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).

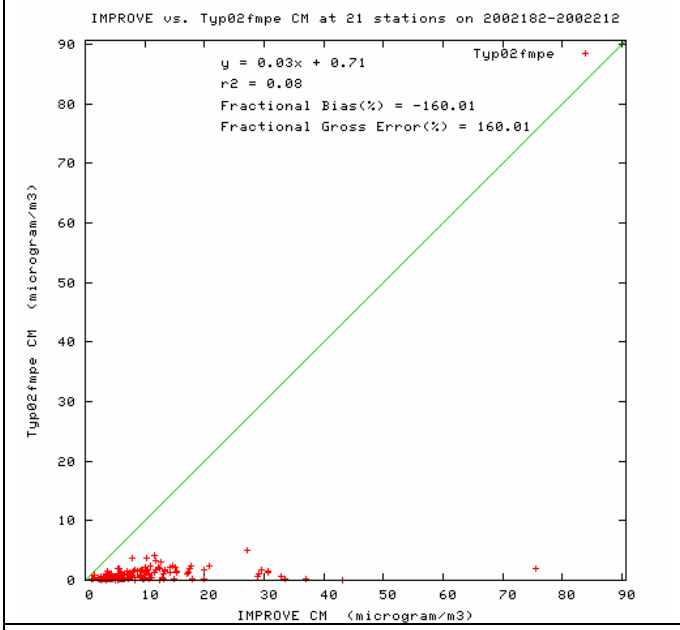
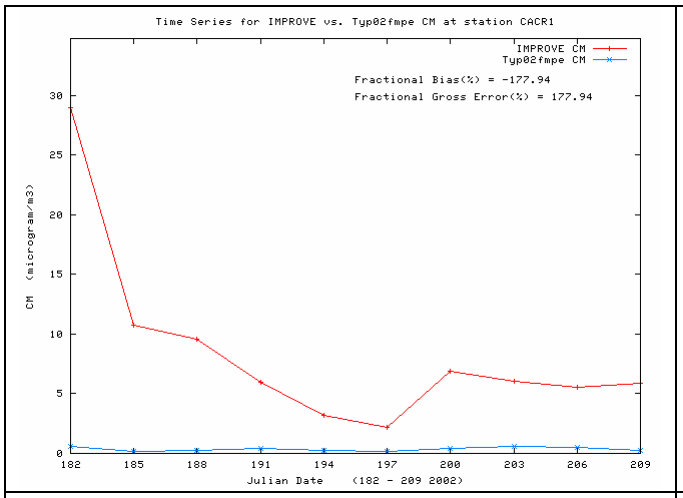
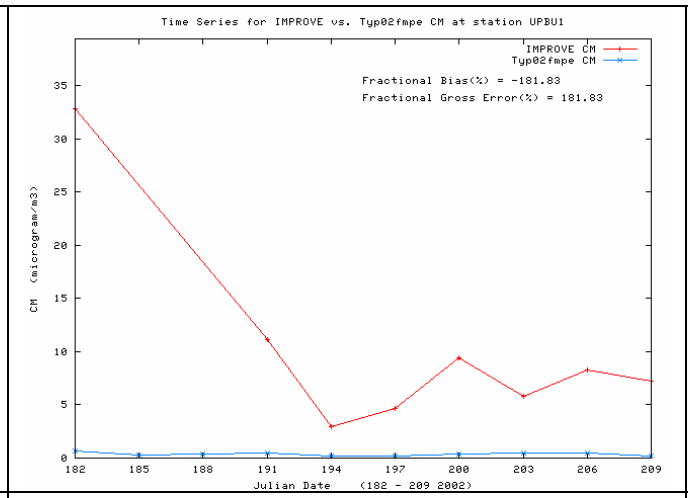
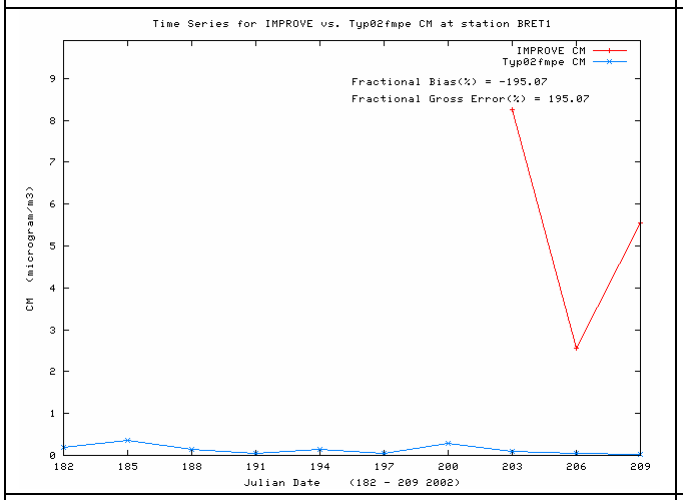
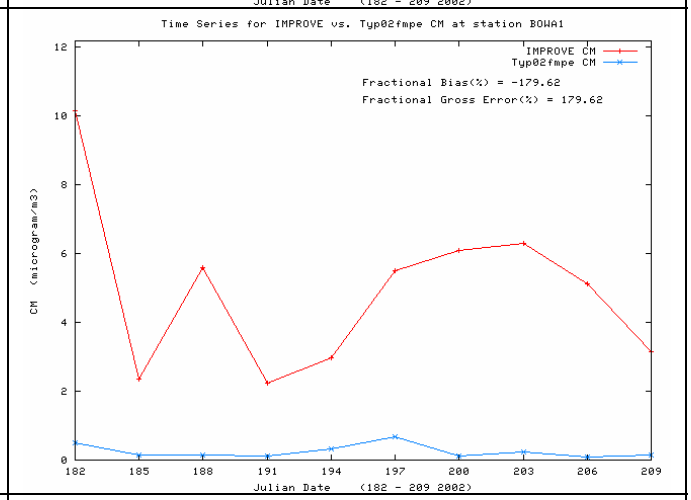


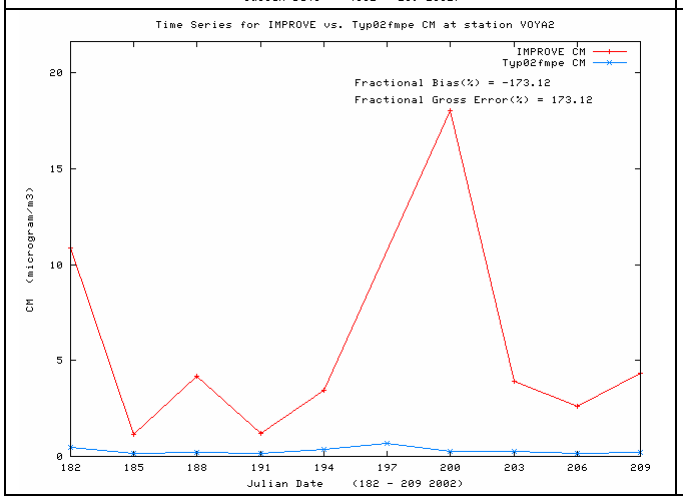
Figure C-36a. Scatter plots of predicted and observed coarse mass (CM) concentrations for July 2002 and sites in the CENRAP region using IMPROVE monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

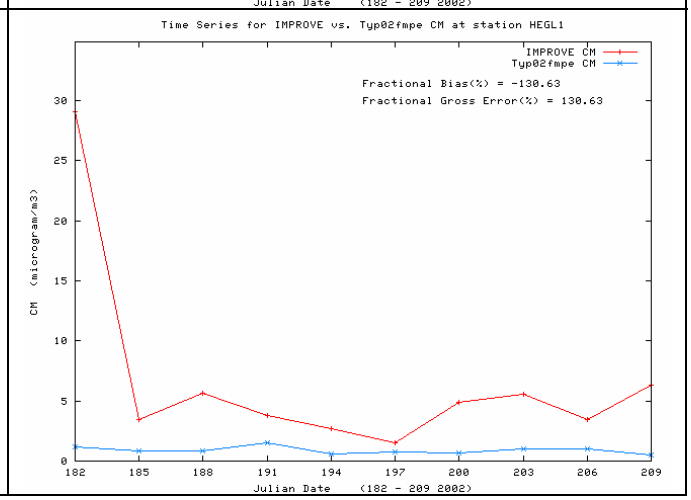

Time Series for IMPROVE vs. Typ02fmpe CM at station CACR1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -177.94
Fractional Gross Error(%) = 177.94
CM (microgram/m3)
Julian Date (182 - 209 2002)


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)

