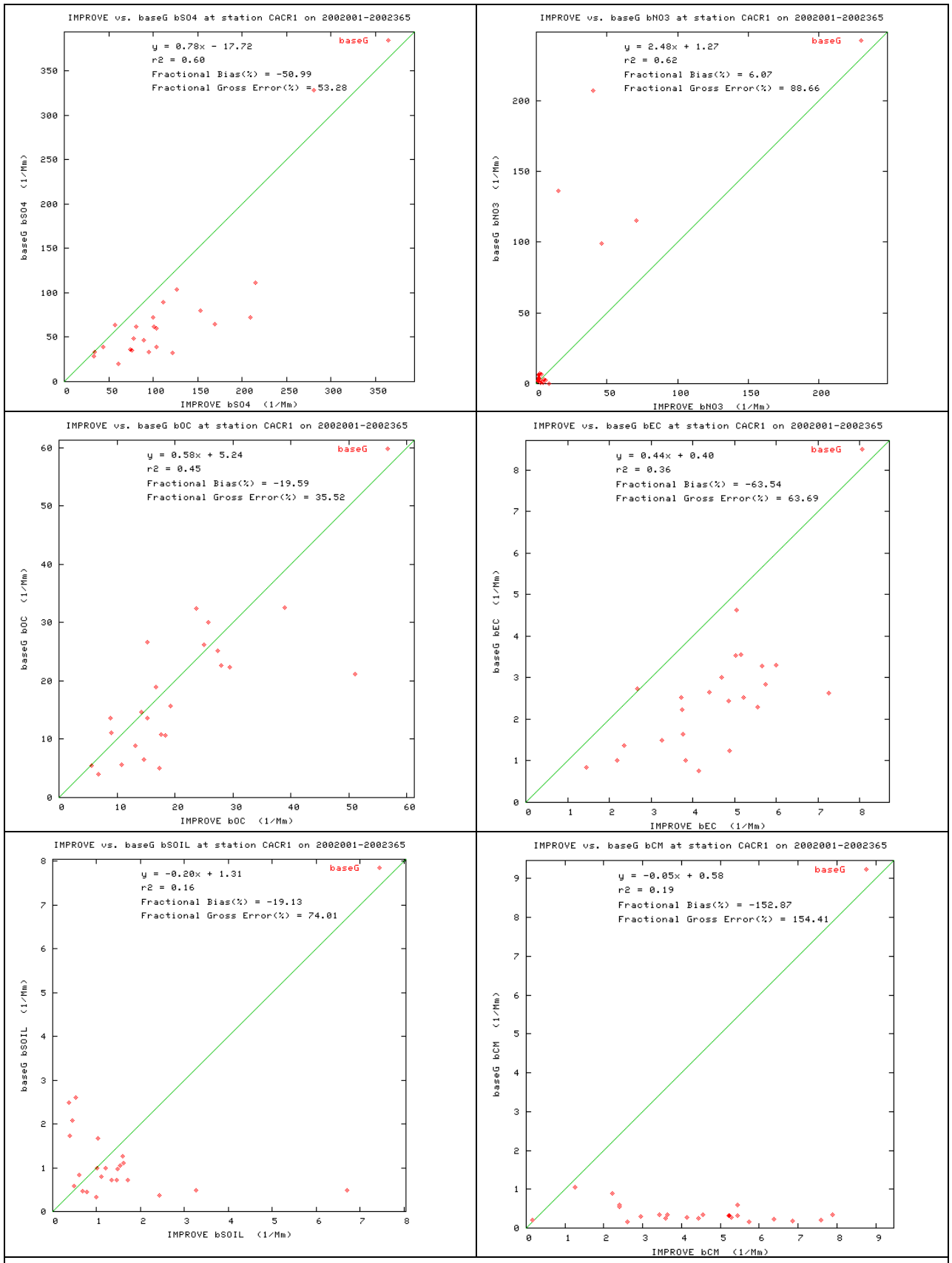


Figure C-48. PM species extinction model performance at Caney Creek (CACR) for the worst 20 percent days during 2002.

