Western Air Quality Modeling Study
Photochemical Grid Model
Final Model Performance Evaluation

Simulation 2011 Base Version B (Base11b)

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TABLES

FIGURES

ACRONYMS AND ABBREVIATIONS

3SAQS	Three State Air Quality Study
3DSW	Three State Data Warehouse
AIRS	Aerometric Information Retrieval System
AMET	Atmospheric Model Evaluation Tool
AMON	Ammonia Monitoring Network
AQS	Air Quality System
BLM	Bureau of Land Management
CAMx	Comprehensive Air Quality Model with Extensions
CASTNet	Clean Air Status and Trends Network
CB6r2	Carbon Bond 6 revision 2
CO	Carbon Monoxide or Colorado
CONUS	Continental United States
CSN	Chemical Speciation Network
CTM	Chemistry-Transport Model
EC	Elemental Carbon Fine Particulate Matter
EPA	Environmental Protection Agency
FB	Fractional Bias
FE	Fractional Error
FRM	Federal Reference Method
HNO_3	Nitric Acid
IMPROVE	Interagency Monitoring of Protected Visual Environments
IWDW	Intermountain West Data Warehouse
JPAD	Jonah-Pinedale Anticline Development
LAI	Leaf Area Index
LCP	Lambert Conformal Conic Projection
MDA1	Daily Maximum 1-hour Average Ozone
MDA8	Daily Maximum 8-hour Average Ozone
MEGAN	Model of Emissions of Gases and Aerosols from Nature
MOVES	Motor Vehicle Emissions Simulator
MPE	Model Performance Evaluation
NADP	National Acid Deposition Program
NEPA	National Environmental Policy Act
NH_3	Gas-phase Ammonia
NH_4	Ammonium Fine Particulate Matter
NM	New Mexico
NMB	Normalized Mean Bias
NME	Normalized Mean Error
NO_2	Nitrogen Dioxide

NO_3	Nitrate Fine Particulate Matter
NPS	National Park Service
NTN	National Trends Network
O_3	Ozone
OA	Organic Aerosol Fine Particulate Matter
OC	Organic Carbon Fine Particulate Matter
PGM	Photochemical Grid Model
$PM_{2.5}$	Particulate Matter with Diameter < 2.5 µm
R-E	Ramboll-Environ, Corporation
SMOKE	Sparse Matrix Operator Kernel Emissions system
SO_2	Sulfur Dioxide
SO_4	Sulfate Fine Particulate Matter
TOMS	Total Ozone Mapping System
UBWOS	Uintah Basin Winter Ozone Study
UGRWOS	Upper Green River Winter Ozone Study
USFS	United States Forest Service
UNC-IE	University of North Carolina Institute for the Environment
UT	Utah
WAQS	Western Air Quality Study
WESTUS	Western U.S. (12-km Domain)
WY	Wyoming

1 EXECUTIVE SUMMARY

The Western Air Quality Study (WAQS) performed photochemical grid modeling for the year 2011 using the Comprehensive Air Quality Model with Extensions (CAMx) version 6.10 and Community Mutiscale Air Quality Model (CMAQ) version 5.0.2. The WAQS completed a second iteration of the 2011 air quality simulation as an improvement over a version A simulation completed early in 2015. This document presents the CAMx and CMAQ 2011 model performance evaluation (MPE) for the WAQS 2011 base year simulation version B (Base11b). We conducted the MPE for ozone (O_3), fine particulate matter ($PM_{2.5}$), wet deposition of sulfur and nitrogen, ammonia, and light extinction. The MPE focuses on the ability of the models to simulate air quality on both regional 12-km and Intermountain West 4-km modeling domains. We evaluated the performance of hourly O_3 as well as daily maximum 1-hour (MDA1) and daily maximum 8-hour average (MDA8) O_3. We also included carbon monoxide (CO), nitrogen dioxide (NO_2), and sulfur dioxide (SO_2) in the evaluation. The $PM_{2.5}$ evaluation includes total $PM_{2.5}$ along with the component species sulfate (SO_4), nitrate (NO_3), ammonium (NH_4), elemental carbon (EC), organic carbon (OC), organic aerosol (OA), and other PM (PM Other). The deposition evaluation focused on total sulfur and oxidized and reduced nitrogen species. Ammonia evaluation is made against the National Acid Deposition Network AMoN observations. Visibility is evaluated against IMPROVE network light extinctions.

The WAQS CAMx and CMAQ Base11b 12-km and 4-km simulations meet performance goals for annual average, summer season, and MDA1 and MDA8 O_3 averaged across all monitoring locations in the modeling domains. On an annual, domain-wide average, the models overestimate (positive biases) hourly O_3, MDA1, and MDA8 at urban sites. At rural sites, CAMx tends to overestimate the observations while CMAQ tends to underestimate the observations. For both models the overall performance (lower bias and error) is better at the rural than at the urban sites. Both models tend to underestimate high observed O_3 concentrations (> 60 ppb) and overestimate the observed O_3 concentrations during the summer season (June-August). On average, the version of CAMx used for the WAQS tends to estimate higher O_3 than CMAQ. This discrepancy may be due to the different photochemical mechanisms used by each model. While winter season high O_3 events are simulated better by CAMx than CMAQ, both models continue to underestimate winter O_3 associated with oil and gas production.

Both models tend to overestimate observed NO_2, although the biases have been reduced in simulation Base11b relative to Base11a. Both models both tend to underestimate CO, although the performance is mixed when looking at the monthly performance in each state. In Utah, Wyoming, and New Mexico the models both tend to underestimate SO_2; the models overestimate SO_2 in Colorado.

On an annual domain-wide basis, CAMx simulation Base11b has moved closer to the PM performance criteria for bias and error for total $PM_{2.5}$, EC, and SO_4 relative to simulation Base11a. Urban OC performance also improved with lower positive biases in simulation

Base11b at the CSN sites. The model performance for NO_3, NH_4 and rural OC (IMPROVE) degraded compared to the Base11a. Both models generally overestimate urban total $PM_{2.5}$ and underestimate rural total $PM_{2.5}$, although some variability in these trends exist on a seasonal and monthly basis. The boundary condition dust corrections in simulation Base11b reduced the overestimates of total $PM_{2.5}$ on an annual basis. This correction degrades spring season PM performance when dust entering the domain from the boundary impacts the observations. The boundary corrections for dust need to be re-examined, particularly in the spring and summer, when their contributions to total $PM_{2.5}$ mass are the greatest. SO_4 is underestimated by CMAQ at rural (IMPROVE) sites, but otherwise shows an increasing tendency to overestimate at all locations as the concentration increases. SO_4 at the urban (CSN) sites is predicted well in the spring and fall, but moderately underestimated in the summer, and significantly overestimated in the winter. While NO_3 performance improves in simulation Base11b relative to Base11a on an annual basis, summer season NO_3 is severely underestimated in simulation Base11b.

CAMx and CMAQ are both systematically underestimating NH_3. As with simulation Base11a, the negative normalized mean biases (CAMx: -70.3%; CMAQ: -62.2%) indicate that the models are not accurately capturing at least one key parameter needed to estimate ambient NH_3. The biases are highest in the winter and summer months and lowest in October and November.

On an annual basis, both models underestimate wet deposition for all species. Sulfate deposition shows the best performance across all sites in the 12-km domain (CAMx NMB: -22.3%; CMAQ NMB: -18.9%), followed by nitrate (CAMx NMB: -49.3%; CMAQ NMB: -38.8%) and ammonium (CAMx NMB: -50.4%; CMAQ NMB: -45.9%). Although the deposition estimates are still low relative to the observations, CMAQ estimates higher deposition than CAMx resulting in smaller negative biases for all species.

Both models underestimate light extinction, although some differences exist between species and in different parts of the modeling domain. CMAQ Base11b estimates higher SO_4, NO_3, and EC extinction than CAMx, resulting in lower biases than CAMx relative to the estimated IMPROVE observed light extinctions for these species. CAMx estimates higher OC and coarse mass light extinction than CMAQ. Even with the removal of sea salt from the boundary conditions, both models overestimate the contributions of sea salt to light extinction. CAMx underestimates the contribution of soil to light extinction, a trend that is likely related to the overcorrection of the boundary condition dust in simulation Base11b.

2 INTRODUCTION

2.1 Background

The Western Air Quality Study (WAQS) includes cooperators from the United States Forest Service (USFS), Bureau of Land Management (BLM), National Park Service (NPS), Environmental Protection Agency (EPA) Region 8 and the state air quality management agencies of Colorado, Utah, New Mexico, and Wyoming. The WAQS is intended to facilitate air resource analyses for federal and state agencies in these states toward improved information for the public and stakeholders as a part of air quality planning, including the National Environmental Policy Act (NEPA). Funded by the EPA, BLM, and the USFS, and with in-kind support from the NPS and Colorado, Utah, and Wyoming state air agencies, by working closely with cooperators and overseeing the various agreements, the main focus of the study is on assessing the environmental impacts of sources related to oil and gas development and production. In particular, the cooperators will use photochemical grid models (PGMs) to quantify the impacts of proposed oil and gas development projects within the Intermountain West on current and future air quality, including ozone and visibility levels in the National Parks and Wilderness Areas.

Air pollutant emissions data analysis and modeling expertise and skills are an integral need of the WAQS participants to support routine application of PGMs during the project period of performance. The WAQS Cooperators have hired the University of North Carolina (UNC) at Chapel Hill and Ramboll-Environ Corporation (Ramboll) to assist in developing the technical data needed to perform the WAQS as well as populate the Intermountain West Data Warehouse (IWDW). The WAQS is an extension of the Three-State Air Quality Study (3SAQS), which was initiated in 2012 to support National Environmental Policy Act (NEPA) impact assessments of oil and gas development projects in the States of Colorado, Utah, and Wyoming.

2.2 Overview

The WAQS project performed photochemical grid modeling (PGM) for the year 2011 using the Comprehensive Air Quality Model with Extensions (CAMx) version 6.10 (ENVIRON, 2014) and the Community Multiscale Air Quality (CMAQ) Model version 5.10. The 3SAQS 2011 Modeling Protocol (UNC and ENVIRON, 2014a) details the CAMx and CMAQ configurations and justification for why they were chosen for the WAQS. This document presents the PGM 2011 model performance evaluation (MPE) for the WAQS 2011 base year simulation version B (Base11b). Simulation Base11b builds off of the 3SAQS version A simulation (3SAQS _Base11a: UNC and ENVIRON, 2015) with updates to the emissions, boundary conditions, and model configurations. We will first present the model input and configuration changes for Base11b relative to Base11a. We will then present a summary of the model performance for the Base11b CAMx and CMAQ simulations, focusing on monitors within a 4-km domain that encompasses the major oil and gas basins of the Intermountain West.

For details on the approach used for the modeling and MPE refer to the 3SAQS 2011a MPE report (UNC and ENVIRON, 2015). Chapter 3 of this report details the methods used to evaluate to 2011b

CAMx and CMAQ simulation. Chapter 4 of this report presents the WAQS Base11b model performance results for ozone and ozone precursors, particulate matter, acid deposition, and visibility.

3 APPROACH

3.1 PGM Science and Input Data Configuration

The WAQS developed 2011 annual CAMx and CMAQ modeling inputs for the 36-km continental U.S. (CONUS), 12-km western U.S. (WESTUS), and 4-km 3-State (3SAQS) domains as shown in Figure 3-1 using Lambert Conformal Conic Projection (LCP) parameters defined in Table 3-1. Along with performing annual two-way grid nesting on all three domains using CAMx, the WAQS 2011b modeling preformed annual one-way grid nesting on all three domains using CMAQ.