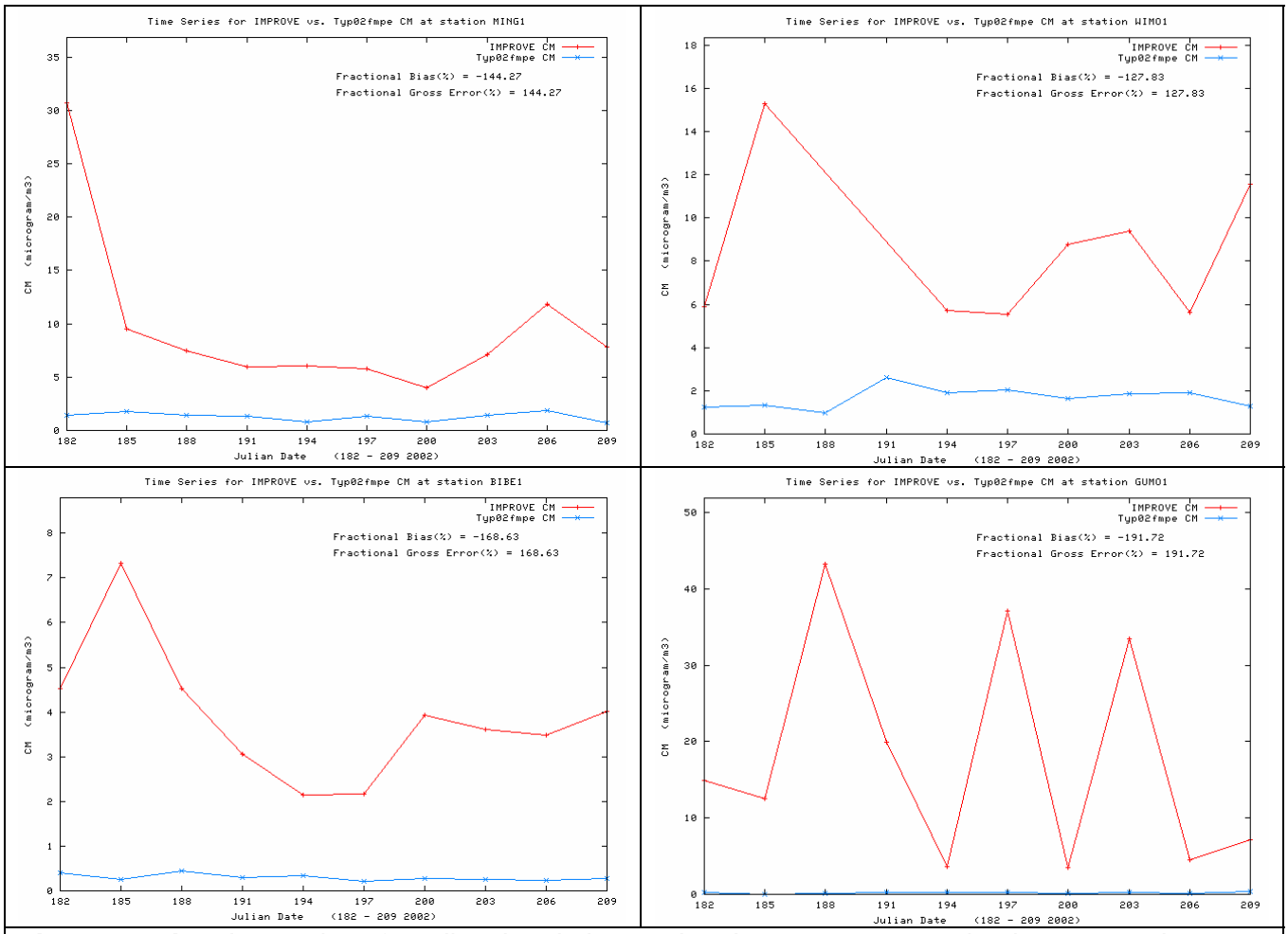


Figure C-36b. Time series of predicted and observed 24-hour coarse mass (CM) concentrations at CENRAP IMPROVE CLASS I AREA sites in July 2002 for CMAQ 2002 36 km Base F base case simulation.

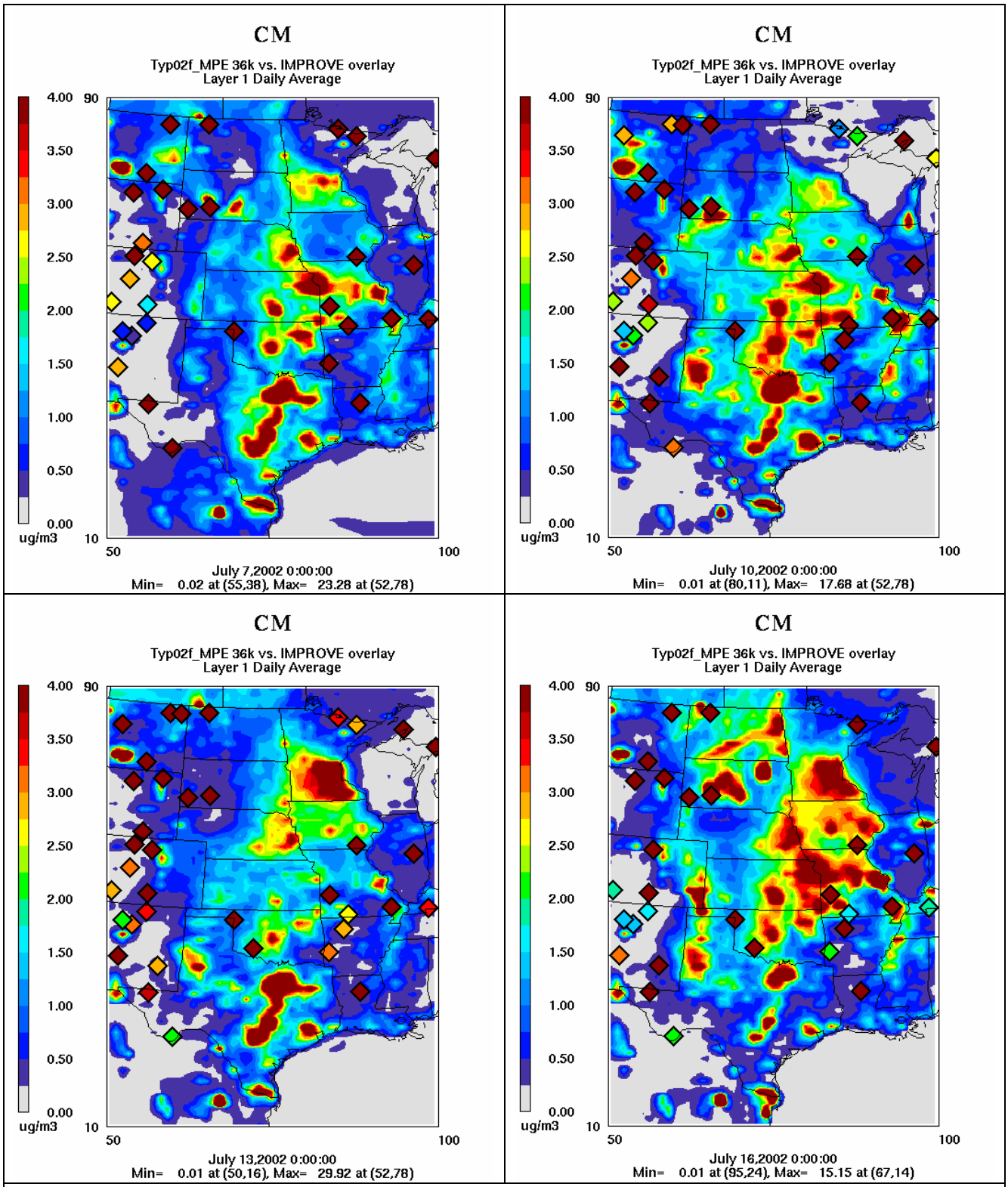


Figure C-36c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour CM concentrations for July 7, 10, 13 and 16, 2002.

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).