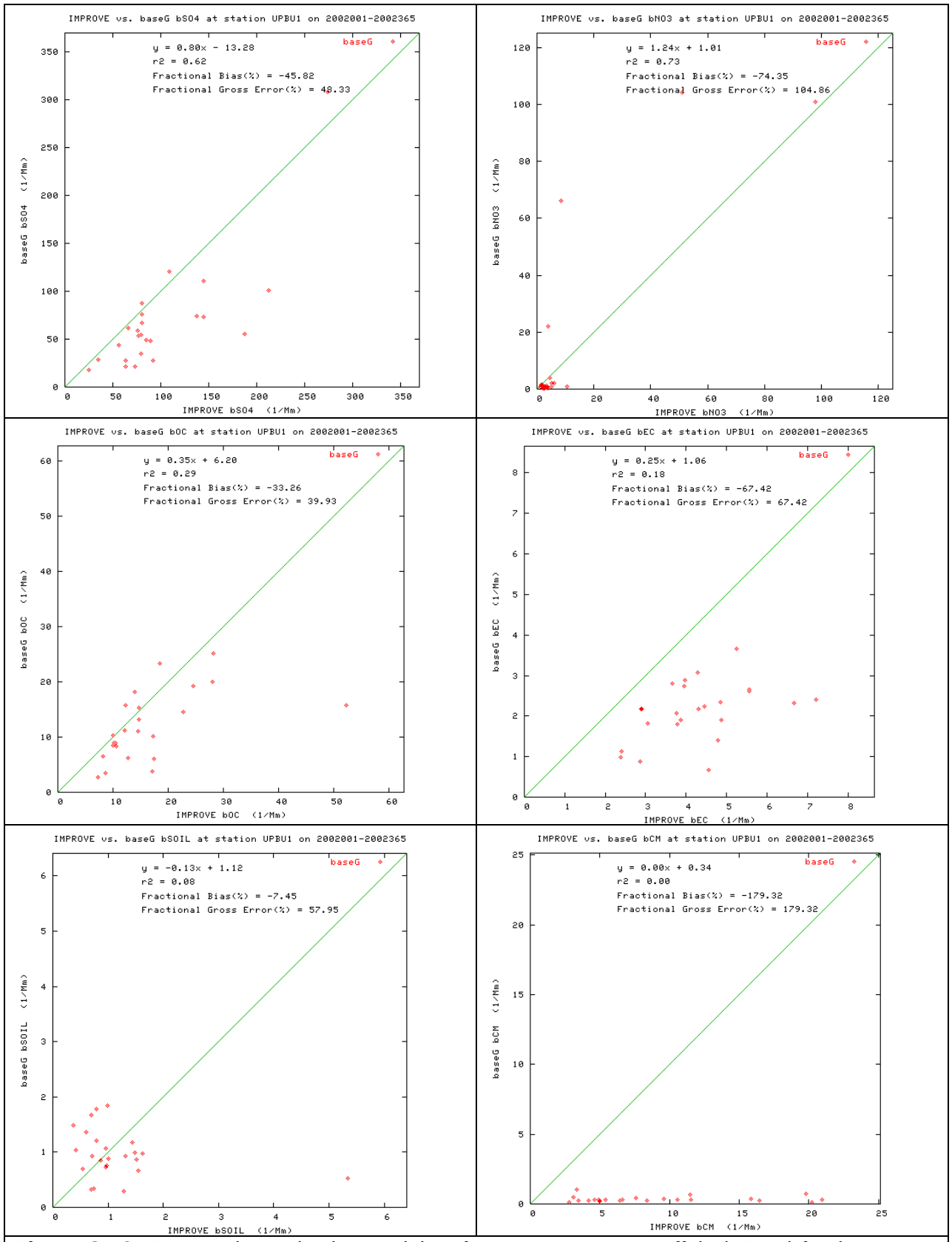


Figure C-49. PM species extinction model performance at Upper Buffalo (UPBU) for the worst 20 percent days during 2002.

C.5.3 Breton Island (BRET), Louisiana

The observed total extinction on the worst 20 percent days at Breton Island is underestimated by -71% (Figure 3-11), which is due to an underestimation of each component of extinction (Figure C-50) by from -50% to -70% (SO4, OMC and Soil) to over -100% (EC and CM). The observed extinction on the worst 20 percent days ranges from 90 to 170 Mm^{-1}, whereas the modeled values drop down to as low as approximately 15 Mm^{-1}. On the best 20 percent days the range of the observed and modeled extinction is similarly (roughly 10 to 50 Mm^{-1}) that results in a reasonably low bias (-22%), but there is little agreement on which days are higher or lower resulting in a lot of scatter and high error (54%).

C.5.4 Boundary Waters (BOWA), Minnesota

There are three types of days during the worst 20 percent days at BOWA, SO4 days, OMC days and NO3 days (Figure 3-12). The two high OMC days are likely fire impact events that the model captures to some extent on one day and not on the other. On the five high (> 20 Mm^{-1}) NO3 extinction days the model predicts the observed extinction well on three days and overestimates by a factor of 3-4 on the other two high NO3 days. SO4 in underestimate by -43% on average across the worst 20 percent days at BOWA.

With the exception of two days, the model reproduces the total extinction for the best 20 percent days at BOWA quite well with a bias and error value of +14% and 22% (Figure 3-12). Without these two days, the modeled and observed extinction both range between 15 and 25 Mm^{-1}.

C.5.5 Voyageurs (VOYA) Minnesota

VOYA is also characterized by SO4, NO3 and OMC days (Figure 3-13). Julian Days 179 and 200 are high OMC days that were also high OMC days at BOWA again indicating impacts from fires in the area that is not fully captured by the model. SO4 and NO3 extinction is fairly good and, without the fire days, OMC performance looks good as well (Figure C-52). On the best 20 percent days there is one day the modeled extinction is much higher than observed and a few others that are somewhat higher, but for most of the best 20 percent days the modeled extinction is comparable to the observed values.