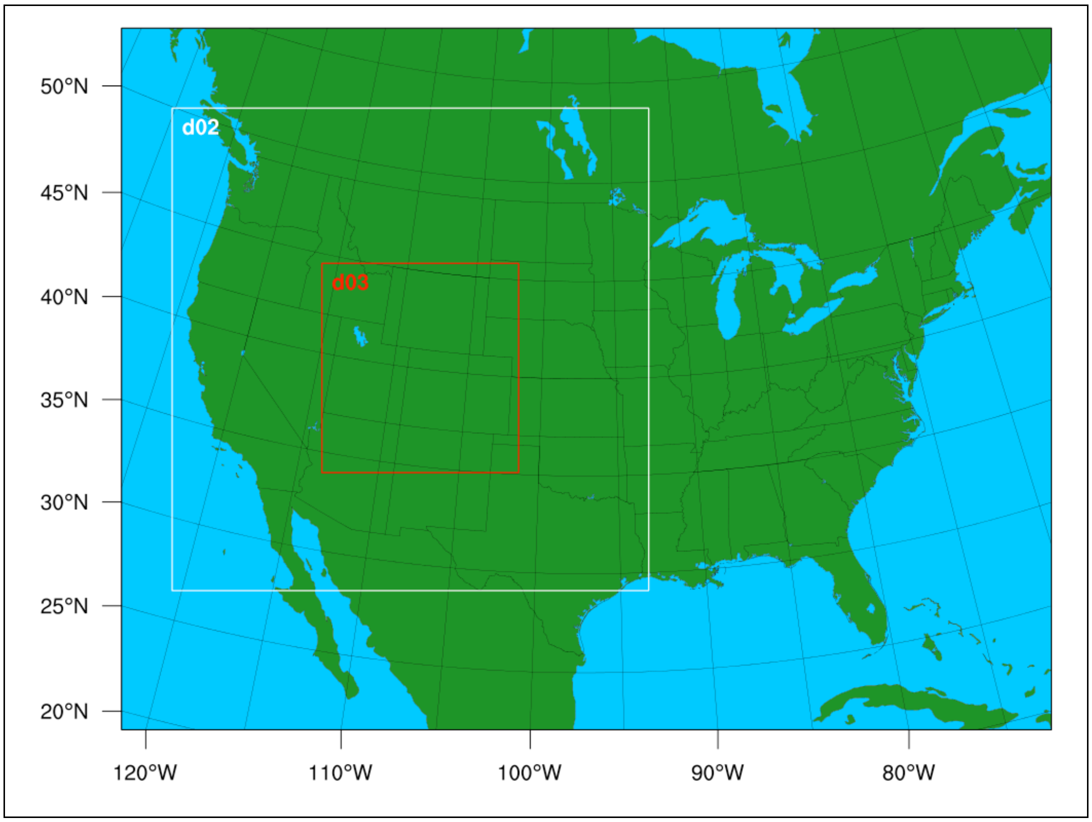


Figure 3-1. 36 km CONUS, 12 km WESTUS, and 4 km 3SAQS processing domain used for developing PGM emission inputs.

Table 3-1. Modeling domain parameters for the WAQS modeling domains.

Parameter	Value
Projection	Lambert-Conformal
1st True Latitude	33 degrees N
2nd True Latitude	45 degrees N
Central Longitude	97 degrees W
Central Latitude	40 degrees N
dX (km)	d01 = 36, d02 = 12, d03 = 4
dY (km)	d01 = 36, d02 = 12, d03 = 4
X-orig (km)	d01 = -2736, d02 = -2388, d03 = -1516
Y-orig (km)	d01 = -2088, d02 = -1236, d03 = -544
# cols	d01 = 148, d02 = 227, d03 = 281
# rows	d01 = 112, d02 = 230, d03 = 299

Table 3-2 summarizes the CAMx version 6.10 (released April 2014) and CMAQ version 5.0.2 (released May 2014) science configurations and options used for the WAQS 2011b modeling. Details of these configurations are available in the 3SAQS 2011 modeling protocol (UNC and ENVIRON, 2014a) and Base11a MPE report (UNC and ENVIRON, 2015)

Details of the changes from Base11a to Base11b are provided below.

Meteorological Inputs: We improved the input meteorology for simulating wintertime inversion layers in the western oil and gas basins. We generated a new WRF simulation for the Base11b modeling that integrates observed snow-cover/snow-depth data from the Snow Data Assimilation System (SNODAS; NHRSC, 2004). This simulation differed from the Base11a WRF simulation that used standard NAM reanalysis snow fields. Bowden et al. (2015) describes how the SNODAS data were integrated into WRF and shows the impact of this configuration on wintertime model performance. We processed the Base11b WRF meteorological fields with version 4.3 of the WRFCAMx processor that improves the calculation of surface albedo from snow. The WRF and WRFCAMx improvements that we applied to simulation Base11b only impact the simulated meteorology when there is snow cover, otherwise the meteorology fields are the same as simulation Base11a. Details of the 3SAQS 2011 WRF meteorology data (Base11a) are available in UNC and ENVIRON (2014c).

Initial/Boundary Conditions: The boundary conditions (BCs) for the 36 km CONUS domain simulation were based on the MOZART[1] global chemistry model. As we observed adverse model performance impacts in simulation Base11a from excessive dust entering the regional modeling domains from the outer boundary, we chose to zero out the dust fields from MOZART when downscaling these data for simulation Base11b. We used the same programs as simulation Base11a to interpolate from the MOZART horizontal and vertical coordinate system to CAMx and to map the MOZART chemical species to the CB6r2 and CB05 chemical mechanisms. We also zeroed out the sea salt particle concentrations in the MOZART BCs.

[1] http://www.acd.ucar.edu/wrf-chem/mozart.shtml

Emissions: We made several changes to the input emissions for simulation Base11b:

- *Fires:* Version 2 of the 2011 DEASCO3 daily point-source inventory with pre-computed plumes
- *Oil and Gas Emissions:* Phase II of the WAQS point and area oil and gas inventory. Point sources, sources in Wyoming, and all sources in the Paradox and Raton Basins are unchanged from simulation Base11a. Fracing emissions were added to the Denver-Julesburg, Piceance, Uinta, North San Juan, and South San Juan basins. Uinta Basin tribal emissions were estimated based on EPA Tribal minor new source review data for the following sources: artificial lift engines, condensate tanks, heaters, oil tanks, pneumatic pumps, condensate truck loading. Added emissions for the Williston and Great Plains Basins.
- *Onroad Mobile Emissions:* Replaced MOVES2010b with MOVES2014 emissions for all U.S. counties
- *Residential Wood Combustion (RWC) Sources*: Reduced all pollutants from RWC sources by 50% due to high wintertime positive biases in primary organic aerosol at urban monitors in simulation Base11a.
- *Other Anthropogenic Emissions*: Replaced the 2011v1 EPA modeling platform used in simulation Base11a with the 2011v2 platform. Changes included agricultural burning reductions in the Midwest, updates to spatial and temporal allocation for many sources, and updates to Canada and Mexico inventories.

Table 3-2. PGM model configurations for WAQS

Science Options	CAMx Base 2011b Configuration	CMAQ Base 2011b Configuration	Difference from Base11a
Model Codes	CAMx v6.10 – April 2014 Release	CMAQ v5.0.2 – May 2014 Release	
Horizontal Grid Mesh	36/12/4 km	36/12/4 km	Same as Base11a
36 km grid	148 x 112 cells	148 x 112 cells	Not used for CMAQ in Base11a
12 km grid	239 x 206 cells	239 x 206 cells	Not used for CMAQ in Base11a
4 km grid	281 x 299 cells	281 x 299 cells	
Vertical Grid Mesh	25 vertical layers, defined by WRF	25 vertical layers, defined by WRF	Same as Base11a
Grid Interaction	36/12/4 km two-way nesting	36/12/4 km one-way nesting	
Initial Conditions	15 day spin-up on 36 km grid	15 day spin-up on 36/12/4 km grids	Same as Base11a
Boundary Conditions	36 km from global chemistry model	36 km from global chemistry model	Modified the MOZART-GEOS5 GCM data by zeroing out the dust and sea salt concentrations from the boundary
Emissions			
Baseline Emissions Processing	SMOKE, MOVES2014 and MEGAN	SMOKE, MOVES2014 and MEGAN	Updated emissions inventory data for most anthropogenic sectors and fires
Sub-grid-scale Plumes	No plume-in-grid	No plume-in-grid	Same as Base11a
Chemistry			Same as Base11a
Gas Phase Chemistry	CB6r2	CB05	
Aerosols	CF2	AERO5	
Meteorological Processor	WRFCAMx v4.3	MCIP	Update for CAMx snow configuration
Horizontal Diffusion	Spatially varying	Spatially varying	Same as Base11a
Vertical Diffusion	CMAQ-like in WRFCAMx	ACM2	Same as Base11a
Diffusivity Lower Limit	Kz_min = 0.1 to 1.0 m^2/s or 2.0 m^2/s	Kz_min = 0.1 to 1.0 m^2/s or 2.0 m^2/s	
Deposition Schemes			Same as Base11a
Dry Deposition	Zhang dry deposition scheme	Models-3 scheme	
Wet Deposition	CAMx-specific formulation	Models-3 scheme	
Numerics			Same as Base11a
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) -- Fast Solver	EBI	
Vertical Advection Scheme	Implicit scheme w/ vertical velocity update	WRF-scheme	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	PPM with Yamartino updates	
Integration Time Step	Wind speed dependent	Wind speed dependent	Same as Base11a

3.2 Model Performance Evaluation Procedures

UNC and ENVIRON (2015) presents the statistical approaches and details about the observational data used to evaluate the model performance for simulation Base11a. We will use the same datasets and approaches to evaluate simulation Base11b. For this MPE report we focus on the average model performance across all sites in the 4-km domain and within the states of Colorado, Utah, Wyoming, and New Mexico. We highlight the model performance impacts of the changes to the model input files made in simulation Base11b relative to Base11a. Similar to the Base11a MPE report, this reported includes an evaluation for ozone (O_3), fine particulate matter ($PM_{2.5}$), wet deposition species, visibility, and ammonia (NH_3). We evaluate the performance of hourly O_3 as well as daily maximum 1-hour (MDA1) and daily maximum 8-hour average (MDA8) O_3. We also include carbon monoxide (CO), nitrogen dioxide (NO_2), and sulfur dioxide (SO_2) gas-phase species in the evaluation. The $PM_{2.5}$ evaluation includes total $PM_{2.5}$ along with the component species sulfate (SO_4), nitrate (NO_3), ammonium (NH_4), elemental carbon (EC), organic carbon (OC), and other PM (PM Other). The deposition evaluation focuses on total sulfur and oxidized and reduced nitrogen species.

While a full description of the MPE goals and criteria for O_3 and PM are provided in UNC and ENVIRON (2015), Table 3-3 summarizes the bias and error goals used for assessing model performance.

Table 3-3. Model performance goals and criteria

Fractional Bias (FB)	Fractional Error (FE)	Comment
≤±15%	≤35%	O_3 model performance goal that would be considered very good model performance
≤±30%	≤50%	PM model performance Goal, considered good PM performance
≤±60%	≤75%	PM model performance Criteria, considered average PM performance. Exceeding this level of performance for PM species with significant mass may be cause for concern.

Monitor site-specific performance metrics for all of the federal and state aerometric networks operating within the 12-km and 4-km modeling domains are available in an electronic docket to this report. The docket is available through the Intermountain West Data Warehouse (IWDW). From the IWDW Model Performance Evaluation Plots page, follow the menus to simulation Base11b (2011→Base11b→AQ) to view the full suite of MPE plots for the CAMx and CMAQ simulations.

4 2011 BASE B MODEL PERFORMANCE EVALUATION

4.1 Gas-Phase Species Model Performance

This section presents regional and statewide gas-phase species model performance across the entire 12-km and 4-km modeling domains. More detailed performance metrics (hourly and site-specific) for the Base11b simulation are available through the IWDW. Model performance for both the CAMx and CMAQ models are presented in this section.