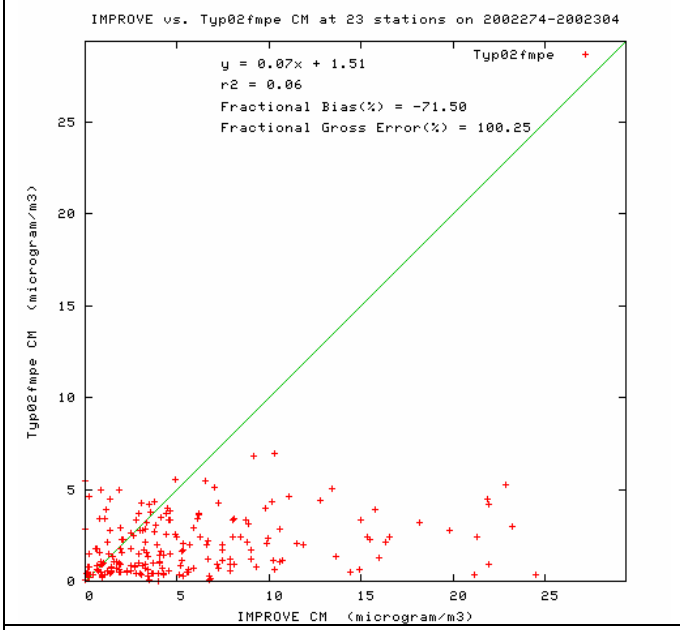
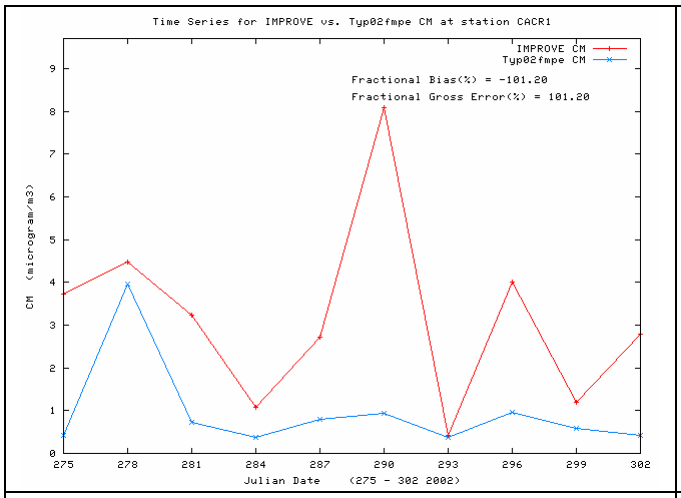
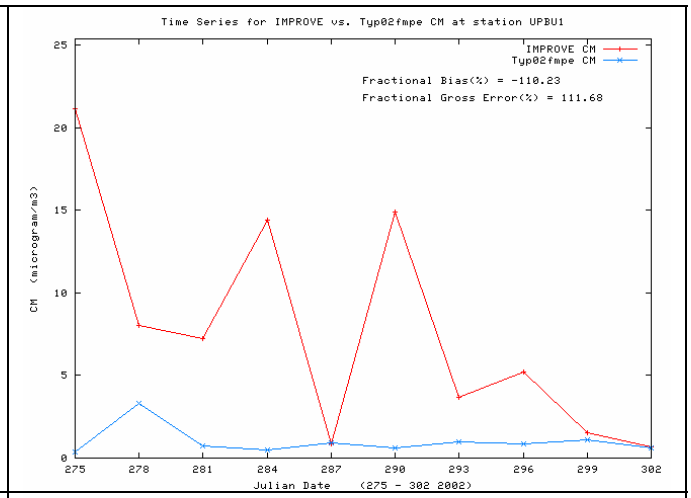
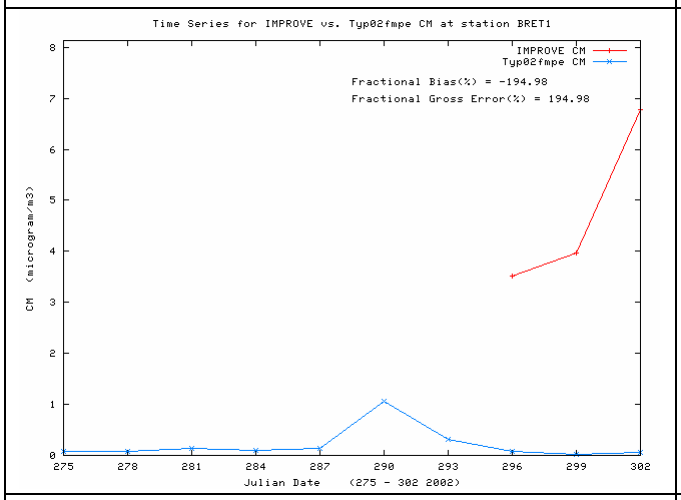
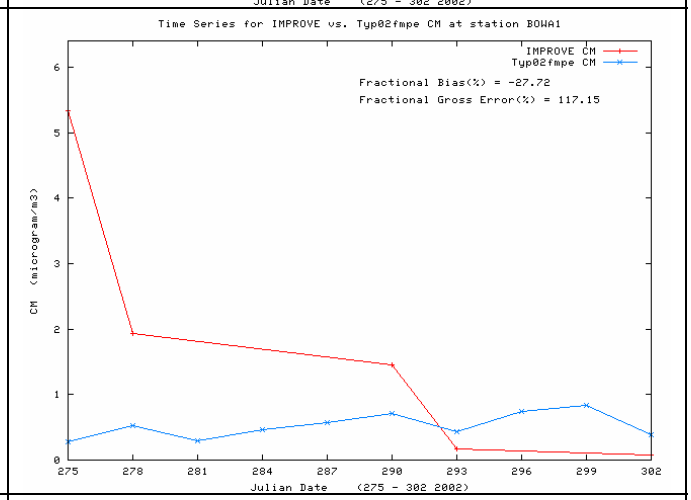


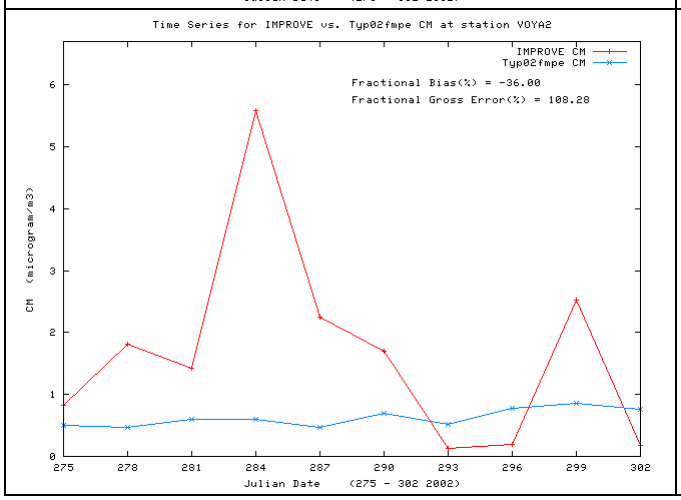
Figure C-37a. Scatter plots of predicted and observed coarse mass (CM) concentrations for October 2002 and sites in the CENRAP region using IMPROVE monitoring networks using the CMAQ 2002 36 km Base F base case simulation.

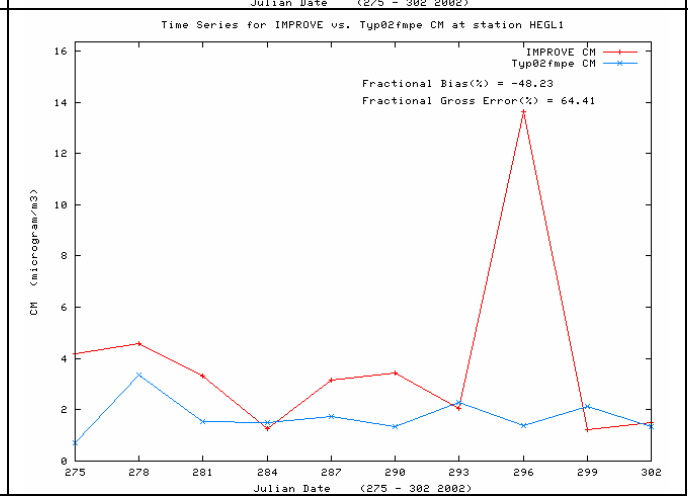

Time Series for IMPROVE vs. Typ02fmpe CM at station CACR1
IMPROVE CM
Typ02fmpe CM
Fractional Bias(%) = -101.20
Fractional Gross Error(%) = 101.20
CM (microgram/m3)
Julian Date (275 - 302 2002)


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)

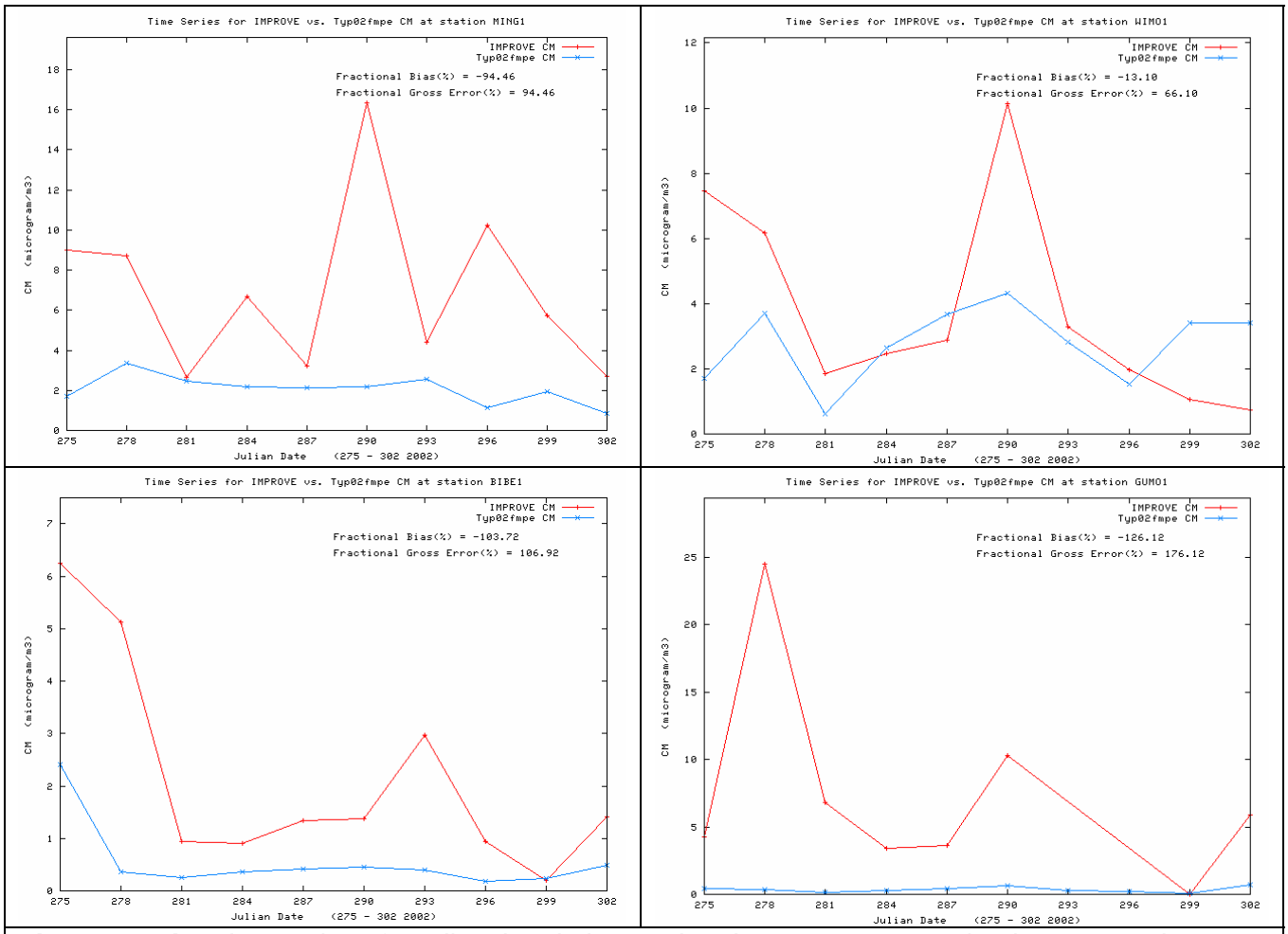


Figure C-37b. Time series of predicted and observed 24-hour coarse mass (CM) concentrations at CENRAP IMPROVE CLASS I AREA sites in October 2002 for CMAQ 2002 36 km Base F base case simulation.