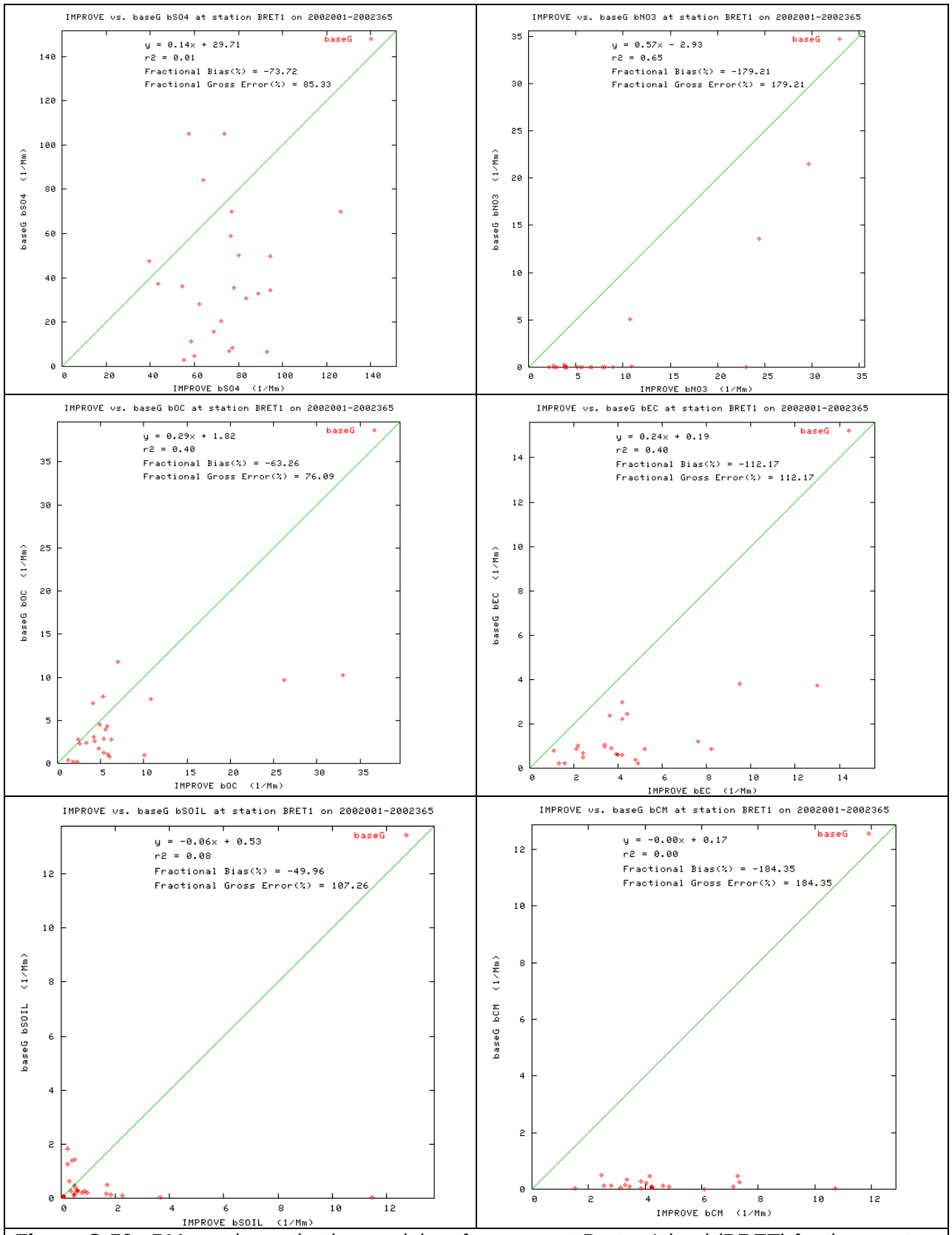


Figure C-50. PM species extinction model performance at Breton Island (BRET) for the worst 20 percent days during 2002.

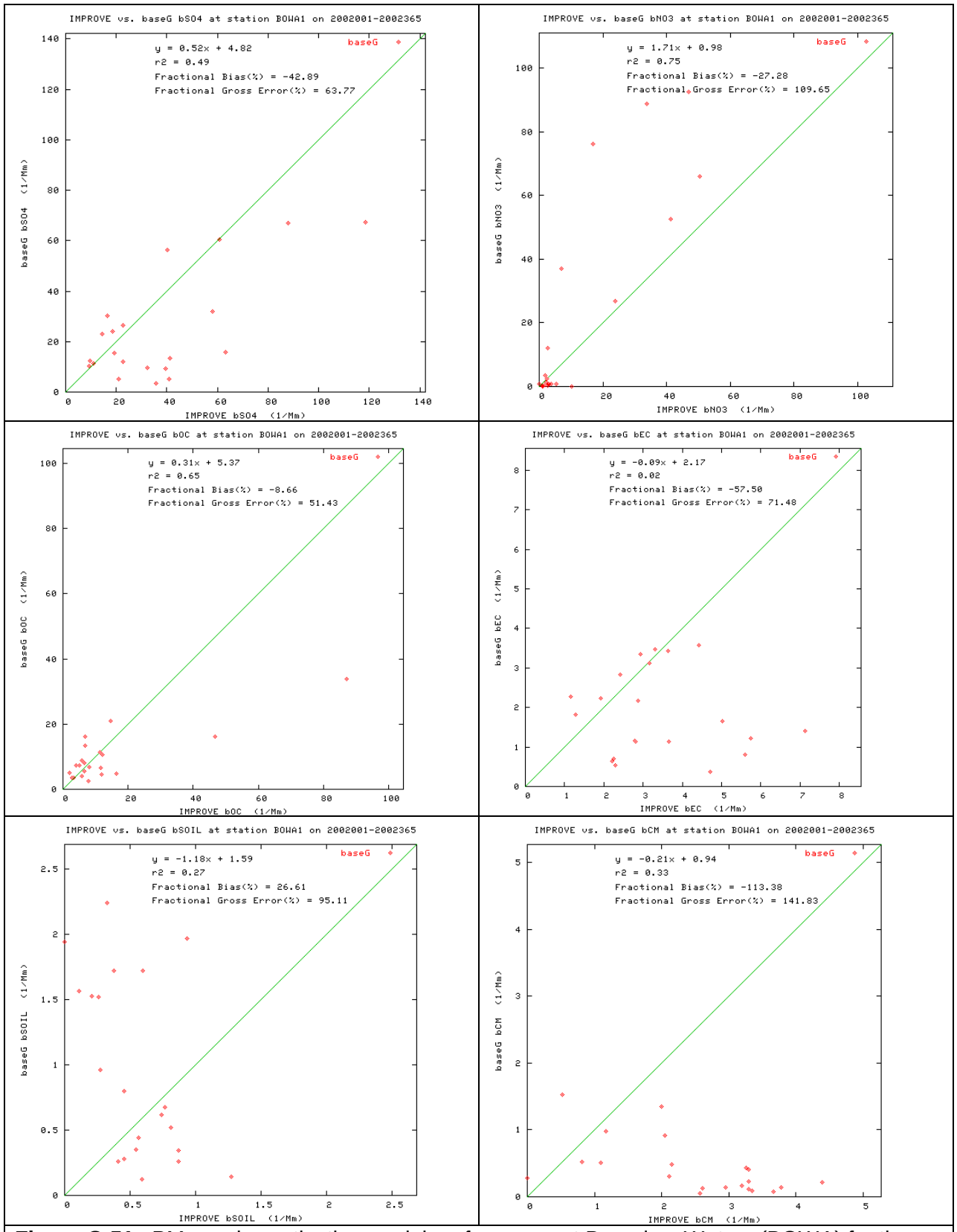


Figure C-51. PM species extinction model performance at Boundary Waters (BOWA) for the worst 20 percent days during 2002.