4.1.1 Section Summary

- The WAQS CAMx and CMAQ Base11b 12-km and 4-km simulations meet the performance goals for annual average and peak daily maximum 1-hour (MDA1) and daily maximum 8-hour average O_3 (MDA8) averaged across the AQS and CASTNet monitoring locations. With the exception of CAMx 12-km model estimates of AQS MDA8 (Fractional Bias = 15.97%), both CAMx and CMAQ meet the performance goal for summer season MDA1 and MDA8 averaged across the AQS and CASTNet monitoring locations.
- On an annual, domain-wide average, CAMx and CMAQ overestimate (positive biases) hourly O_3, MDA1, and MDA8 averaged across the AQS sites. Across the CASTNet sites, CAMx tends to overestimate the observations while CMAQ tends to underestimate the observations. For both models the overall performance (lower bias and error) is better across the CASTNet sites than the AQS sites.
- Both models tend to underestimate high observed O_3 concentrations (> 60 ppb).
- Both models tend to overestimate the observed summer season O_3 concentrations.
- On average, the version of CAMx used for the WAQS tends to estimate higher O_3 than CMAQ. This difference may be due to the different photochemical mechanisms used by each model.
- The models fail to predict a dip in the O_3 concentrations observed during July 2011 across both the AQS and CASTNet monitoring networks. The result of this performance deficit are systematic overestimates in both models (positive biases) through most of the second half of the year.
- Observed winter high O_3 concentrations are underestimated by both models.
- Both models overestimate fall O_3 concentrations.
- Both models tend to overestimate observed NO_2, although the biases have been reduced in simulation Base11b relative to Base11a.
- Both models tend to underestimate CO, although the performance is mixed when looking at the monthly performance in each state.
- In Utah, Wyoming, and New Mexico the models both tend to underestimate SO_2; the models overestimate SO_2 in Colorado.

4.1.2 WAQS Base11b 12-km Domain Model Performance

Table 4-1 includes bias and error metrics for CAMx O_3 simulations at sites averaged across the 12-km modeling domain. The rows labeled AQS Hourly and CNET Hourly are performance statistics for hourly O_3 at the AQS and CASTNet monitors, respectively. The rows labeled AQS MDA1 and CNET MDA1 are statistics for daily maximum 1 hour O_3 at each network; AQS MDA8 and CNET MDA8 are daily maximum 8-hour average O_3. Values in red indicate performance metrics for which CAMx misses the model performance goals. Values in purple indicate performance metrics for which CAMx misses the model performance criteria. The WAQS CAMx Base11b 12-km domain-wide model performance for O_3 meets the performance goals (NMB ≤±15% and NME ≤±35%) for annual average, summer season (June – August), and peak (> 60 ppb) daily maximum 1-hour (MDA1) and daily maximum 8-hour average O_3 (MDA8) averaged across the AQS and CASTNet monitoring locations. The simulation misses the performance goals only for annual and summer season hourly O_3 averaged across all AQS monitors in the 12-km domain.

Several key points of CAMx O_3 model performance across the 12-km domain include:

- Fractional bias (FB=19.9%), fractional error (FE=41.6%), and Normalized Mean Bias (NMB=18.3%) for AQS hourly O_3 are the only performance metrics for which CAMx misses the performance goals, although they are within the performance criteria. 3SAQS simulation Base11a also missed these performance goals for hourly O_3.
- On an annual, domain-wide average, CAMx has a positive bias for hourly O_3, MDA1, and MDA8 across both the AQS and CASTNet sites; the overall performance (lower bias and error) is better across the CASTNet sites than the AQS sites.
- When a 60 ppb observed O_3 concentration threshold is applied, the model biases switch from positive to negative at all sites. Although the model performance improves across the AQS sites and degrades at the CASTNet sites at ozone values >60 ppb, CAMx still achieves the ozone performance goals. At these higher observed concentrations, CAMx has lower biases across the AQS sites than at the CASTNet sites.
- Model performance for O_3 degrades slightly (i.e. higher bias and error) during the ozone season (June-August), relative to the annual performance, at the AQS sites. CAMx has a positive bias during the summer period.

Table 4-2. includes the CMAQ bias and error metrics for observed O_3 at sites averaged across the 12-km modeling domain.

Several key points of CMAQ O_3 model performance across the 12-km domain include:

- The WAQS CMAQ Base11b 12-km domain-wide ozone model performance meets the performance goals for annual average, summer season, and peak MDA1 and MDA8 across the AQS and CASTNet monitoring locations. CMAQ only misses the fractional error (FE) performance goal for annual and summer season hourly AQS O_3.
- On an annual, domain-wide average, CMAQ has positive biases averaged across the AQS sites and negative biases across the CASTNet sites; the overall performance (lower bias and error) is better across the CASTNet sites than the AQS sites.
- When a 60 ppb observed O_3 concentration threshold is applied, the model biases are negative in all networks. At these higher observed concentrations, CMAQ has lower biases across the AQS sites than at the CASTNet sites.
- Model performance for O_3 improves slightly (i.e. lower bias and error) during the ozone season (June-August), relative to the annual performance, averaged across the AQS sites. CMAQ has positive biases at the AQS sites and negative biases across the CASTNet sites during the summer period.

Figure 4-1 includes annual 12-km domain-wide scatter plots (CAMx and CMAQ vs. observations) for all AQS and CASTNet sites in the 12-km domain. The figure includes MDA8 O_3 performance for CAMx and CMAQ, with and without a 60 ppb concentration threshold applied to the observations. Both CAMx and CMAQ have positive biases (i.e. overestimates) in simulating the observed AQS O_3 values; CAMx has a higher NMB than CMAQ (CAMx: 13.9%, CMAQ: 8.8%). Across the CASTNet sites, CAMx tends to overpredict MDA8 O_3 (NMB: 3.7%) and CMAQ tends to underpredict MDA8 O_3 (NMB: -1.1%). CAMx and CMAQ both tend to underpredict MDA8 O_3 on the days with high O_3 measurements (>60 ppb). CAMx has a lower average NMB across both the AQS and CASTNet sites relative to CMAQ on the high O_3 days.

The quantile-quantile (Q-Q) plots shown in Figure 4-2 include MDA8 O_3 concentrations at AQS and CASTNet sites for both simulations 3SAQS Base11a and WAQS Base11b. The Q-Q plots show the unpaired distribution of simulated MDA8 O_3 concentrations plotted against observed concentrations. Note that the 3SAQS Base11a simulation did not produce 12-km CMAQ results. These plots illustrate that both CAMx and CMAQ overestimate the observations across all concentrations at the AQS sites. In the WAQS Base11b simulation CMAQ has a tendency to estimate higher concentrations than CAMx at the upper end of the observed AQS concentration distribution. At the CASTNet sites, CAMx and CMAQ overestimate the low observed values (<60 ppb) and underestimates high observed values (>60 ppb). While Q-Q distributions for the Base11a and Base11b CAMx simulations are similar, CMAQ tends to estimate lower MDA8 O_3 concentrations at the lower end of the CASTNet concentration distribution and higher MDA8 O_3 concentrations at the upper end of the distribution.

Figure 4-3 and Figure 4-4 show monthly CAMx model performance for MDA8 at the AQS and CASTNet sites in the 12-km domain, respectively. The bias-concentration plots in these figures show monthly NMB plotted as bars (left y-axis) and the monthly average concentrations plotted as lines (right y-axis); the observed monthly average concentrations are plotted as the black line. The CAMx and CMAQ biases are positive in all months averaged across the AQS sites, with the CMAQ biases consistently lower than CAMx, particularly in the summer months. While the CAMx simulations also overpredict the MDA8 O_3 concentrations in all months across the CASTNet sites, CMAQ underpredicts MDA8 O_3 across these sites during January through June. CMAQ also has consistently lower monthly biases than CAMx in simulating MDA8 O_3 across the CASTNet sites.

Table 4-1. 12-km domain ozone performance indicators for CAMx simulation Base2011b

Species	Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod
	Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)	(ppb)	(ppb)
O3	AQS Hourly	19.90	41.6	6.06	11.4	18.30	34.5	33.10	39.20
	CNET Hourly	12.20	22.3	3.56	8.3	8.51	19.8	41.80	45.40
	AQS MDA1	10.70	18.5	4.38	9.2	8.96	18.7	48.80	53.20
	CNET MDA1	2.62	13.2	0.72	6.7	1.39	12.9	51.70	52.40
	AQS MDA8	15.00	21.1	5.91	9.3	13.90	21.2	44.00	49.90
	CNET MDA8	5.09	13.9	1.86	6.5	3.81	13.4	48.70	50.50
O3 > 60 ppb	AQS MDA1	-4.30	12.9			-3.50	12.8		
	CNET MDA1	-9.73	13.2			-9.20	12.7		
	AQS MDA8	-2.95	11.7			-2.20	11.6		
	CNET MDA8	-9.04	12.1			-8.50	11.6		
June-August O3	AQS Hourly	22.17	37.3	7.52	12.8	20.07	34.0	37.67	45.17
	CNET Hourly	14.40	24.5	4.58	9.9	10.12	21.7	45.70	50.27
	AQS MDA1	11.23	20.2	5.27	11.7	9.34	20.6	56.80	62.10
	CNET MDA1	2.04	14.6	0.35	8.5	0.63	14.3	59.47	59.80
	AQS MDA8	15.97	22.0	7.46	11.6	14.70	22.8	50.87	58.33
	CNET MDA8	5.26	15.0	2.15	8.1	3.94	14.6	55.27	57.40

Table 4-2. 12-km domain ozone performance indicators for CMAQ simulation Base2011b

Species	Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod
	Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)	(ppb)	(ppb)
O3	AQS Hourly	7.89	41.4	2.92	10.4	8.81	31.4	33.10	36.00
	CNET Hourly	1.26	24.2	-0.49	8.5	-1.17	20.4	41.80	41.30
	AQS MDA1	6.77	17.9	2.98	8.6	6.03	17.5	49.40	52.40
	CNET MDA1	-1.67	13.7	-1.24	6.8	-2.38	13.2	52.00	50.80
	AQS MDA8	9.59	19.5	3.90	8.3	8.77	18.8	44.50	48.40
	CNET MDA8	-0.24	14.1	-0.53	6.5	-1.09	13.2	48.90	48.40
O3 > 60 ppb	AQS MDA1	-6.00	15.2			-4.5	15.0		
	CNET MDA1	-12.00	15.9			-10.7	14.9		
	AQS MDA8	-11.70	15.4			-10.8	14.1		
	CNET MDA8	-12.50	14.9			-11.2	13.6		
June-August O3	AQS Hourly	5.27	35.8	2.33	10.8	6.25	28.8	37.63	39.97
	CNET Hourly	-1.01	26.0	-1.49	9.9	-3.17	21.6	45.67	44.17
	AQS MDA1	5.21	18.5	2.64	10.4	4.66	18.2	56.77	59.40
	CNET MDA1	-4.41	14.8	-2.77	8.5	-4.62	14.3	59.43	56.70
	AQS MDA8	8.28	19.1	3.91	9.5	7.73	18.7	50.83	54.70
	CNET MDA8	-2.39	14.2	-1.58	7.6	-2.83	13.7	55.27	53.67