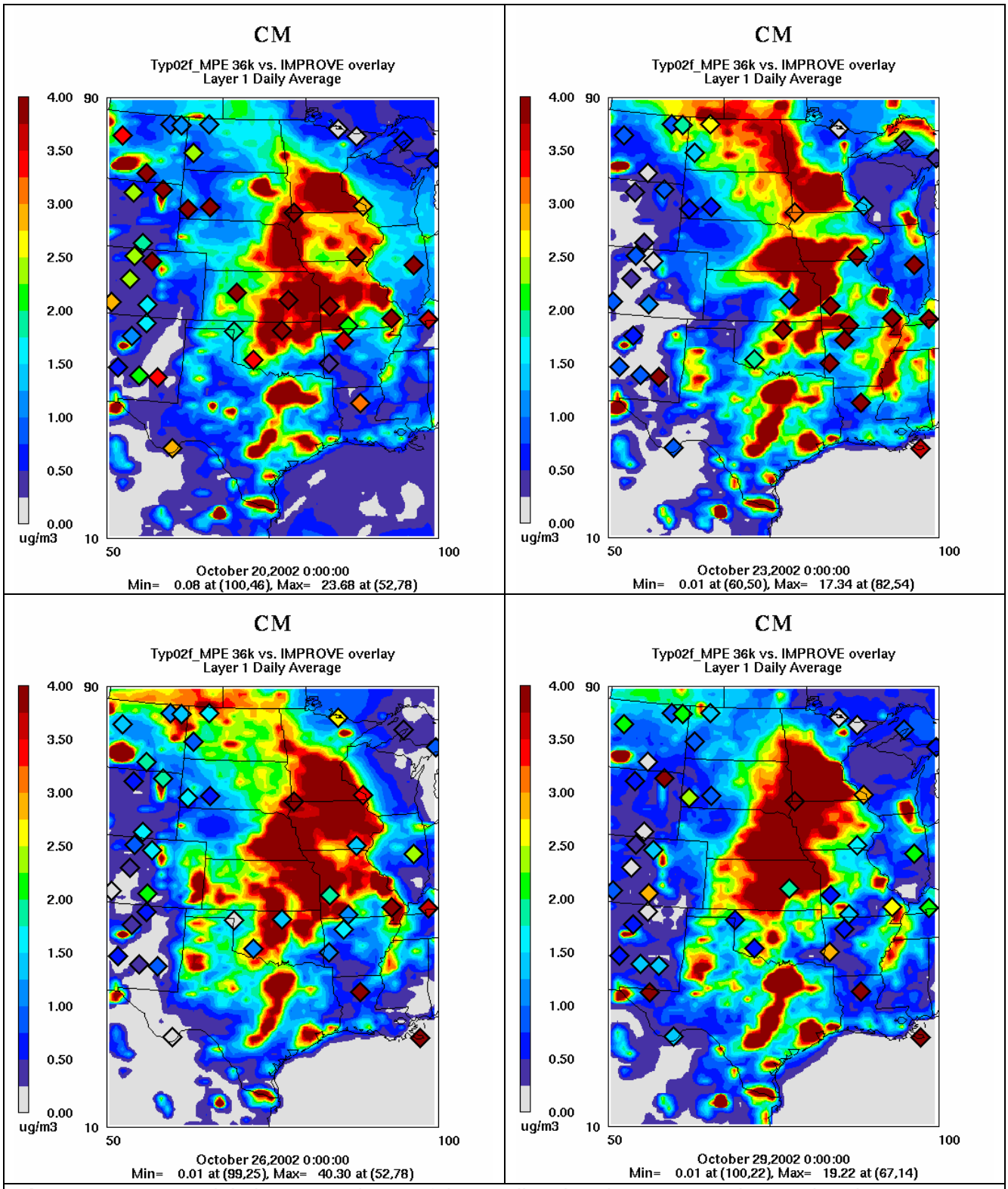


Figure C-37c. Spatial plot comparisons of the predicted and IMPROVE observed 24-hour CM concentrations for October 20, 23, 26 and 29, 2002.

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.

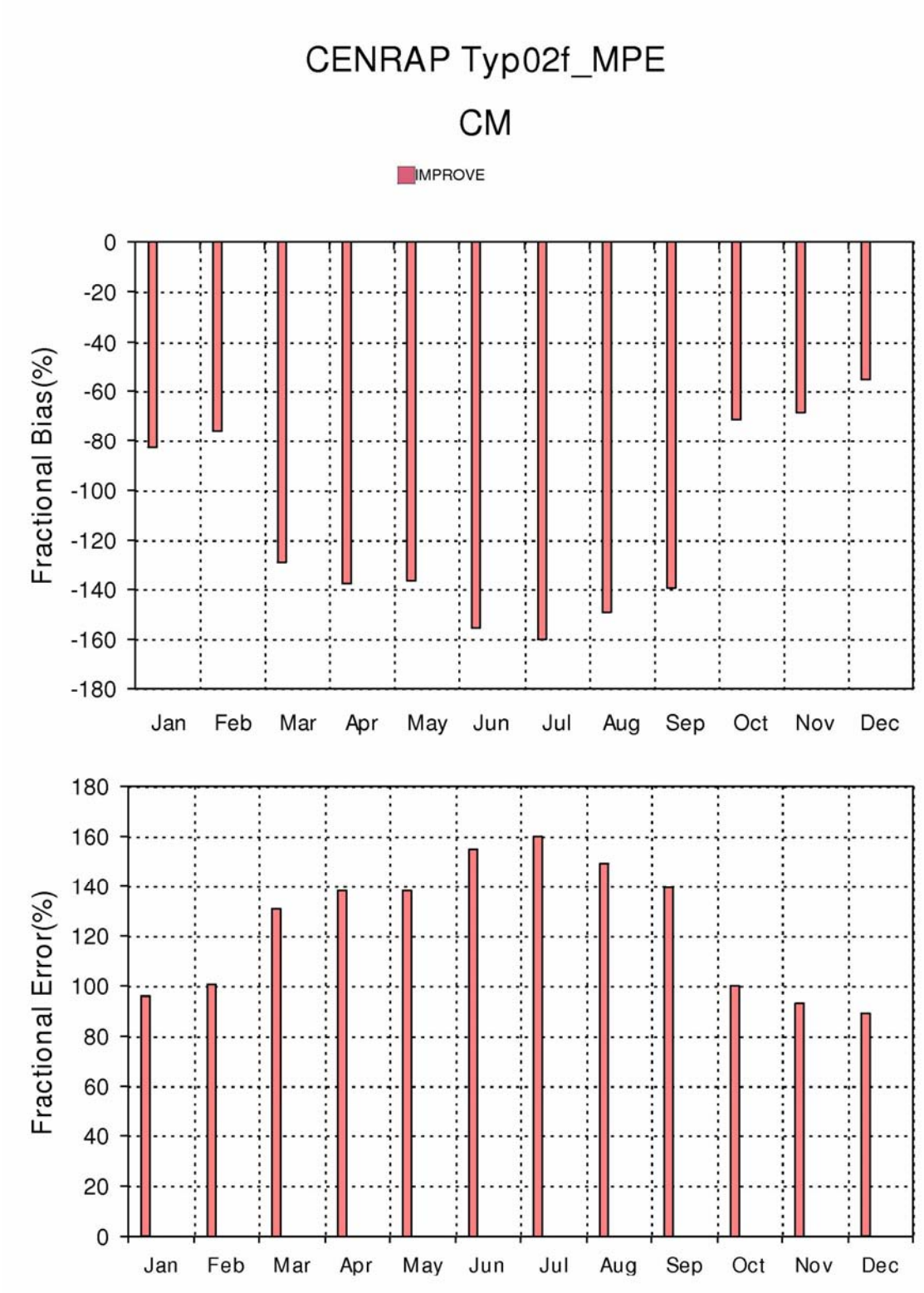


Figure C-38. Monthly CM fractional bias (top) and fractional gross error (bottom) statistical measures for IMPROVE monitoring sites in the CENRAP region.