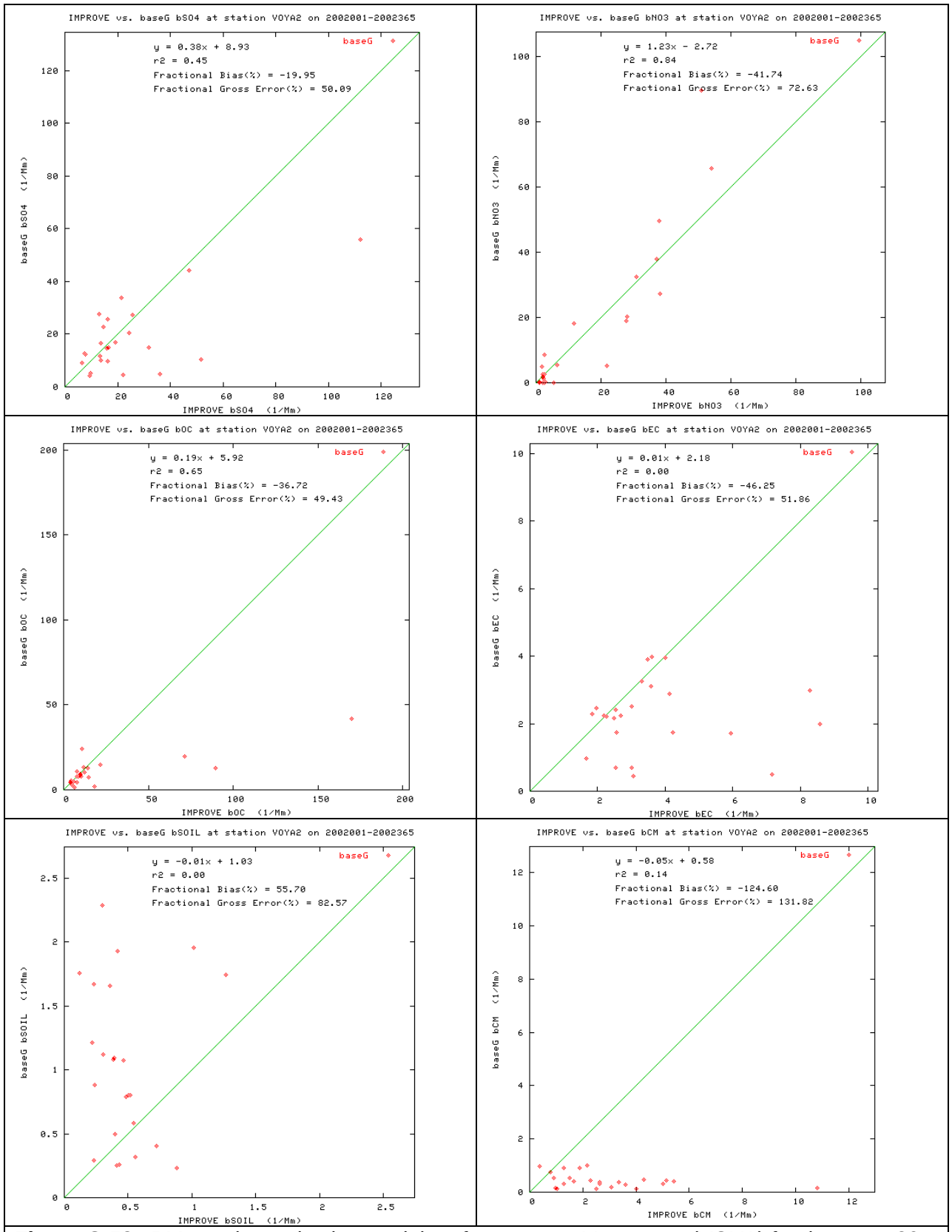


Figure C-52. PM species extinction model performance at Voyageurs (VOYA) for the worst 20 percent days during 2002.

C.5.6 Hercules Glade (HEGL) Missouri

On most of the worst 20 percent days at HEGL the observed extinction ranges from 120 to 220 Mm^{-1} whereas model extinction ranging from 50 to 170 Mm^{-1} (Figure 3-14). However, there is one extreme day with extinction approaching 400 Mm^{-1} that the model does a very good job in replicating. Over all the days there is a modest underestimation bias in SO4 (-39%) and OMC (-39%) extinction, larger underestimation bias in EC (-62%) and CM (-118%) extinction and overestimation bias in Soil (+30%) extinction (Figure C-53).

On the best 20 percent days there is one day where the model overstates the observed extinction by approximately a factor of four and a handful of other days that the model overstates the extinction by a factor of 2 or so, but most of the days both the model and observed extinction sites are around 40 Mm^{-1} plus or minus about 10 Mm^{-1}. On the best 20 percent days when the observed extinction is overstated it is due to overstatement of the NO3.

C.5.7 Mingo (MING) Missouri

The worst 20 percent days at Ming are mainly high SO4 days with a few high NO3 days that the model reproduces reasonably well resulting in low bias (+10%) and error (38%) for total extinction (Figure 3-15). The PM species specific performance is fairly good with low bias for SO4 (+4%), good agreement with NO3 on high NO3 days except for one day, low OMC (+23%) and EC (+3%) bias and larger bias in EC (+37%) and CM (-105%) extinction (Figure C-54).

For the best 20 percent days, there is one day the model is way to high due to overstated NO3 extinction and a few other days the model overstates the observed extinction that is usually due to overrated NO3, but on most of the best 20 percent days the modeled extinction is comparable to the observed values. This results in low bias (+12%) and error (36%) for total extinction at MING for the best 20 percent days.