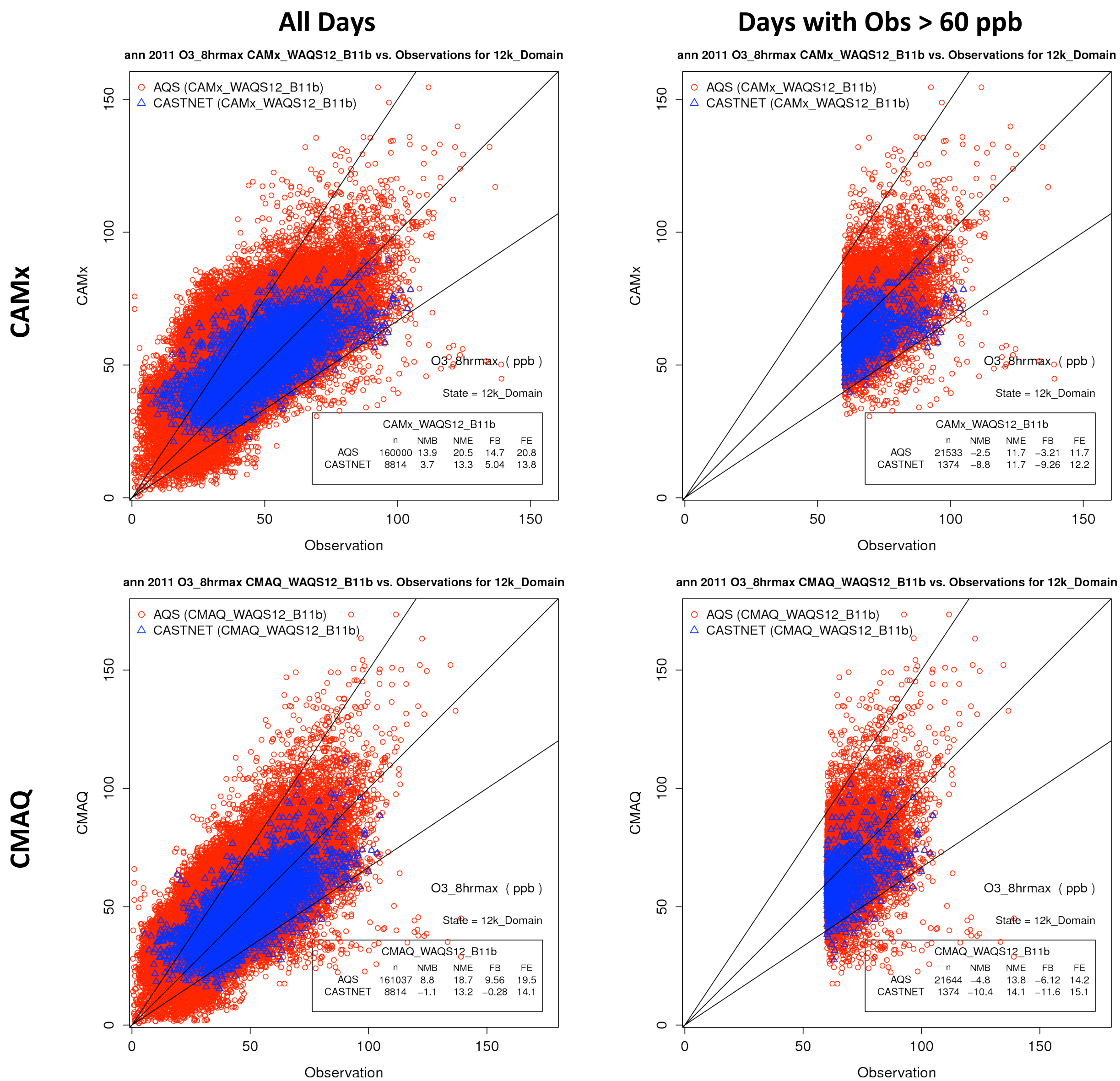


Figure 4-1. WAQS 2011 CAMx (top) and CMAQ (bottom) model performance for MDA8 O_3 for all AQS (red) and CASTNet (blue) sites in the 12-km domain.

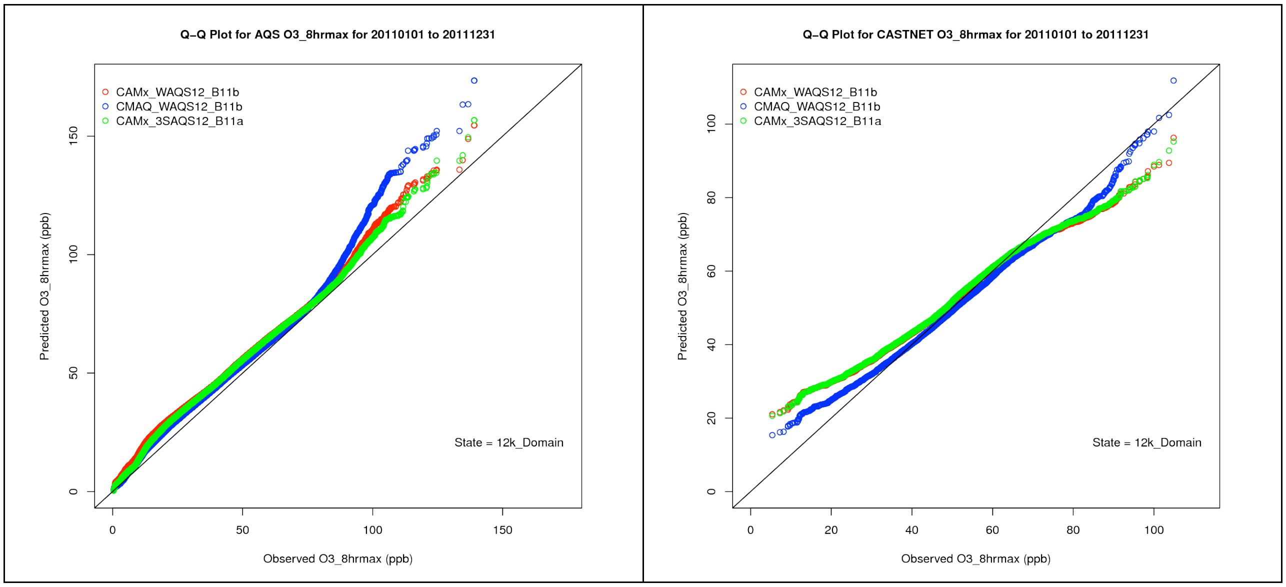


Figure 4-2.Q-Q plots of 2011 MDA8 for the 12-km modeling domain at the AQS (left) and CASTNet (right) monitoring networks.

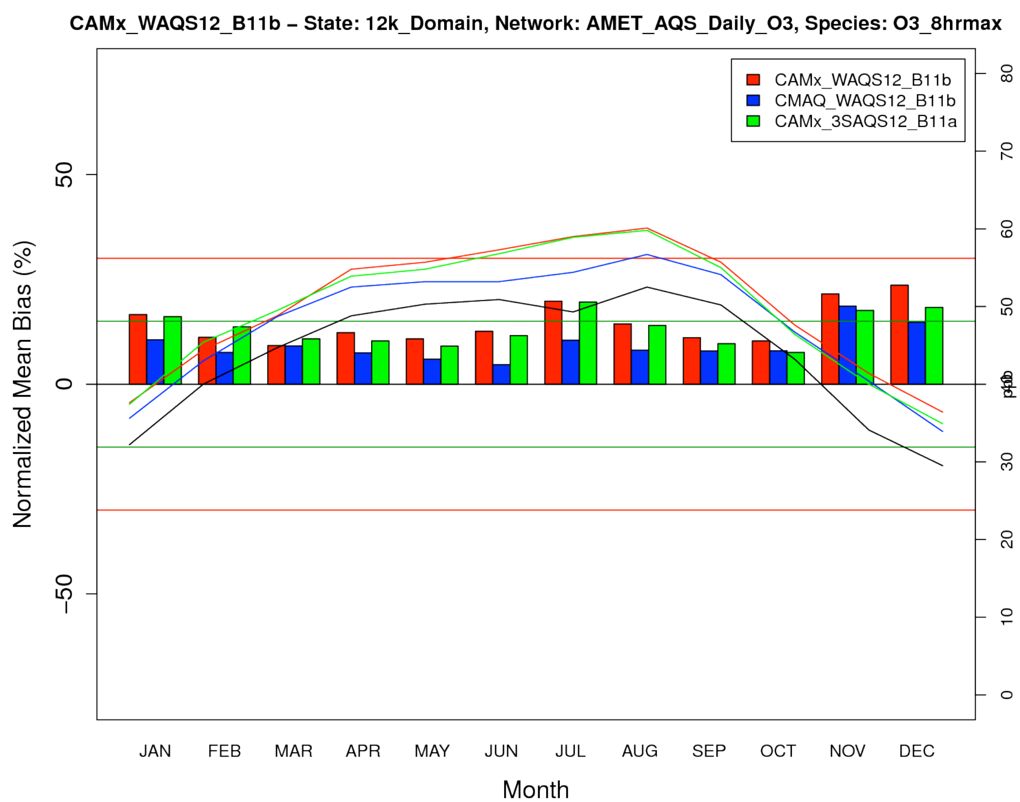


Figure 4-3. 12-km domain AQS MDA8 mean monthly bias (bars) and concentration (lines).

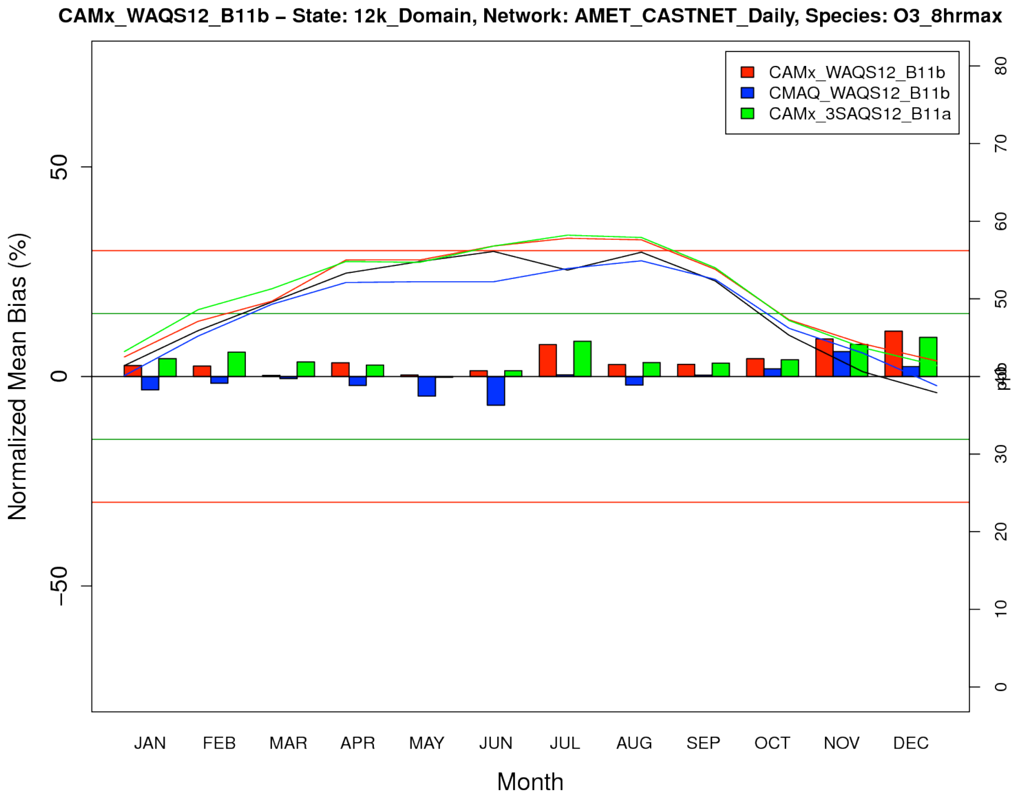


Figure 4-4. 12-km domain CASTNet MDA8 mean monthly bias (bars) and concentration (lines).

4.1.3 WAQS Base11b 4-km Domain Model Performance

Averaged across all sites in the WAQS 4-km domain, the WAQS CAMx and CMAQ Base11b simulations meet the performance goals for hourly O_3, MDA1 O_3, and MDA8 O_3. Table 4-3 includes CAMx bias and error metrics for observed ozone averaged across all monitoring sites in the 4-km modeling domain. Several key points of CAMx O_3 model performance across the 4-km domain include:

- All of the bias and error metrics for hourly, MDA1, and MDA8 O_3 meet the performance goals. Low positive annual biases indicate that on average CAMx tends to slightly overestimate the observations across the year. While individual sites and specific time periods will show different performance trends, averaged across the full year at all of the monitoring sites in the 4-km domain, CAMx tends to overestimate the observed ozone concentrations. Several of the error metrics approach the middle to upper end of the performance goal (35%), indicating that there are compensating biases in the model that are suppressing the averaged bias metrics.
- On an annual, domain-wide average, CAMx has a positive bias for hourly O_3, MDA1, and MDA8 across both the AQS and CASTNet sites; overall, the model performs better at the CASTNet sites, with lower average errors and biases compared to the AQS sites
- When a 60 ppb observed O_3 concentration threshold is applied, the model biases increase and switch from positive to negative.
- Model performance for O_3 improves across the AQS sites and degrades slightly at the CASTNet sites in the ozone season (June-August) relative to the full year.