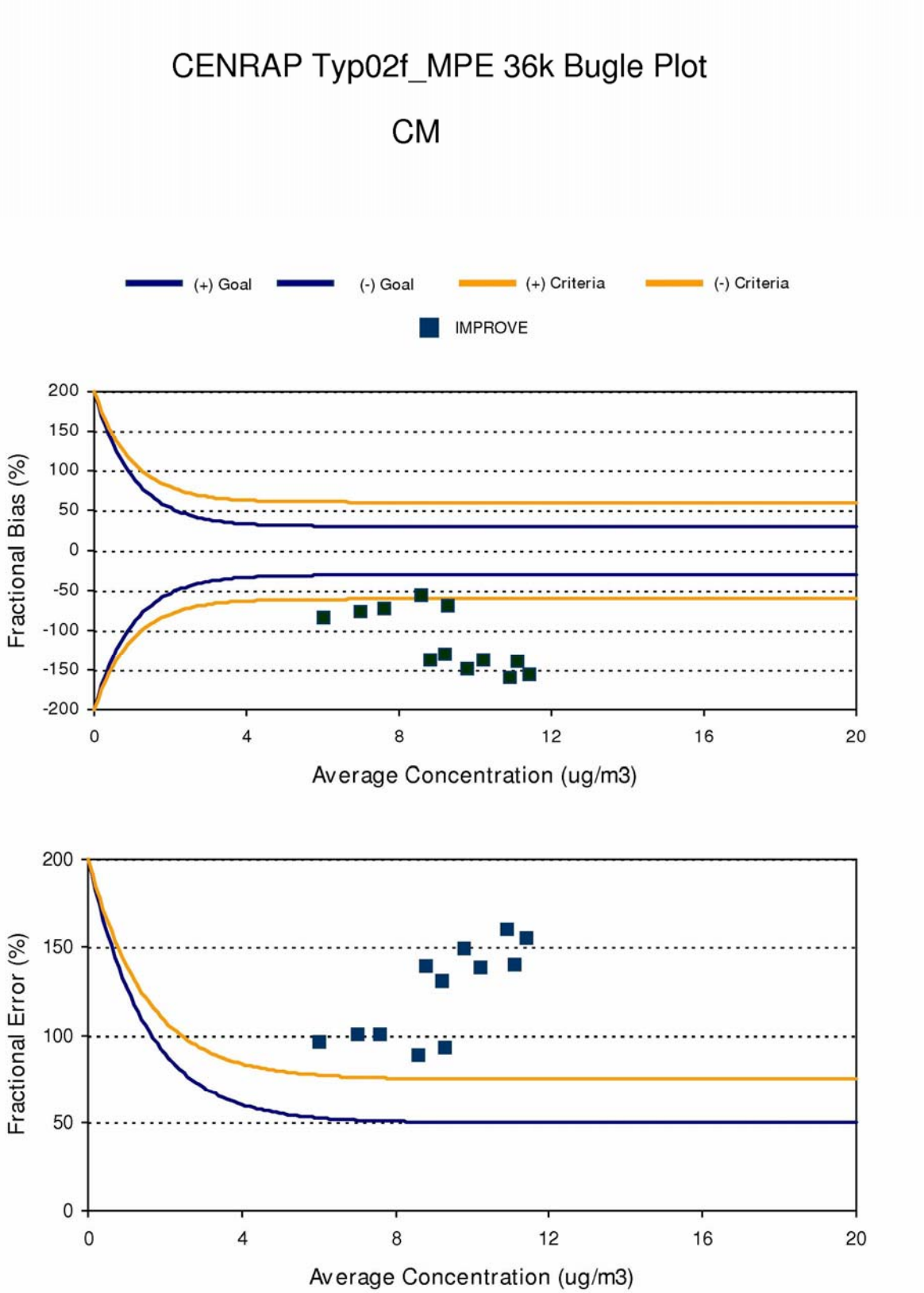


Figure C-39. Bugle Plots of monthly fractional bias (top) and fractional gross error (bottom) and comparisons with model performance goals and criteria for CM and IMPROVE monitoring sites in the CENRAP region.

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.

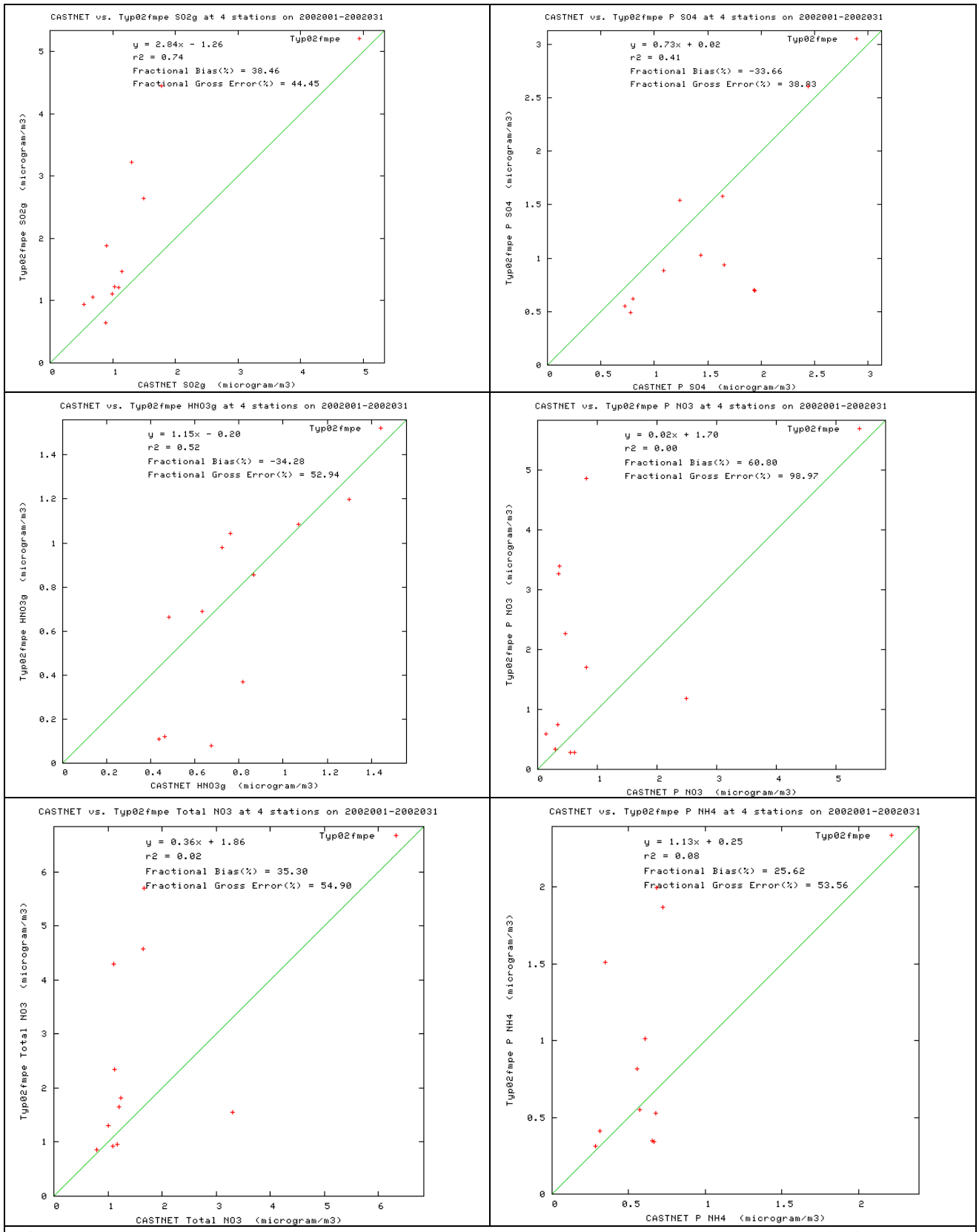


Figure C-40. January 2002 performance at CENRAP CASTNet sites for SO2 (top left), SO4 (top right), HNO3 (middle left), NO3 (middle right), Ttoal NO3 (bottom left) and NH4 (bottom right).

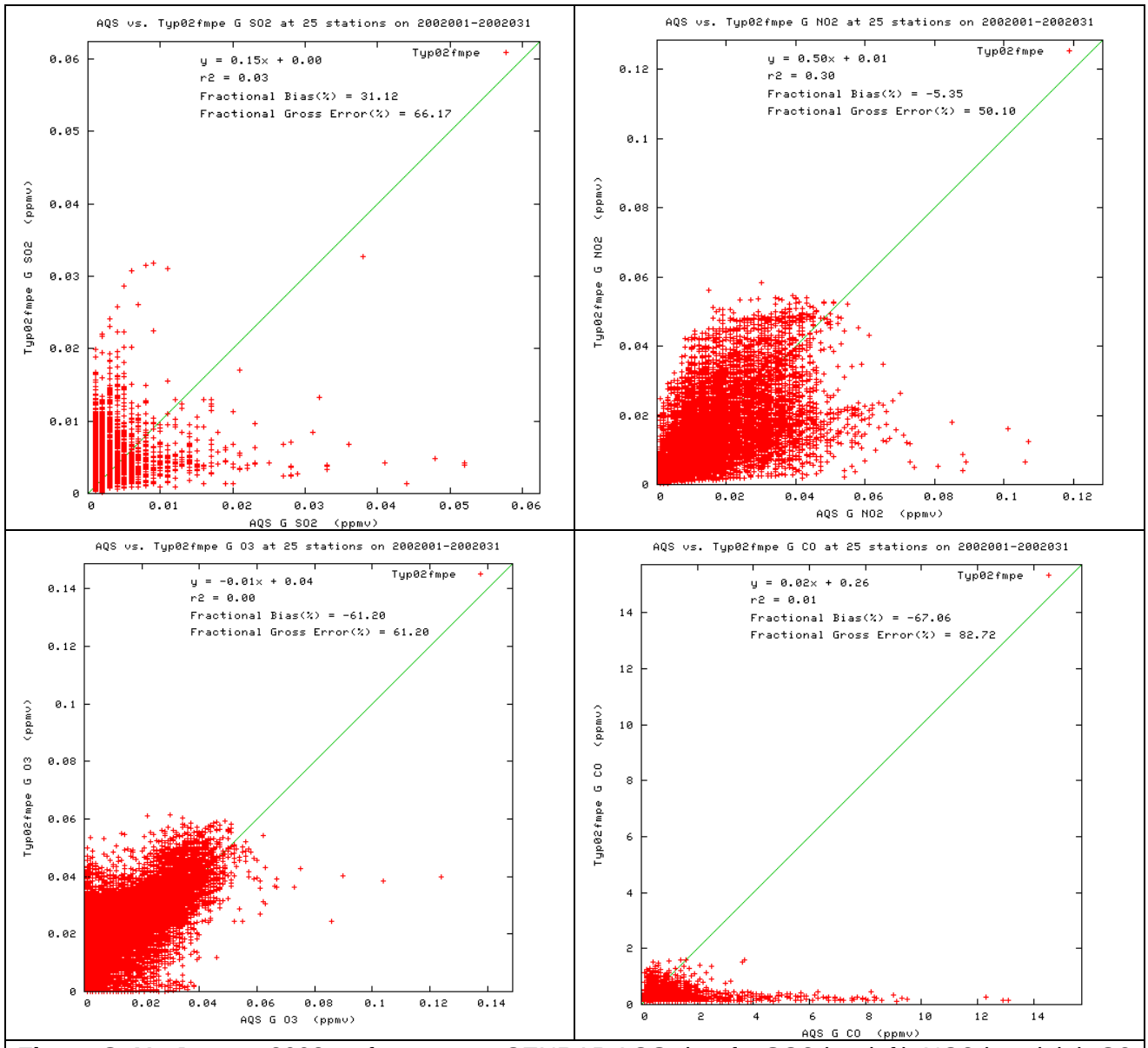


Figure C-41. January 2002 performance at CENRAP AQS sites for SO2 (top left), NO2 (top right), O3 (bottom left) and CO (bottom right).