C.5.8 Wichita Mountains (WIMO), Oklahoma

With the exception of an over-prediction on day 344 due to NO3, observed total extinction on the worst 20 percent days at WIMO is understated with a bias of -42% (Figure 3-16) that is primarily due to an underestimation of extinction due to SO4 (-48%) and OMC (-69%) (Figure C-55).

CMAQ total extinction performance for the average of the best 20 percent days at WIMO is characterized by an overestimation bias (+21%) on most days that is primarily due to NO3 over-prediction on several days. Again the modeled range of extinction on the best 20 percent days (12-60 Mm^{-1}) is much greater than observed (20-35 Mm^{-1}).

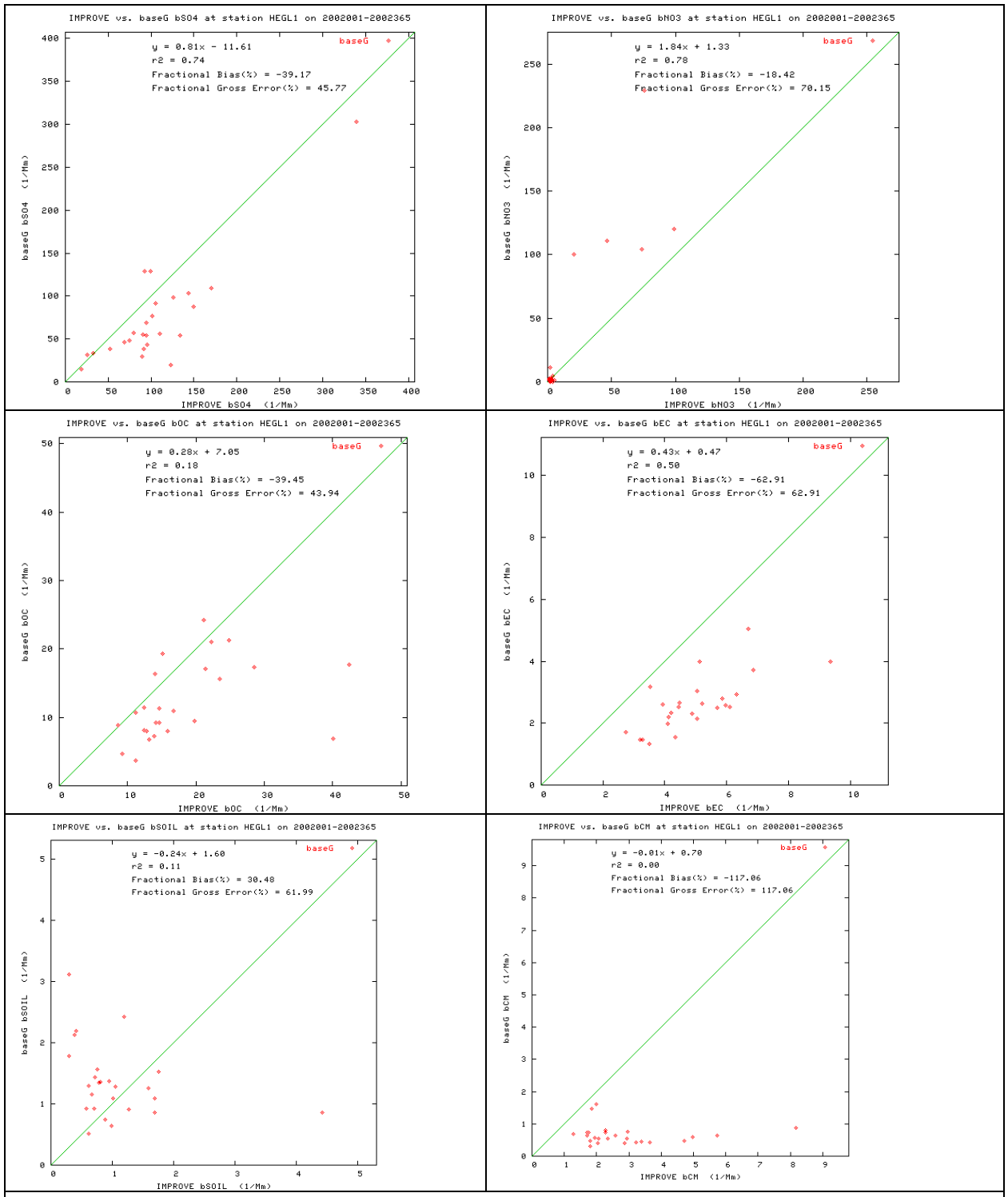


Figure C-53. PM species extinction model performance at Hercules Glade (HEGL) for the worst 20 percent days during 2002.