Table 4-4 includes CMAQ bias and error metrics for observed ozone averaged across all monitoring sites in the 4-km modeling domain. Several key points of CMAQ O_3 model performance across the 4-km domain include:

- All of the bias and error metrics for hourly, MDA1, and MDA8 O_3 meet the performance goals. Several of the error metrics approach the middle to upper end of the performance goal (35%), indicating that there are compensating biases in the model that are suppressing the averaged bias metrics.
- On an annual, domain-wide average, CMAQ has positive biases for hourly O_3, MDA1, and MDA8 across the AQS sites and negative biases across the CASTNet sites; CMAQ does not appear to perform better at one of the networks over the other
- When a 60 ppb observed O_3 concentration threshold is applied, the model biases increase and switch from positive to negative.
- CMAQ performance for O_3 does not change considerably during the ozone season (June-August) relative to the full year.

Figure 4-5 includes annual scatter plots (CAMx and CMAQ vs. observations) for all AQS and CASTNet sites in the 4-km domain. The figure includes MDA8 O_3 performance for both CMAQ and CAMx with and without a 60 ppb concentration threshold applied to the observations. CAMx has a slight positive bias for both networks, with higher NMB at the AQS sites (NMB: 5.2%) compared to the CASTNet sites (NMB: 0.9%). CMAQ also has low biases for both networks, with a positive bias at the AQS sites (NMB: 1.1%) and a negative bias at the CASTNet sites (NMB: -3.1%). On the days with elevated O_3 measurements (>60 ppb), CAMx and CMAQ both have a negative biases (i.e. underestimates), with CAMx exhibiting lower NMB than CMAQ at both the AQS and CASTNet sites.

Figure 4-6 compares the CAMx and CMAQ monthly mean MDA8 NMB for the AQS sites in the 4-km domain for simulations Base11a and Base11b. Superimposed on the bars of the monthly, domain-average NMB are lines with the monthly mean observed (black) and modeled MDA8 concentrations. This figure shows that the model performance is similar in simulations Base11a and Base11b for each model. In most months the CAMx NMB increases slightly in Base11b relative to Base11a. The CMAQ NMB decreases slightly in simulation Base11b relative to Base11a. Averaged across all AQS sites in the 4-km domain, CAMx has low biases during the first half of the year (January-June) and higher biases in the second half of the year (July-December). During the same periods, CMAQ has negative biases from January through June and positive biases from July through December.

The concentration lines in Figure 4-6 also illustrates the trend in the 4-km domain, monthly average model performance for O_3. Where the models all simulate increases in O_3 from June to July, the observations decrease in July. After higher observed O_3 values in August, a trend also simulated by the models, the observations fall off through the rest of the year with concentrations that are systematically 5-10% lower than the models. Additional research into the actual cause of the July O_3 dip (e.g. cooler or wetter meteorological conditions that are not being correctly simulated by the models) may lend insight into why this trend is being missed in the models.

Figure 4-7 compares the CAMx and CMAQ monthly mean MDA8 NMB for the CASTNet sites in the 4-km domain for simulations Base11a and Base11b. Similar performance trends as the AQS sites persist at the CASTNet sites with a switch in model performance from negative biases in the first half of the year to positive biases in the second half of the year. Like at the AQS sites, a similar trend in the observed O_3 at the CASTNet sites shows a dip in concentrations in July, an increase in August, and then decreasing O_3 through the end of the year. The average model biases are generally lower at the rural CASTNet sites than at the AQS sites with all months and all models falling well below the O_3 bias goal of 15%.

Table 4-3. 4-km domain ozone performance indicators for CAMx simulation Base2011b

Species	Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod
	Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)	(ppb)	(ppb)
O3	AQS Hourly	13.1	27.9	3.7	9.4	9.4	24.2	38.9	42.5
	CNET Hourly	3.2	12.5	1.3	5.8	2.7	12.2	47.1	48.4
	AQS MDA1	3.2	12.4	0.4	7.2	0.8	13.7	52.4	52.8
	CNET MDA1	-0.1	9.4	-0.2	5.2	-0.3	9.6	54.3	54.1
	AQS MDA8	6.0	13.5	1.6	7.0	3.3	14.6	48.2	49.8
	CNET MDA8	1.1	9.2	0.5	4.8	0.9	9.2	51.9	52.3
O3 > 60 ppb	AQS MDA1	-6.63	11.9			-6.2	11.6		
	CNET MDA1	-8.11	11.5			-7.5	10.9		
	AQS MDA8	-6.75	11.5			-6.3	11.1		
	CNET MDA8	-7.77	10.5			-7.2	9.9		
June-August O3	AQS Hourly	15.4	24.7	5.0	10.3	11.5	23.4	44.2	49.2
	CNET Hourly	4.2	14.1	1.8	7.0	3.6	13.7	51.2	52.9
	AQS MDA1	2.2	11.5	-0.1	8.3	-0.1	13.4	61.7	61.7
	CNET MDA1	-1.4	10.0	-0.9	6.1	-1.4	10.0	61.2	60.2
	AQS MDA8	5.4	11.7	1.7	7.7	3.1	13.7	56.5	58.2
	CNET MDA8	0.2	9.4	0.1	5.4	0.3	9.3	57.7	57.8

Table 4-4. 4-km domain ozone performance indicators for CMAQ simulation Base2011b

Species	Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod
	Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)	(ppb)	(ppb)
O3	AQS Hourly	6.8	27.9	1.9	8.8	4.8	22.5	39.2	41.0
	CNET Hourly	-2.2	14.3	-1.1	6.5	-2.3	13.7	47.1	46.0
	AQS MDA1	-0.5	13.6	-0.4	6.9	-0.7	13.2	52.4	52.0
	CNET MDA1	-3.9	11.3	-2.1	6.1	-3.8	11.2	54.3	52.2
	AQS MDA8	1.4	14.2	0.5	6.5	1.1	13.5	48.2	48.7
	CNET MDA8	-3.2	11.0	-1.6	5.6	-3.1	10.8	51.9	50.3
O3 > 60 ppb	AQS MDA1	-10.3	15.0			-9.3	14.0		
	CNET MDA1	-12.2	15.2			-11.0	14.0		
	AQS MDA8	-11.7	15.4			-10.4	14.1		
	CNET MDA8	-12.5	14.9			-11.2	13.6		
June-August O3	AQS Hourly	9.2	24.4	3.2	9.6	7.4	21.7	44.2	47.4
	CNET Hourly	-1.5	16.4	-0.8	7.9	-1.4	15.5	51.2	50.3
	AQS MDA1	-0.2	13.0	-0.1	8.0	-0.2	12.9	61.7	61.6
	CNET MDA1	-4.6	12.3	-2.6	7.3	-4.1	12.0	61.2	58.5
	AQS MDA8	2.0	12.7	1.1	7.1	2.0	12.6	56.5	57.6
	CNET MDA8	-3.7	11.8	-1.9	6.6	-3.2	11.4	57.7	55.7

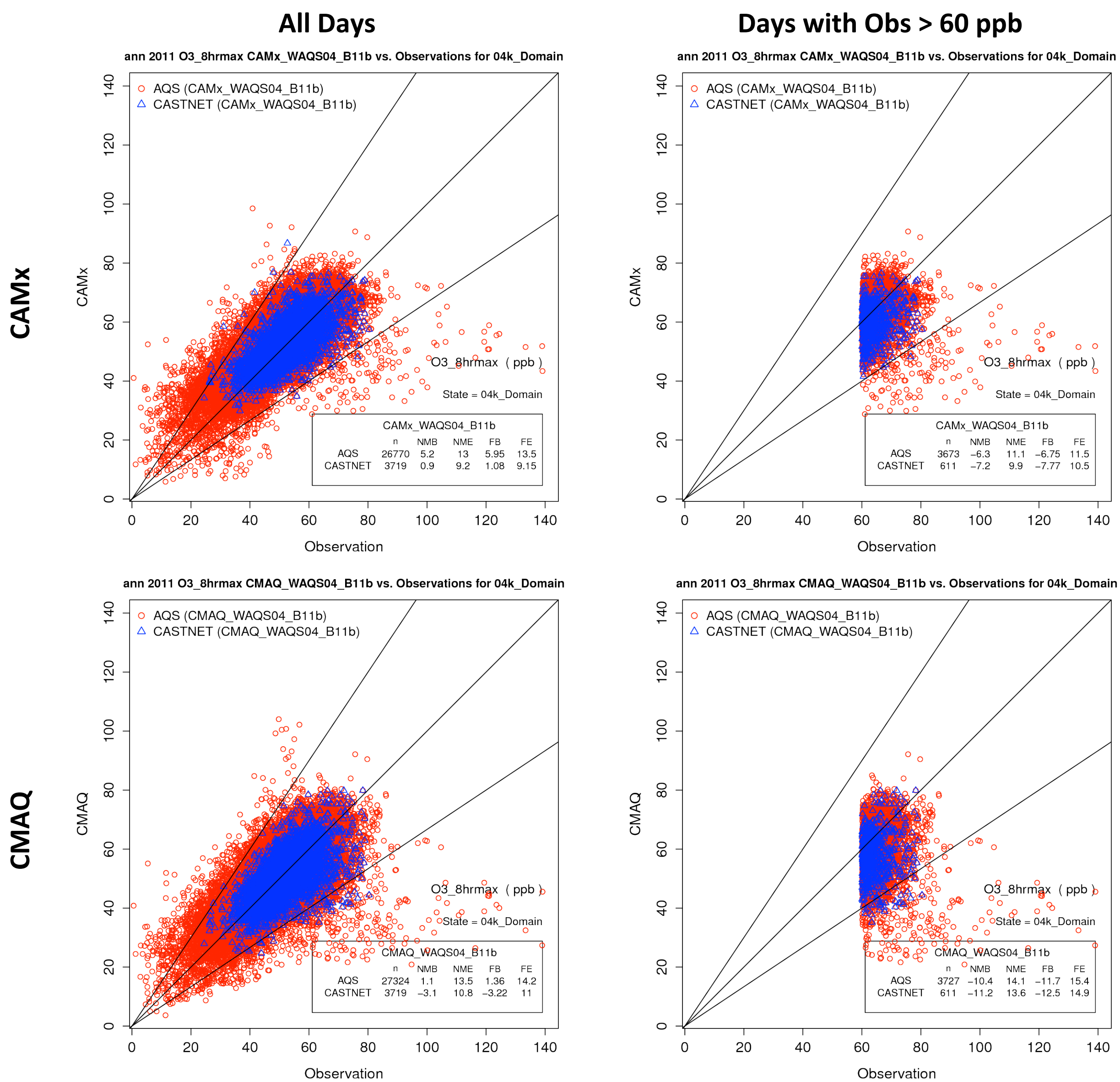


Figure 4-5. WAQS 2011 CAMx (top) and CMAQ (bottom) model performance for MDA8 O_3 for all AQS (red) and CASTNet (blue) sites in the 4-km domain.

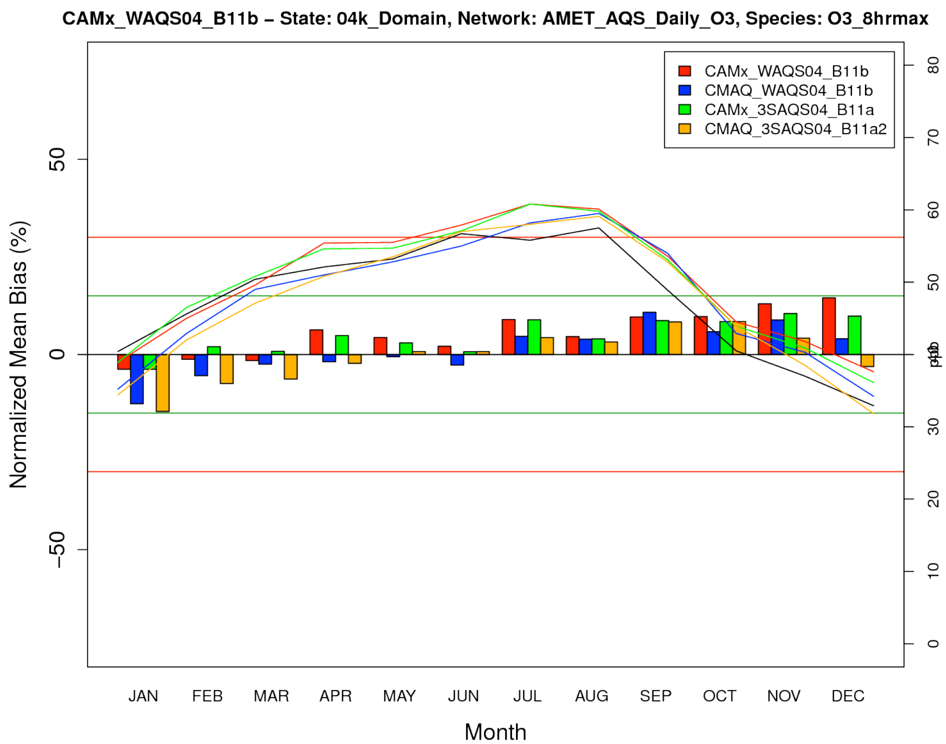


Figure 4-6. AQS 4-km domain MDA8 mean monthly bias (bars) and concentrations (lines).