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.

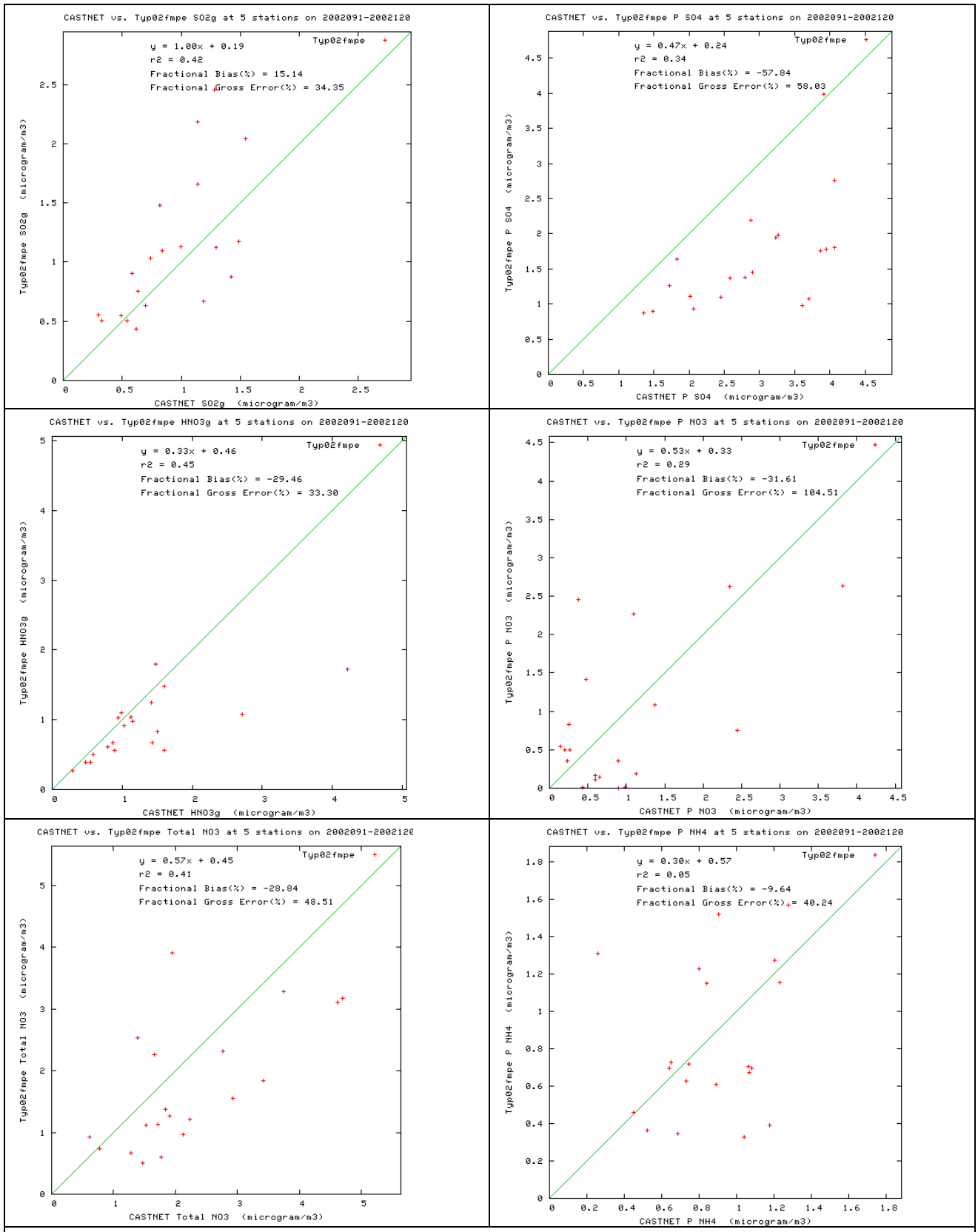


Figure C-42 April 2002 performance at CENRAP CASTNet sites for SO2 (top left), SO4 (top right), HNO3 (middle left), NO3 (middle right), Total NO3 (bottom left) and NH4 (bottom right).

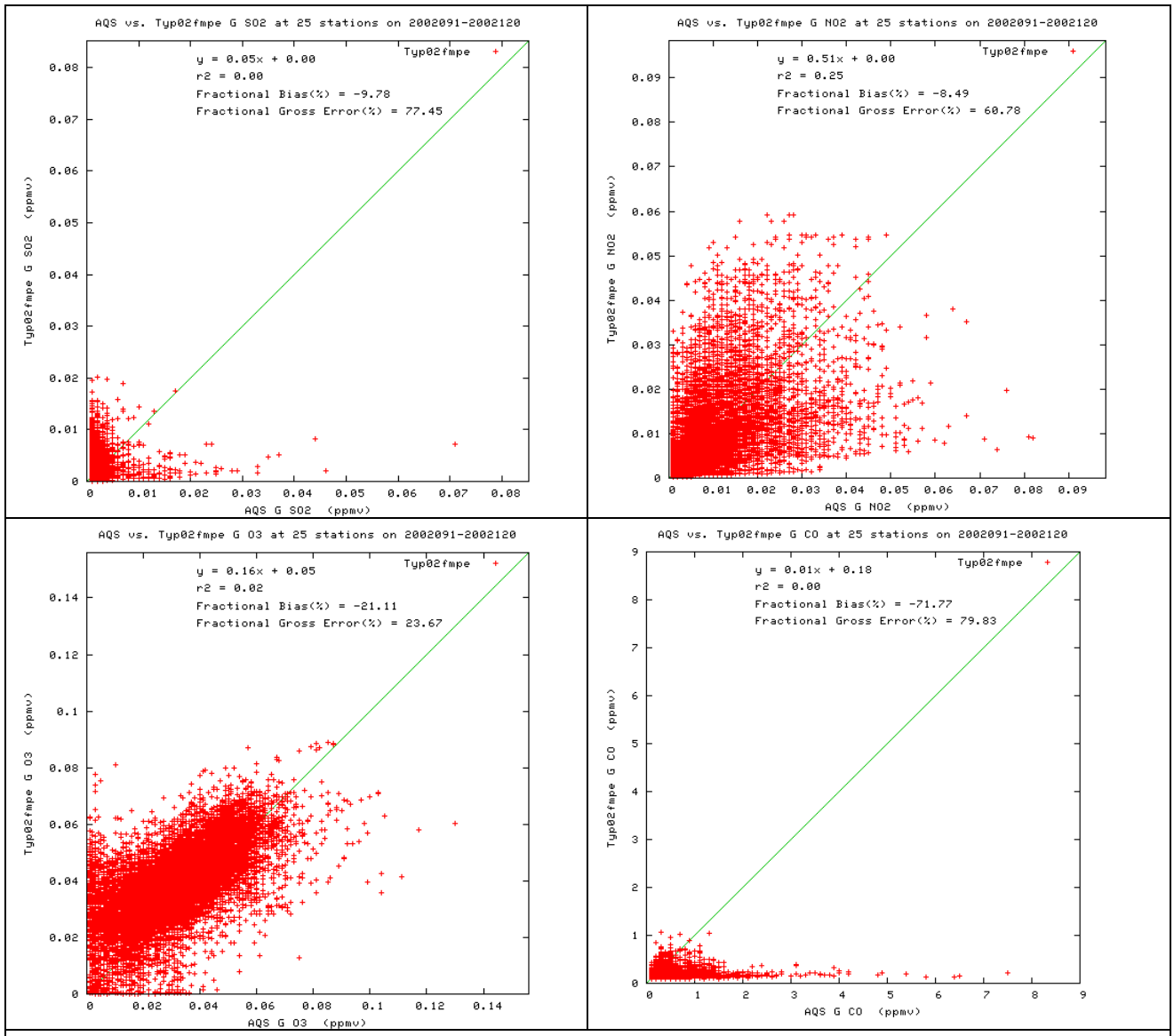


Figure C-43 April 2002 performance at CENRAP AQS sites for SO2 (top left), NO2 (top right), O3 (bottom left) and CO (bottom right).

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%).