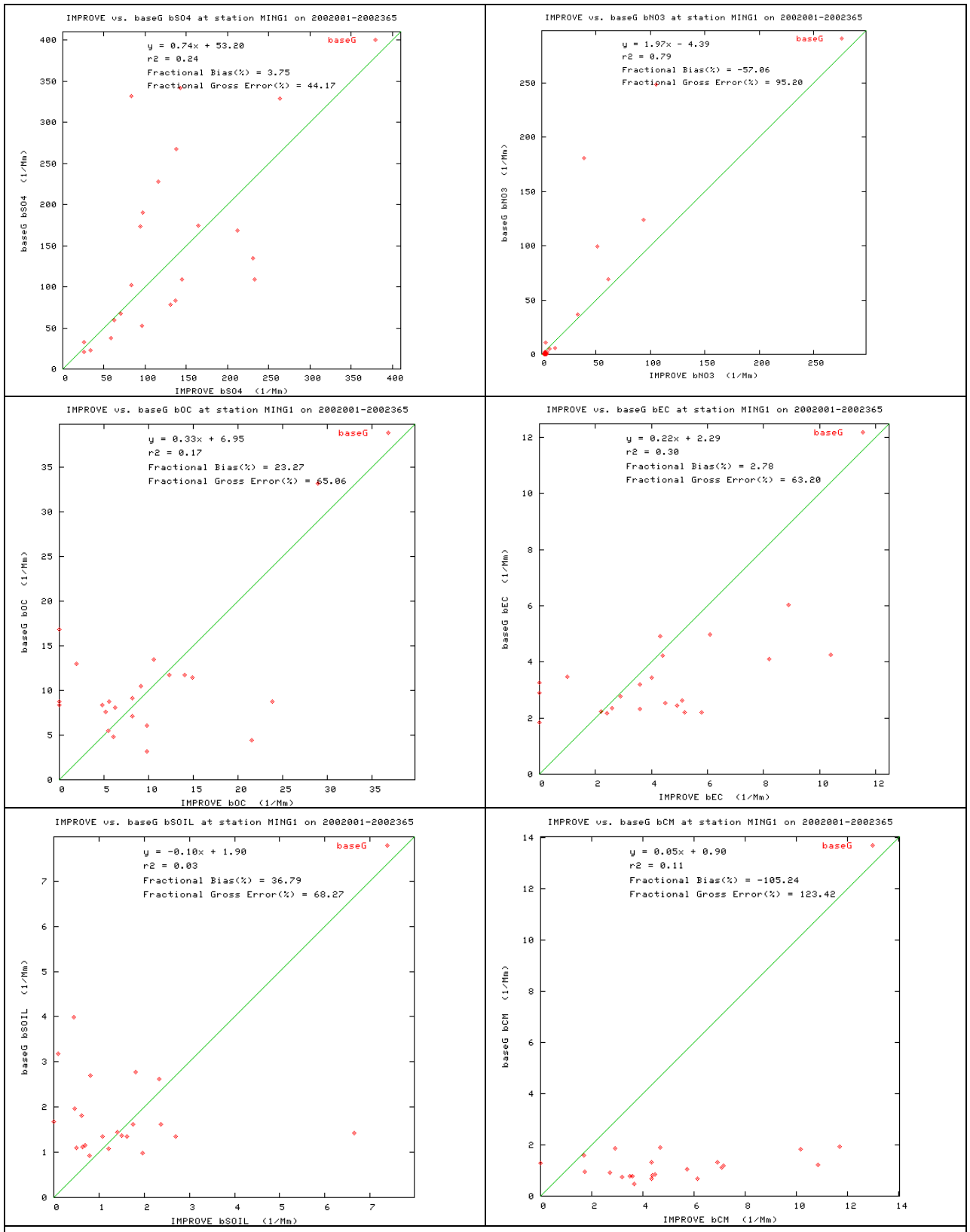


Figure C-54. PM species extinction model performance at Mingo (MING) for the worst 20 percent days during 2002.

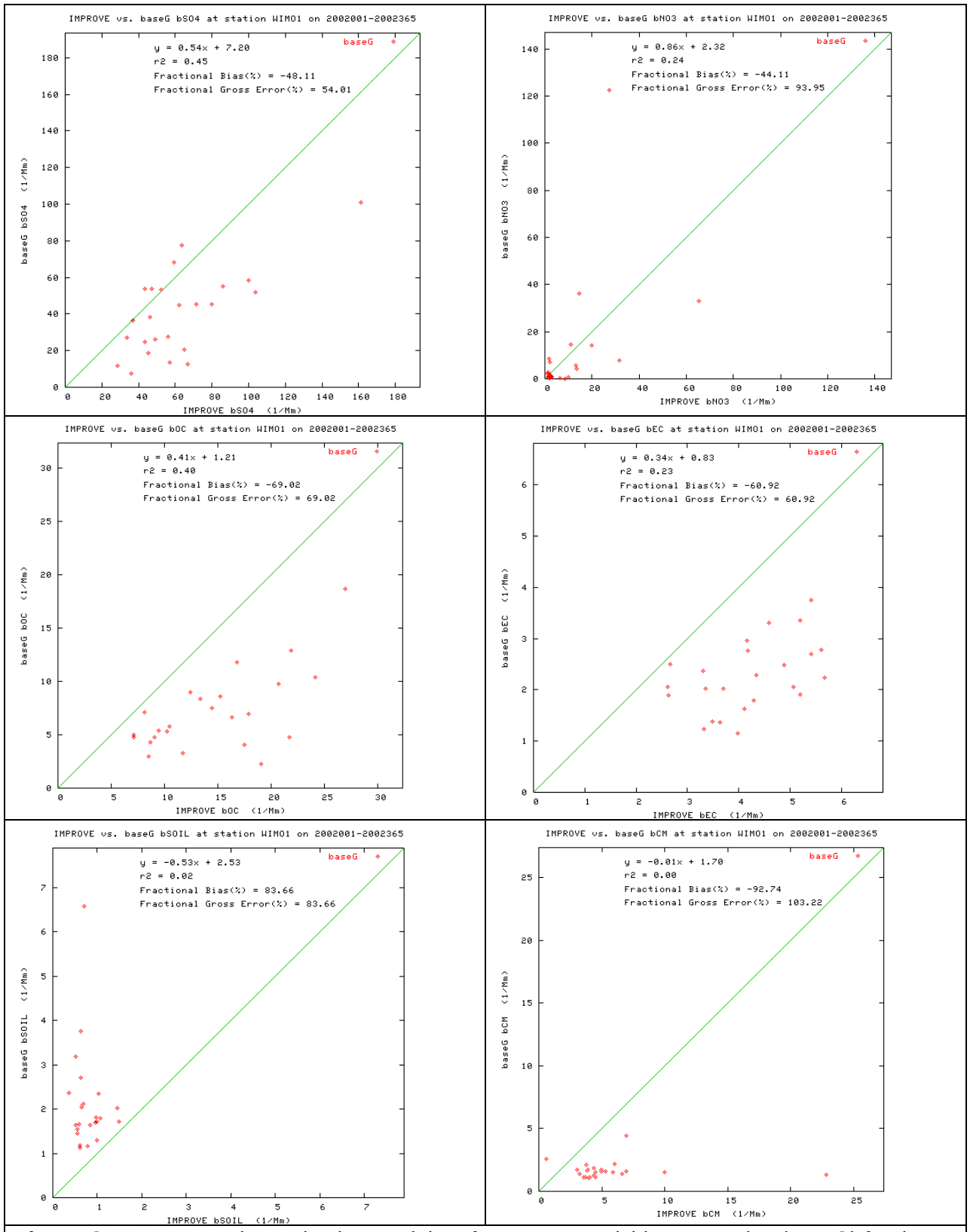


Figure C-55. PM species extinction model performance at Wichita Mountains (WIMO) for the worst 20 percent days during 2002.