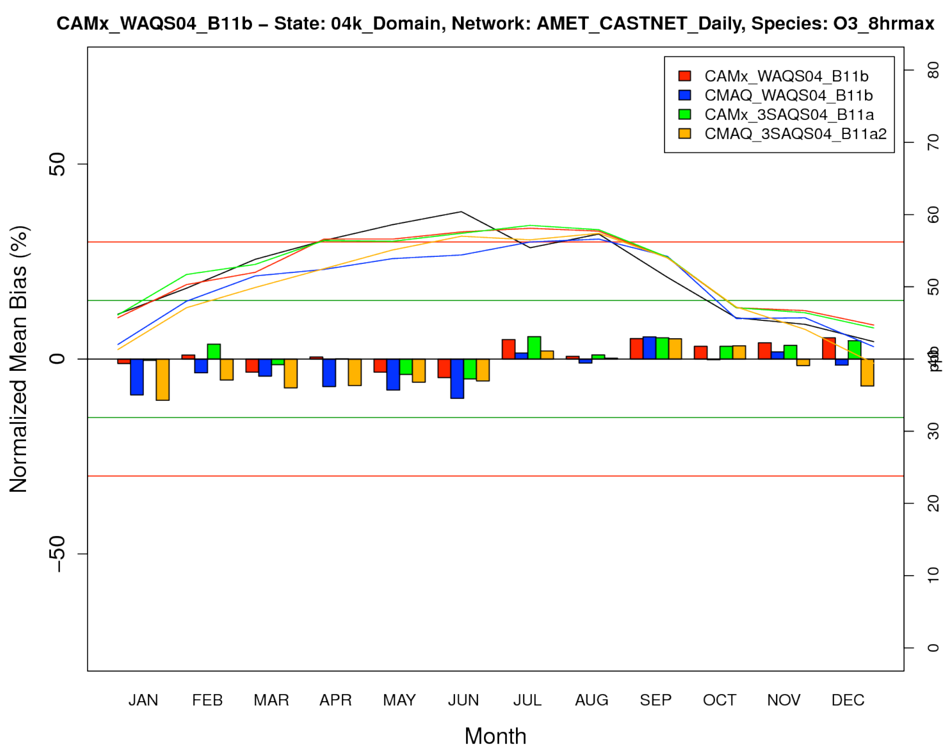


Figure 4-7. CASTNet 4-km domain MDA8 mean monthly bias (bars) and concentrations (lines)

4.1.4 WAQS Base11b State-Level 4-km Model Performance

The model performance metrics in this section illustrate the 4-km grid resolution O_3 model performance at monitors within each of the states of Colorado, New Mexico, Utah, and Wyoming. Both statewide performance and model performance at select sites are discussed. Additional site-level performance plots are available through the IWDW.

Table 4-5 highlights MDA8 O_3 performance for both CAMx and CMAQ averaged across all AQS monitors within each state. Annual average, O_3 season, and peak MDA8 O_3 are shown for each state. As seen in the 4-km domain-wide performance metrics, CAMx predicts higher O_3 than CMAQ. As the models tend to overestimate the observed O_3, for all but the peak O_3 metrics, the higher predictions in CAMx produce higher biases than CMAQ. With the models underestimating the peak O_3, the higher CAMx predictions produce lower negative biases then CMAQ. A possible explanation for the differences in O_3 model performance between CAMx and CMAQ is the use of different photochemical mechanisms in each model. The Base11b CAMx simulation used the Carbon Bond mechanism version 6, revision 2 (CB6r2); the Base11b CMAQ simulation used Carbon Bond version 5 (CB05).

Figure 4-8 are soccer plots comparing the CAMx and CMAQ Base11b seasonal MDA8 O_3 performance averaged across all AQS sites in each state included in the 4-km domain. Soccer plots compare the normalized mean error (NME) and NMB for a simulation and include performance goal lines that look similar to soccer goal posts. The best model performance falls within the inner goal lines on the plots, illustrating model performance where NMB < ±15% and NME < 35%. A few performance trends are highlighted by these plots:

- The models tend to underestimate winter O_3, particularly in Utah and Wyoming. The CMAQ winter O_3 underestimates are more severe than CAMx.
- The statewide model performance for both models is within the performance goals in the spring and summer
- Both models overestimate fall O_3 in all states

Figure 4-9 shows similar soccer plots for the MDA8 observations in the CASTNet network of monitors.

Figure 4-10 through Figure 4-13 are Q-Q and monthly box and whisker plots showing MDA8 O_3 performance at the AQS and CASTNet monitors in Colorado, New Mexico, Utah, and Wyoming. The box and whisker plots compare the monthly mean, 25^{th}-75^{th}, and 5^{th}-95^{th} percentile of MDA8 O_3 concentrations in the observations and for the CAMx and CMAQ Base11a and Base11b simulations. These plots highlight not only the trends in the mean model performance but they illustrate the model skill at the tails of the concentration distributions.
The Q-Q plots shown in these figures illustrate that all simulations underestimated the high observed values of MDA8 O_3, particularly at the AQS sites. The inability of CAMx and CMAQ to reproduce MDA8 values greater than 100 ppb at the AQS sites is attributable primarily to winter O_3 events, particularly in Utah and Wyoming. While simulation Base11a was not

configured to simulate winter high O_3 events, simulation Base11b included enhancements to the WRF meteorology data and to the processing of the WRF data for input to CAMx to improve the simulation of winter high O_3 events (Bowden et al., 2015). Improvements to the simulation of the upper-end of the observed O_3 distribution in Base11b can be attributed to these winter meteorology model enhancements.

Figure 4-14 through Figure 4-17 are monthly bias-concentration plots for Colorado, New Mexico, Utah, and Wyoming. These plots compare simulations Base11a and Base11b for both CAMx and CMAQ. The bias-concentration plots in these figures show monthly NMB plotted as bars (left y-axis) and the monthly average concentrations plotted as lines (right y-axis); the observed monthly average concentrations are plotted as the black line. As with the 4-km domain average bias-concentration plots, the state average plots illustrate that both CAMx and CMAQ performed similarly in the two simulations (i.e. CAMx performance is similar in Base11a and Base11b). The differences between the models (i.e. CAMx vs CMAQ) is amplified in the state level performance metrics. A few highlights of the model performance in these plots include:

- The annual average model performance for the Colorado AQS sites listed in Table 4-5 indicates a much lower bias for CMAQ (NMB: 0.9%) than for CAMx (NMB: 6.3%). The monthly NMB plot for Colorado AQS sites in Figure 4-14 shows that on a monthly average basis CAMx overestimates MDA8 O_3 in most months, while CMAQ tracks the observations more closely, particularly in February through August.
- Figure 4-15 and Figure 4-16 show that the underestimation of MDA8 O_3 in the winter months in Utah and Wyoming is less severe in CAMx than in CMAQ.
- Where July was identified previously as a transitional month in the model performance (see discussion above about the July observed O_3 dip), O_3 model performance in New Mexico changes in June. Figure 4-17 shows that the trend in observed MDA8 O_3 at AQS sites in New Mexico begins to flatten out in May. The models do not capture this trend and continue to estimate increasing O_3 through the summer months. The failure of the models to follow the observed O_3 trends at the New Mexico AQS sites results in positive biases from June through December that approach or exceed the model performance goal of 15% NMB.

Table 4-5. State-level ozone performance indicators for 4-km WAQS simulation 2011b

Species		Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod
		Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)	(ppb)	(ppb)
AQS MDA8	CO	CAMx	6.6	14.0	3.0	6.4	6.3	13.2	48.2	51.2
		CMAQ	1.1	13.4	0.4	6.04	0.9	12.5	48.2	48.7
	UT	CAMx	4.6	14.8	1.3	6.8	2.6	13.8	49.4	50.6
		CMAQ	-0.7	15.8	-1.0	7.17	-2.0	14.5	49.4	48.4
	WY	CAMx	3.2	10.8	1.3	5.2	2.8	10.9	47.7	49.0
		CMAQ	-2.9	13.6	-1.4	6.36	-2.9	13.3	47.7	46.3
	NM	CAMx	9.1	13.8	4.2	6.4	8.9	13.6	47.4	51.6
		CMAQ	6.0	14.6	3.1	6.74	6.5	14.2	47.4	50.5
AQS MDA8 Jul-Aug	CO	CAMx	5.1	11.5	2.8	6.9	4.7	11.6	59.8	62.6
		CMAQ	0.7	11.9	0.2	7.0	0.4	11.8	59.8	60.0
	UT	CAMx	1.1	10.1	0.6	5.7	1.1	10.2	56.3	56.9
		CMAQ	-1.2	11.5	-0.5	6.4	-0.8	11.3	56.3	55.9
	WY	CAMx	6.0	10.2	3.0	5.4	5.8	10.3	51.9	54.9
		CMAQ	1.0	12.6	0.6	6.5	1.2	12.5	51.9	52.5
	NM	CAMx	11.8	14.4	6.9	8.5	12.2	15.1	56.8	63.8
		CMAQ	7.9	13.7	4.6	8.0	8.1	14.2	56.8	61.4
AQS MDA8 >60ppb	CO	CAMx	-3.6	8.7			-3.4	8.6		
		CMAQ	-8.8	12.5			-7.9	11.7		
	UT	CAMx	-15.8	18.2			-14.6	17.0		
		CMAQ	-21.3	24.3			-18.2	21.2		
	WY	CAMx	-15.6	16.9			-14.6	16.0		
		CMAQ	-24.2	25.8			-21.2	22.8		
	NM	CAMx	-6.8	11.5			-6.3	11.1		
		CMAQ	-4.1	9.7			-3.6	9.4		