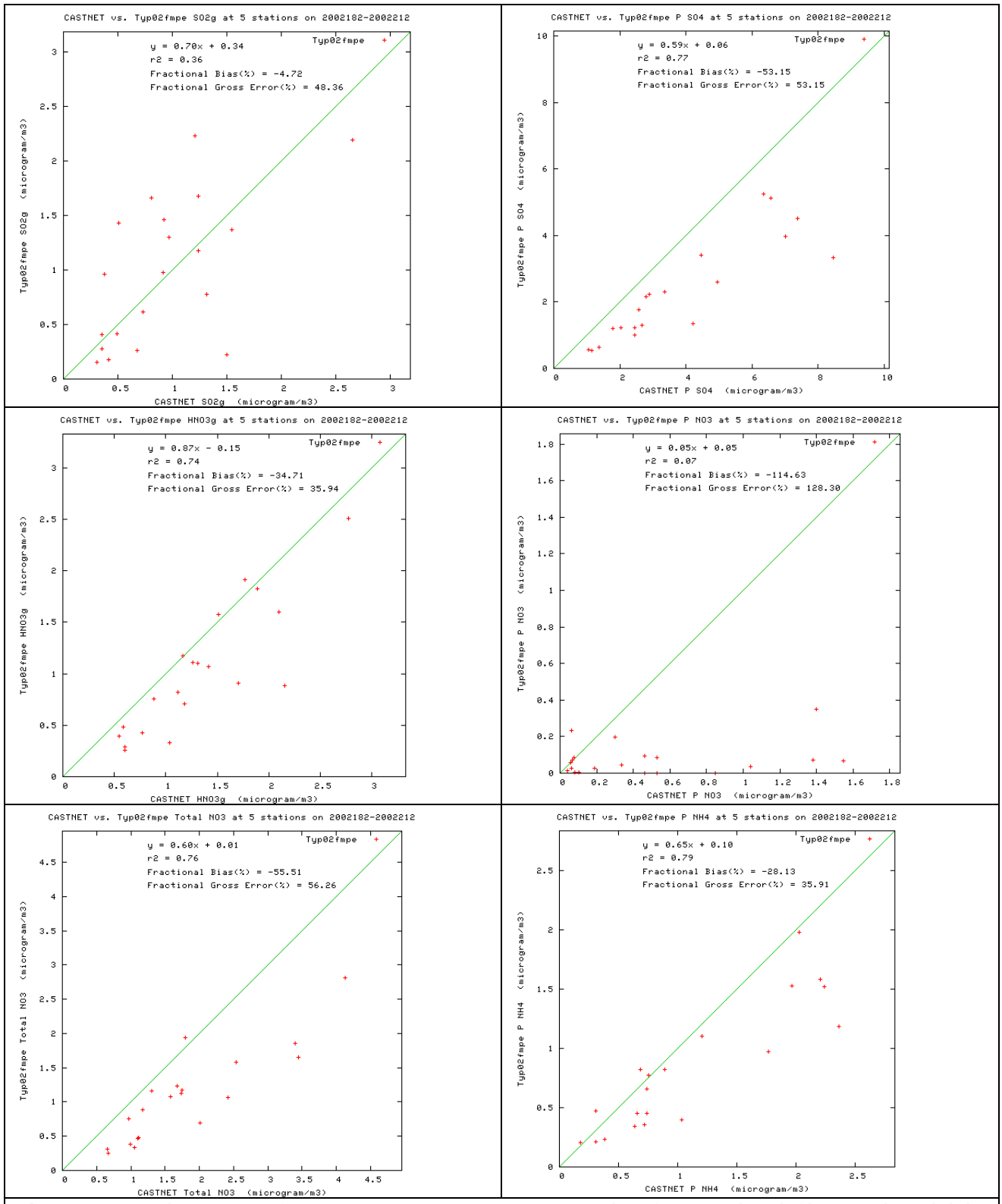


Figure C-44 July 2002 performance at CENRAP CASTNet sites for SO2 (top left), SO4 (top right), HNO3 (middle left), NO3 (middle right), Total NO3 (bottom left) and NH4 (bottom right).

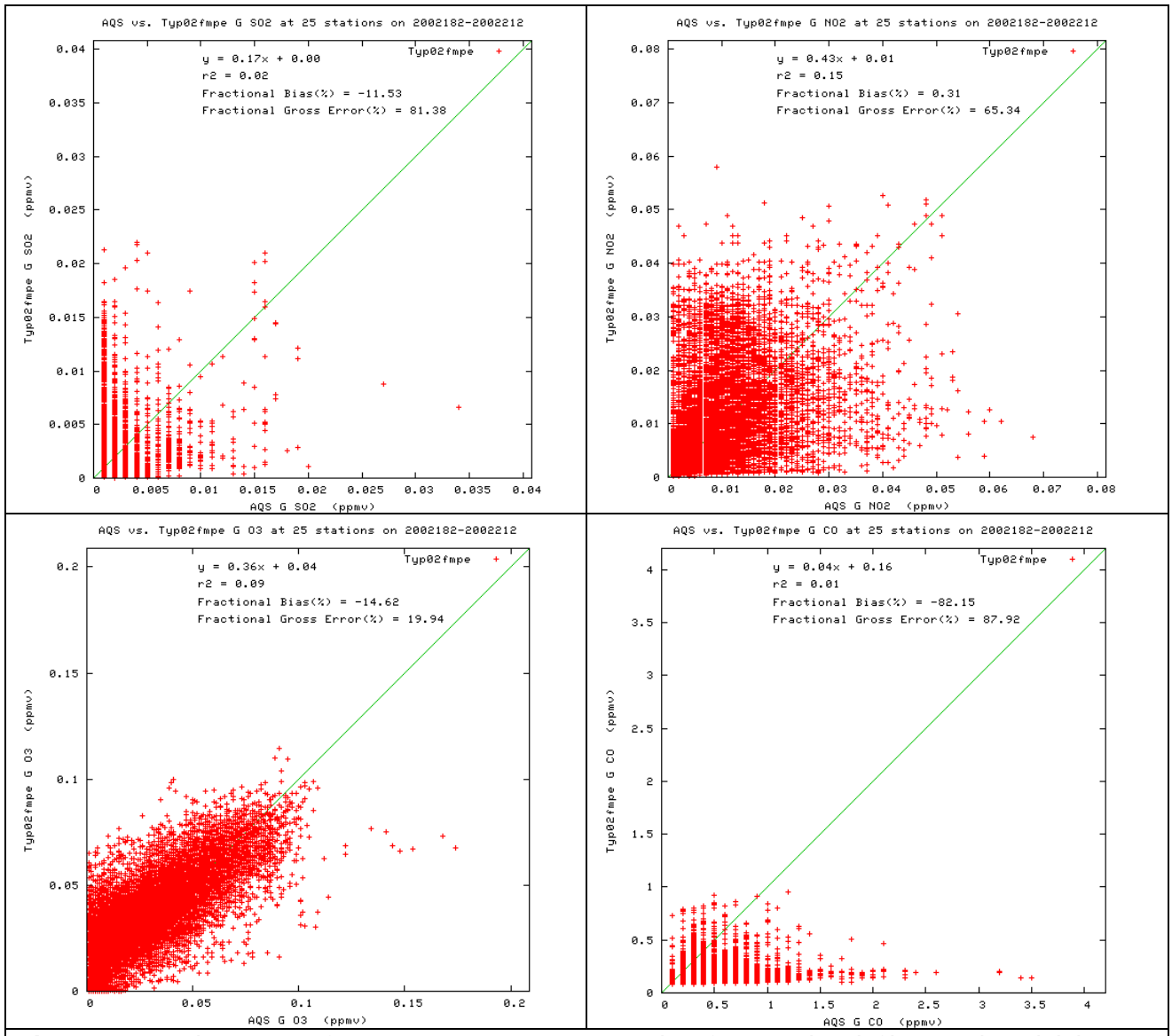


Figure C-45 July 2002 performance at CENRAP AQS sites for SO2 (top left), NO2 (top right), O3 (bottom left) and CO (bottom right).

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.