C.5.9 Big Bend (BIBE) Texas

The observed extinction on the worst 20 percent days at BIBE is under-predicted on almost every day resulting in a fractional bias value of -72% (Figure 3-17). Every component of extinction is underestimated on average for the worst 20 percent days (Figure C-56) with the underestimation bias ranging from -24% (OMC) to -162% (CM). SO4 extinction, that typically represents the largest component of the total extinction is understated by -94%.

The model does a better job in predicting the total extinction at BIBE for the best 20 percent days with average fractional bias and error values of +13% and 19% (Figure 3-17). With the exception of one day that the observed extinction is overestimated by approximately a factor of 2, the modeled and observed extinction on the best 20 percent days at BIBE are both within 12 to 25 Mm^{-1}. However, there are some mismatches with the components of extinction with the model estimating much lower contributions due to Soil and CM.

C.5.10 Guadalupe Mountains (GUMO) Texas

Most of the worst 30 percent days at GUMO are dust days with high Soil and CM that is not at all captured by the model (Figure 3-18). Extinction due to Soil and CM on the worst 20 percent days is underestimated by -105% and -191%, respectively (Figure C-57). Better performance is seen on the best 20 percent days with bias and error for total extinction of 8% and 21%, but the model still understates Soil and CM.

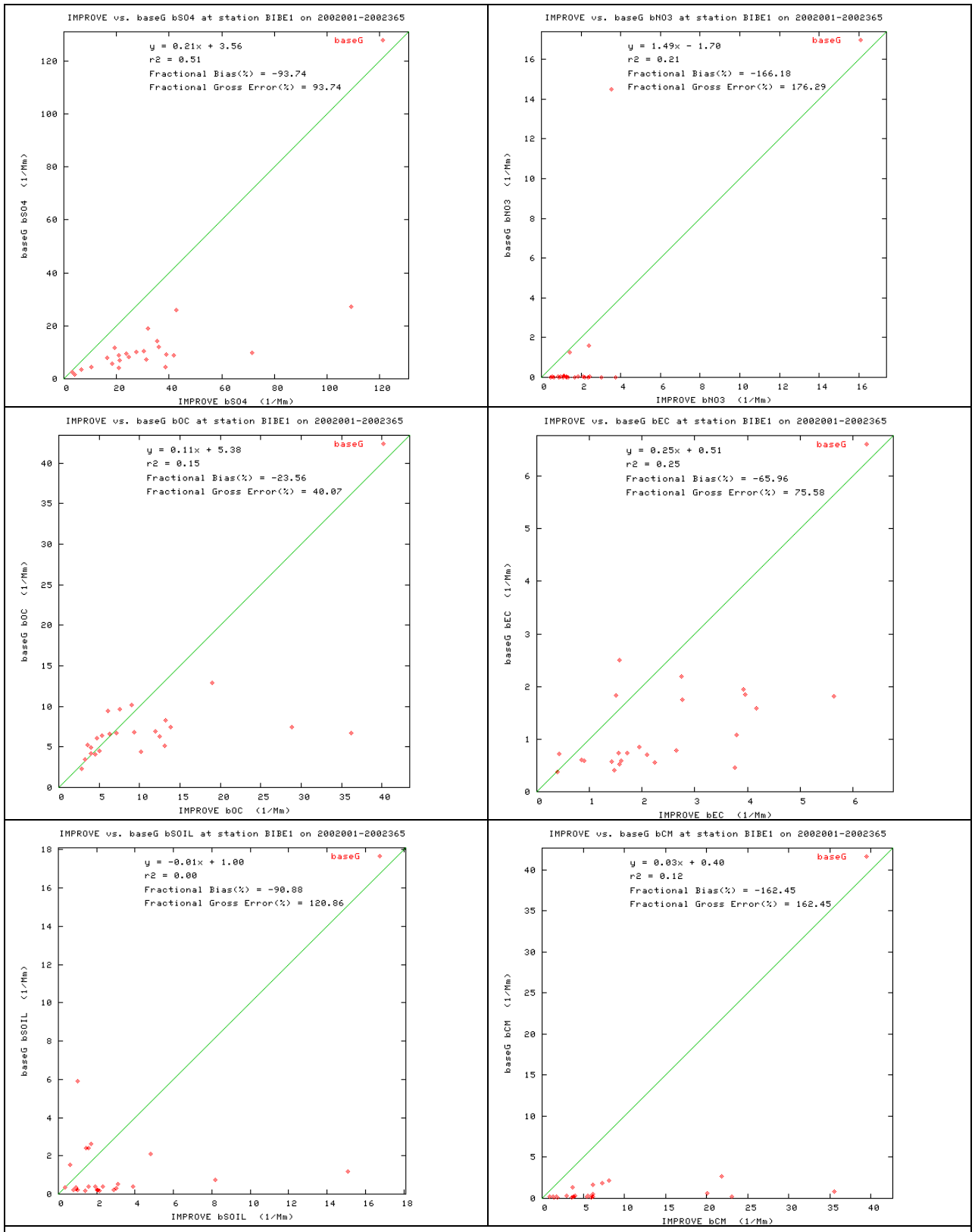


Figure C-56. PM species extinction model performance at Big Bend (BIBE) for the worst 20 percent days during 2002.