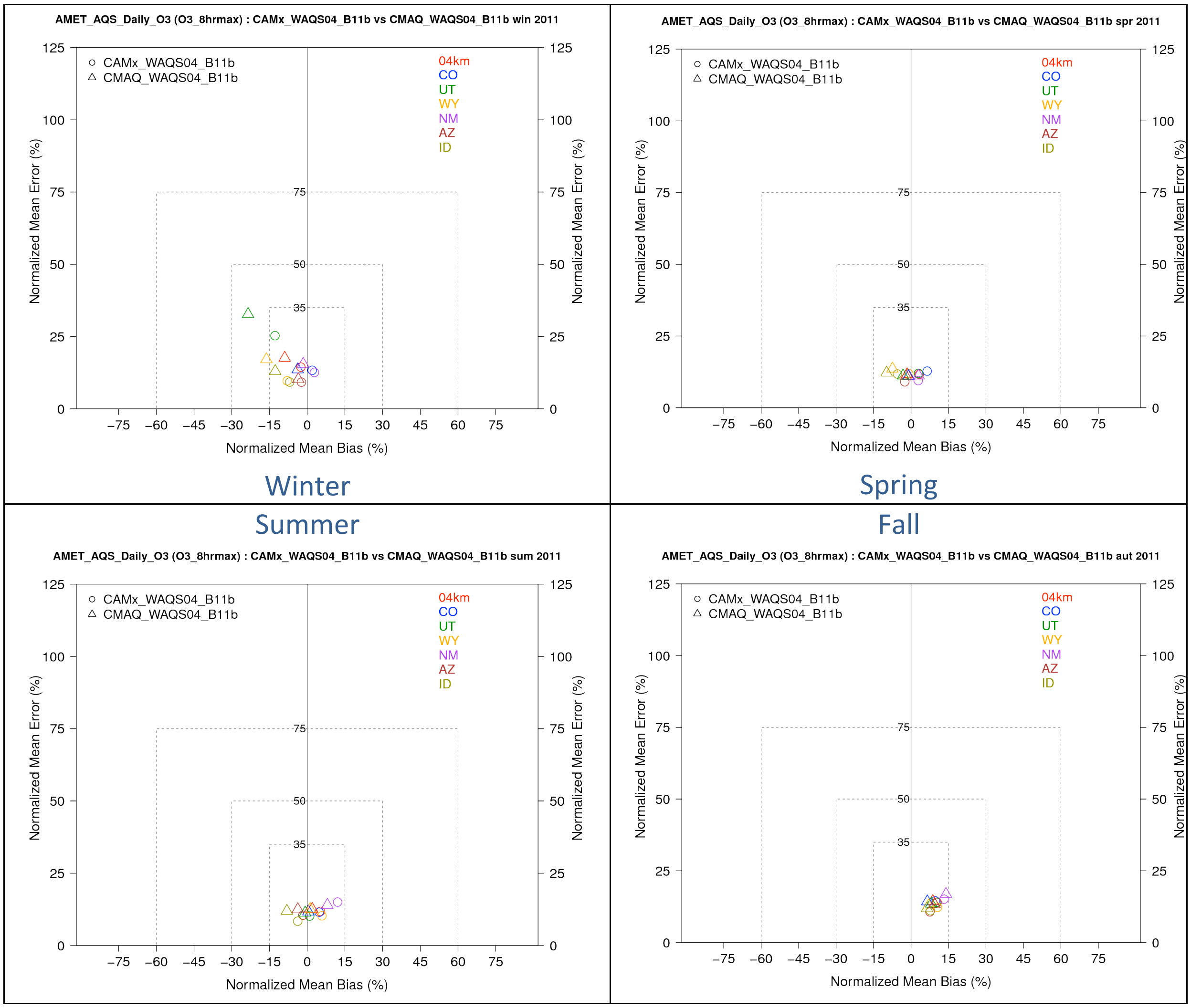


Figure 4-8. Seasonal and state average MDA8 error and bias soccer plots at AQS sites.

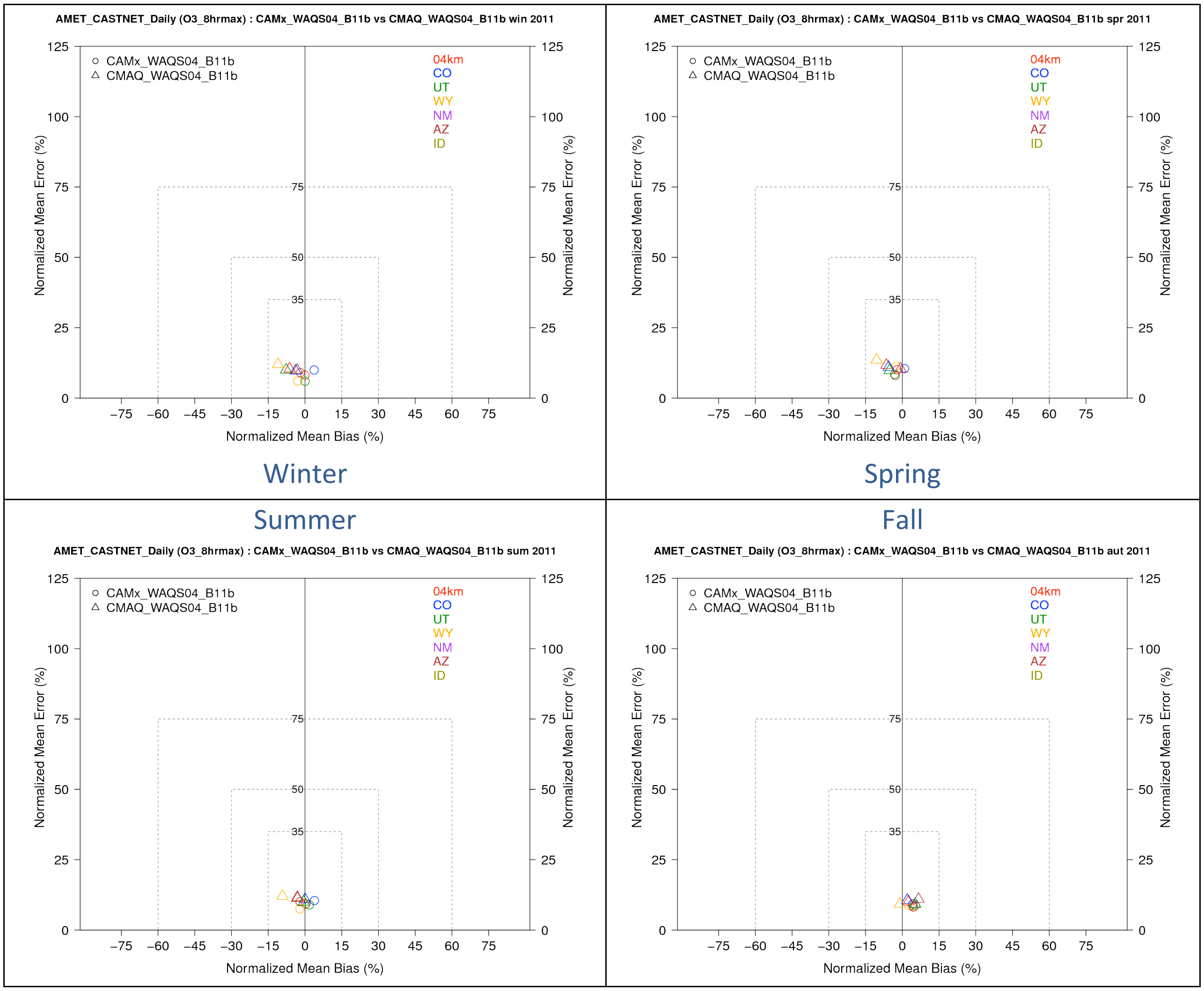


Figure 4-9. Seasonal and state average MDA8 error and bias soccer plots at CASTNet sites.

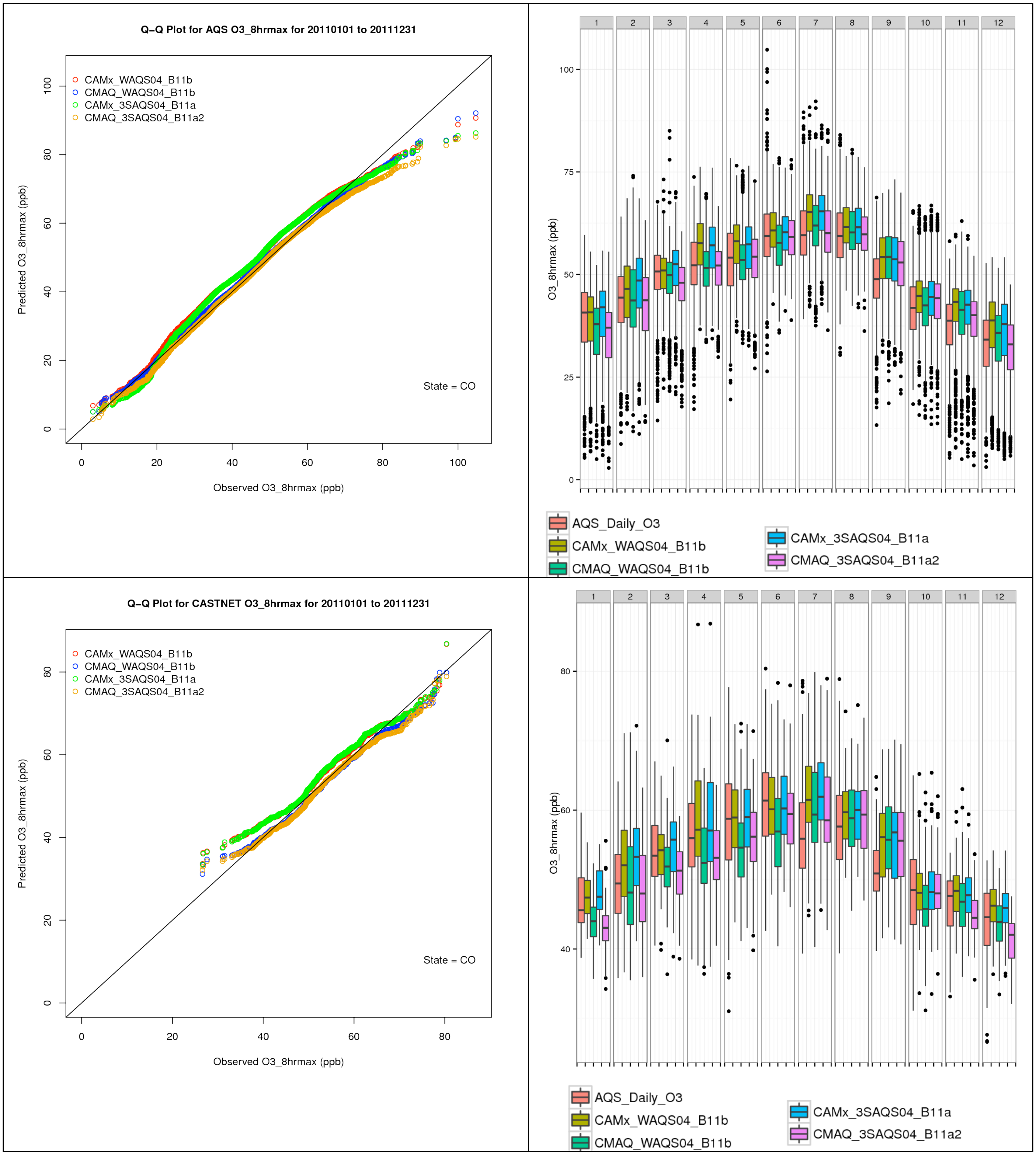


Figure 4-10. Q-Q and monthly box-whisker plots comparing Base11a and Base11b MDA8 concentrations at Colorado AQS (top) and CASTNet sites (bottom)