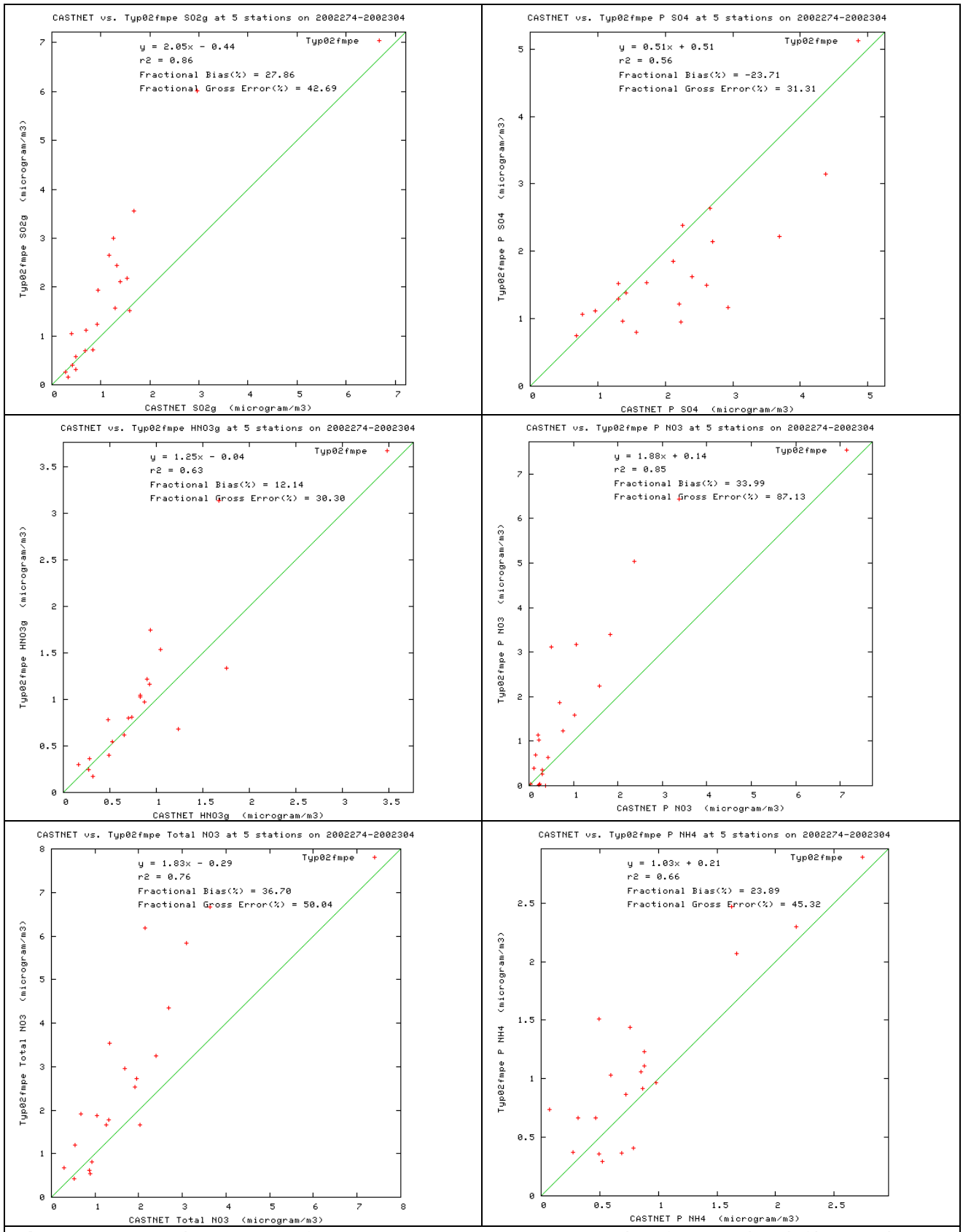


Figure C-46 October 2002 performance at CENRAP CASTNet sites for SO2 (top left), SO4 (top right), HNO3 (middle left), NO3 (middle right), Total NO3 (bottom left) and NH4 (bottom right).

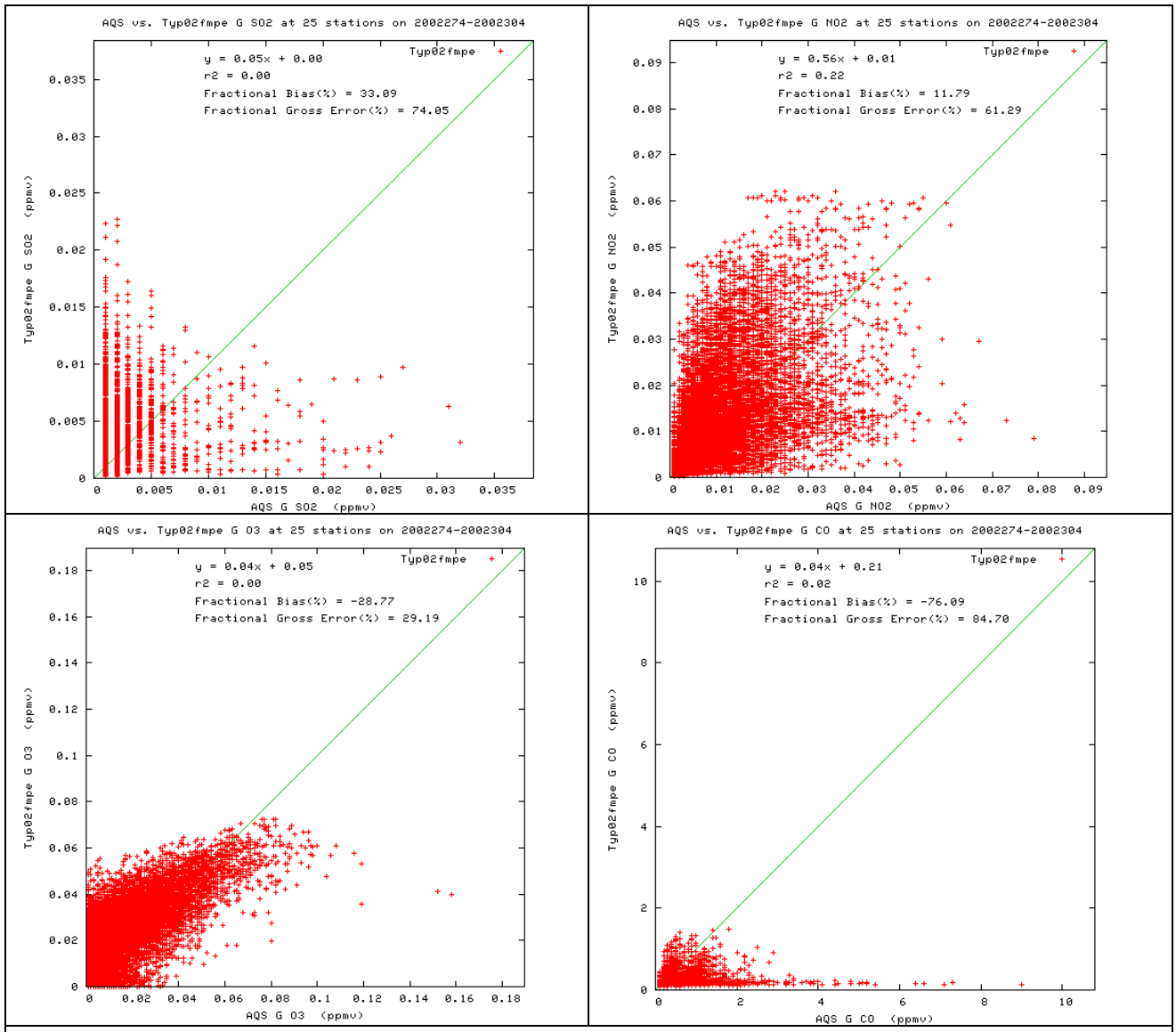


Figure C-47 October 2002 performance at CENRAP AQS sites for SO2 (top left), NO2 (top right), O3 (bottom left) and CO (bottom right).

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.

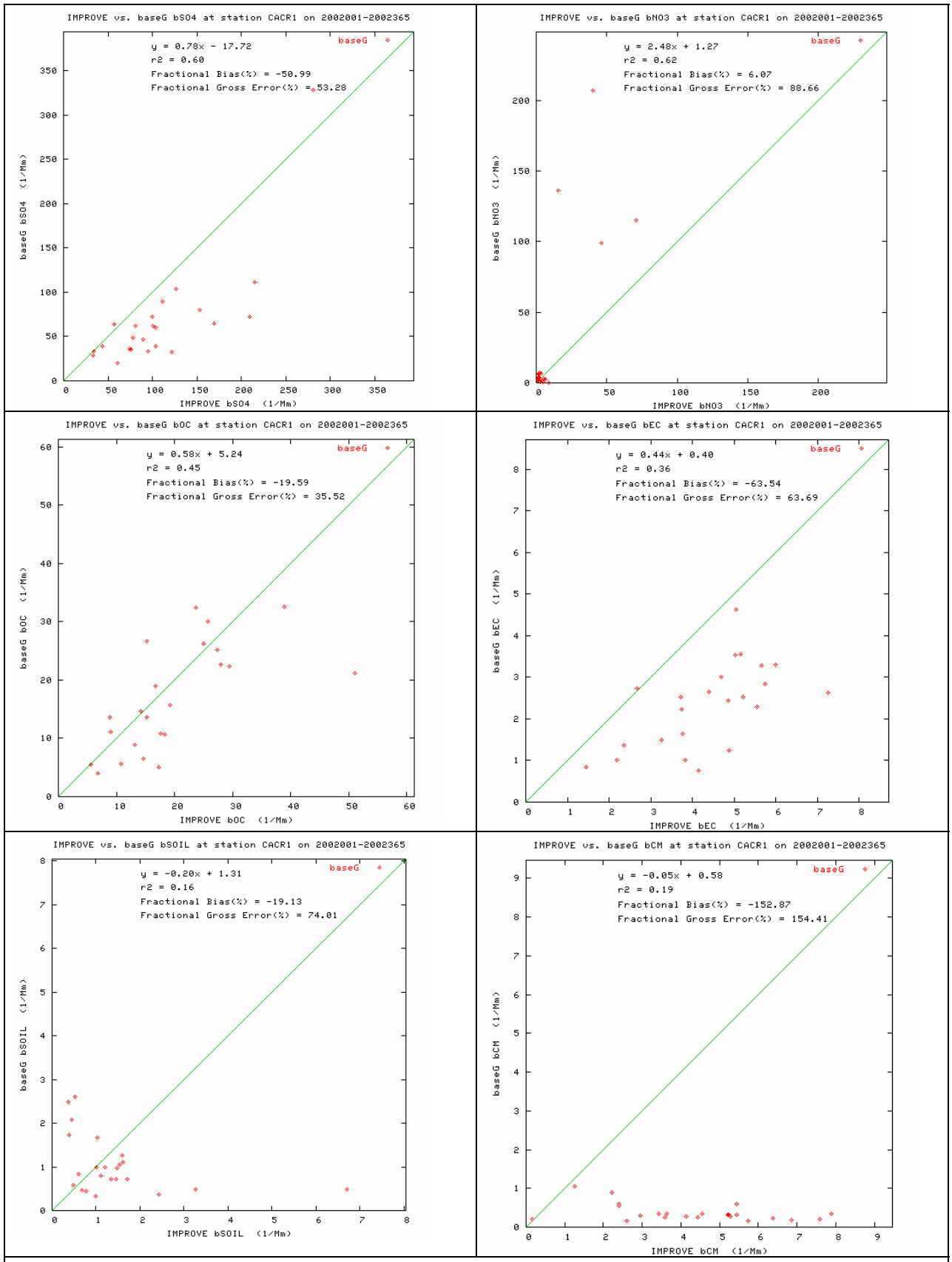


Figure C-48. PM species extinction model performance at Caney Creek (CACR) for the worst 20 percent days during 2002.