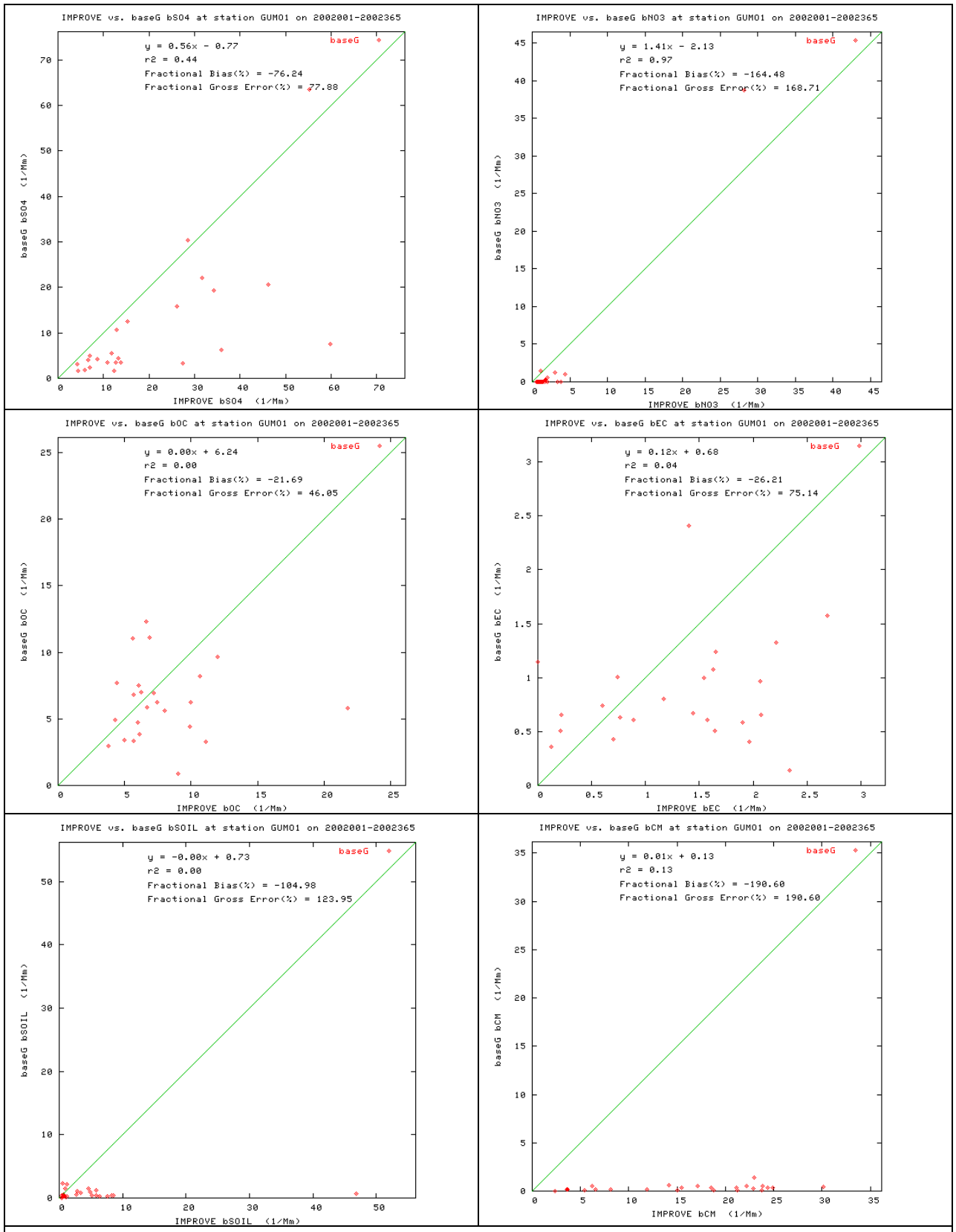


Figure C-57. PM species extinction model performance at Guadalupe Mountains (GUMO) for the worst 20 percent days during 2002.

C.6 Model Performance Evaluation Conclusions

The model performance evaluation reveals that the model is performing best for SO4, OMC and EC. Soil performance is mixed with winter overestimation bias but lower bias but high error in the summer. CM performance is poor year round. The operational evaluation reveals that SO4 performance usually achieves the PM model performance goal and always achieves the model performance criteria, although it does have an underestimation bias that is greatest in the summer. NO3 performance is characterized by a winter overestimation bias with an even greater summer underestimation bias. However, the summer underestimation bias occurs when NO3 is very low and it is not an important component of the observed or predicted PM and visibility impairment. Performance for OMC meets the model performance goal year round at the IMPROVE sites, but is characterized by an underestimation bias at the more urban STN sites. EC exhibits very low bias at the STN sites and a summer underestimation bias at the IMPROVE sites, but meets the model performance goal throughout the year. Soil has a winter overestimation bias that exceeds the model performance goal and criteria raising questions whether the model should be used for this species. Finally, CM performance is extremely poor with an under-prediction bias that exceeds the performance goal and criteria. We suspect that much of the CM concentrations measured at the IMPROVE sites is due to highly localized emissions that can not be simulated with 36 km regional modeling.

Performance for the worst 20 percent days at the CENRAP Class I areas is generally characterized by an underestimation bias. Performance at the BRET, BIBE and GUMO Class I areas for the worst 20 percent days is particularly suspect and care should be taken in the interpretation of the visibility projections at these three Class I areas.

The CMAQ 2002 36 km model appears to be working well enough to reliably make future-year projections for changes in SO4, NO3, EC and OMC at the rural Class I areas. Performance for Soil and especially CM is suspect enough that care should be taken in interpreting these modeling results. The model evaluation focused on the model's ability to predict the components of light extinction mainly at the Class I areas. Additional analysis would have to be undertaken to examine the model's ability to treat ozone and fine particulate to address 8-hour ozone and $PM_{2.5}$ attainment issues.