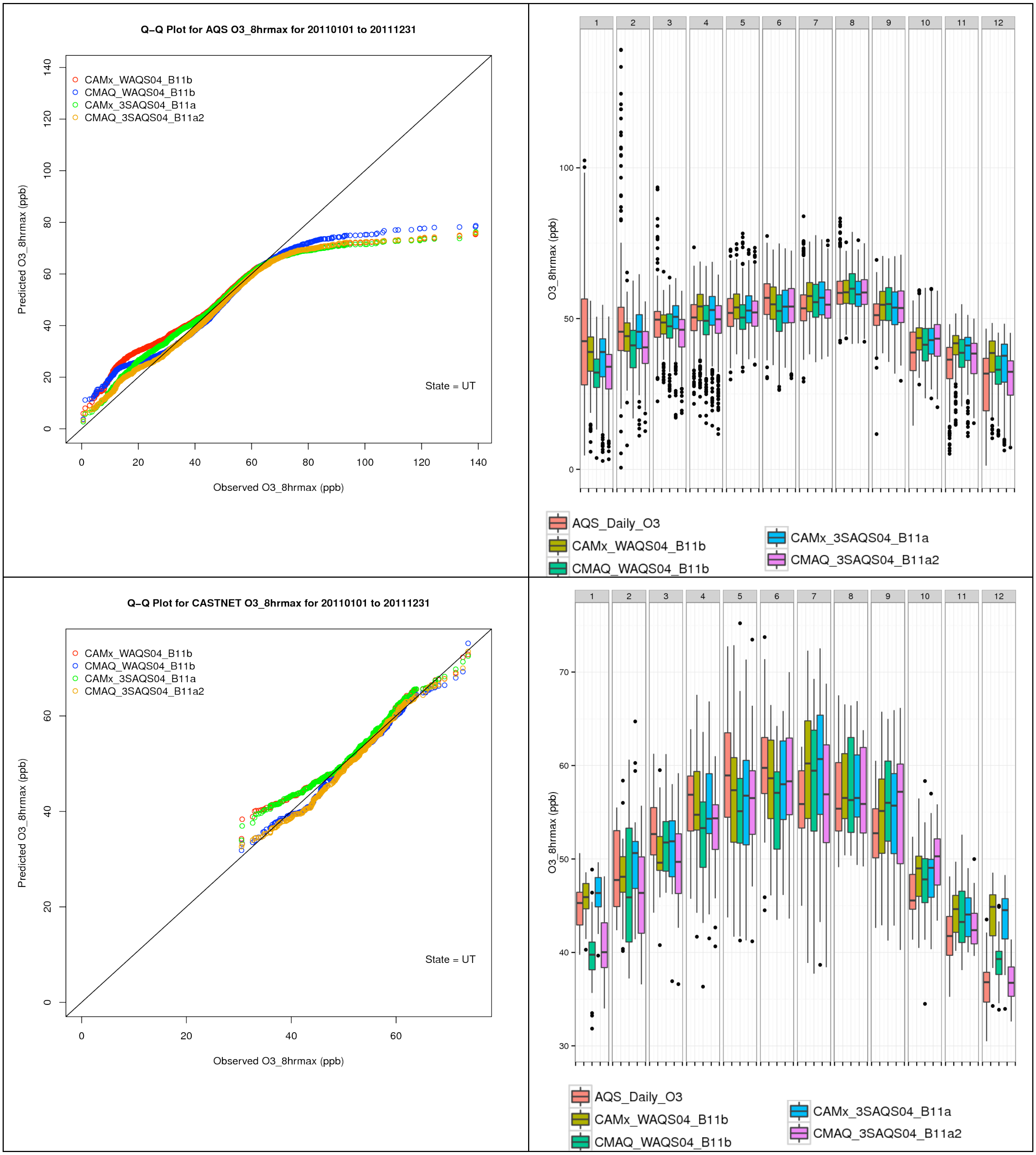


Figure 4-11. Q-Q and monthly box-whisker plots comparing Base11a and Base11b MDA8 concentrations at Utah AQS (top) and CASTNet sites (bottom)

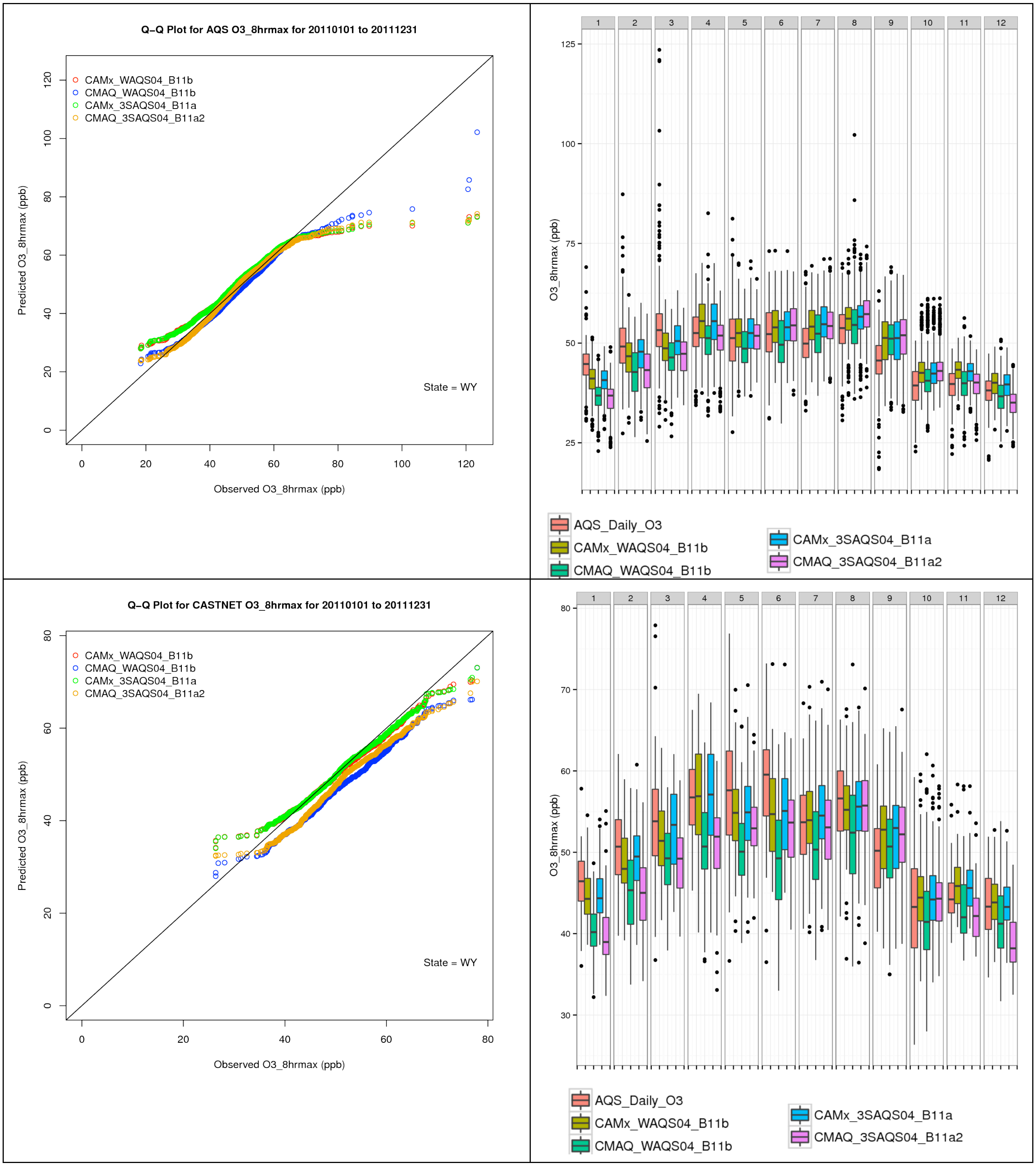


Figure 4-12. Q-Q and monthly box-whisker plots comparing Base11a and Base11b MDA8 concentrations at Wyoming AQS (top) and CASTNet sites (bottom)

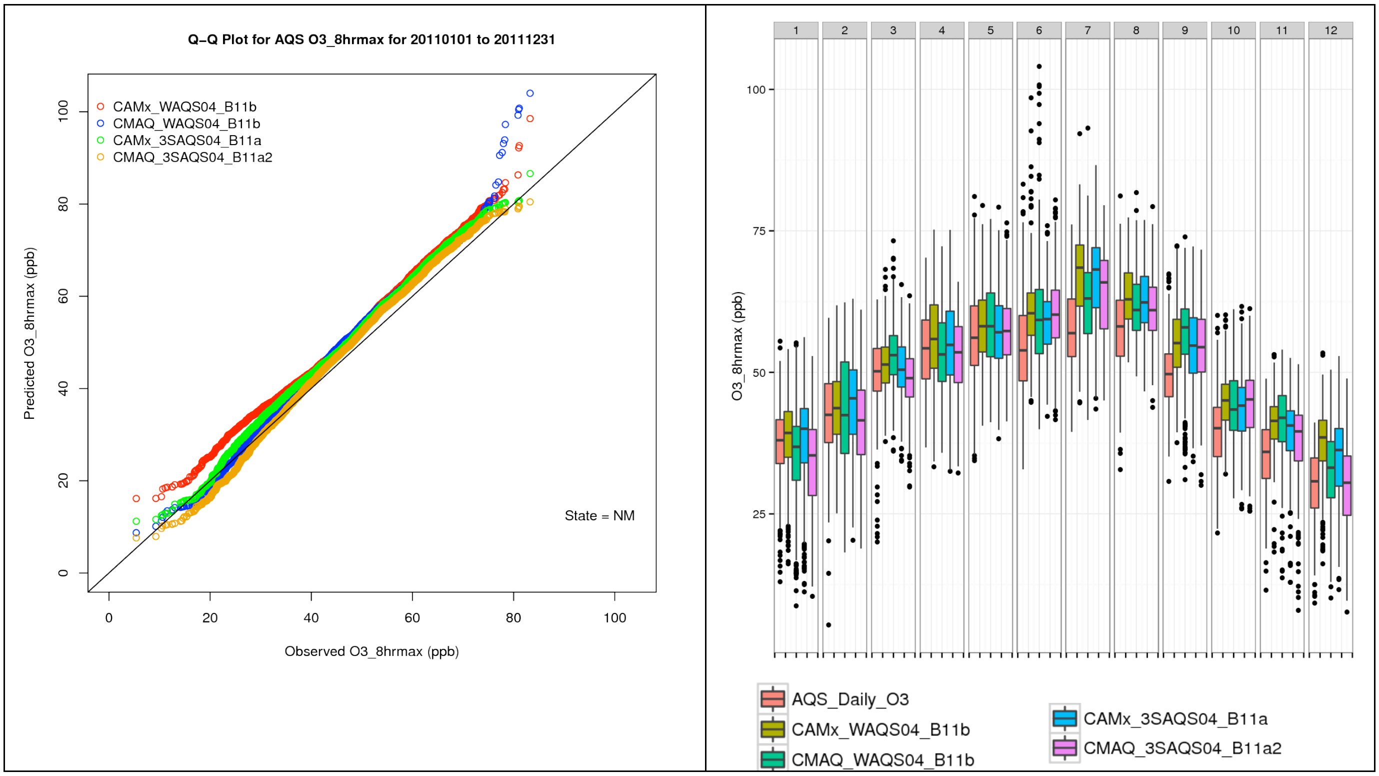


Figure 4-13. Q-Q and monthly box-whisker plots comparing Base11a and Base11b CAMx MDA8 concentrations at New Mexico AQS sites

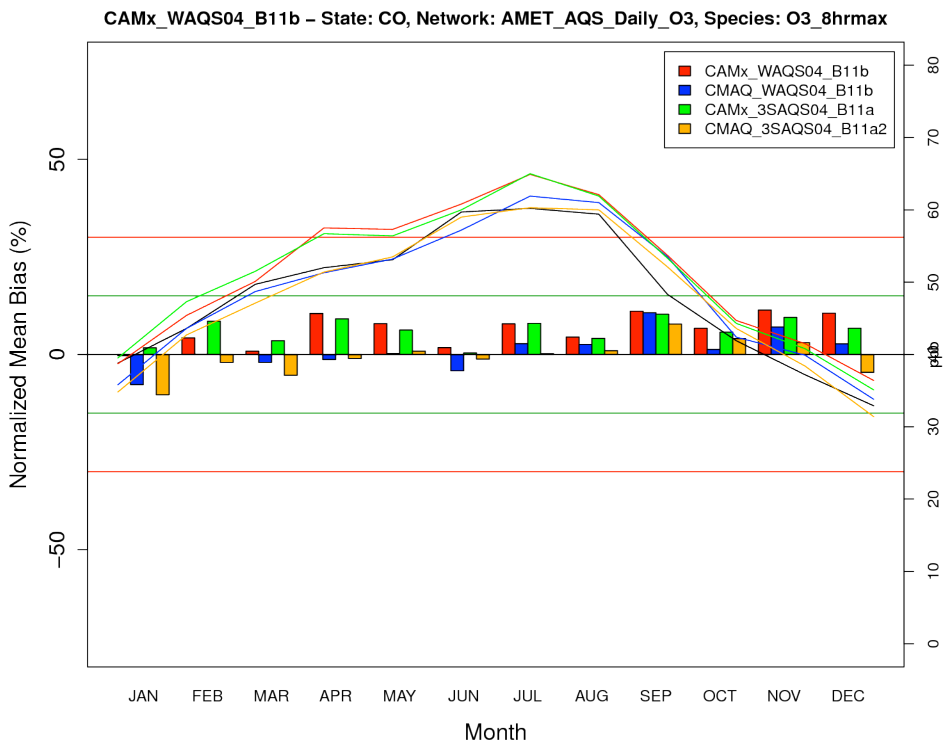


Figure 4-14. Bias-concentration plot for MDA8 predictions at AQS sites in Colorado.

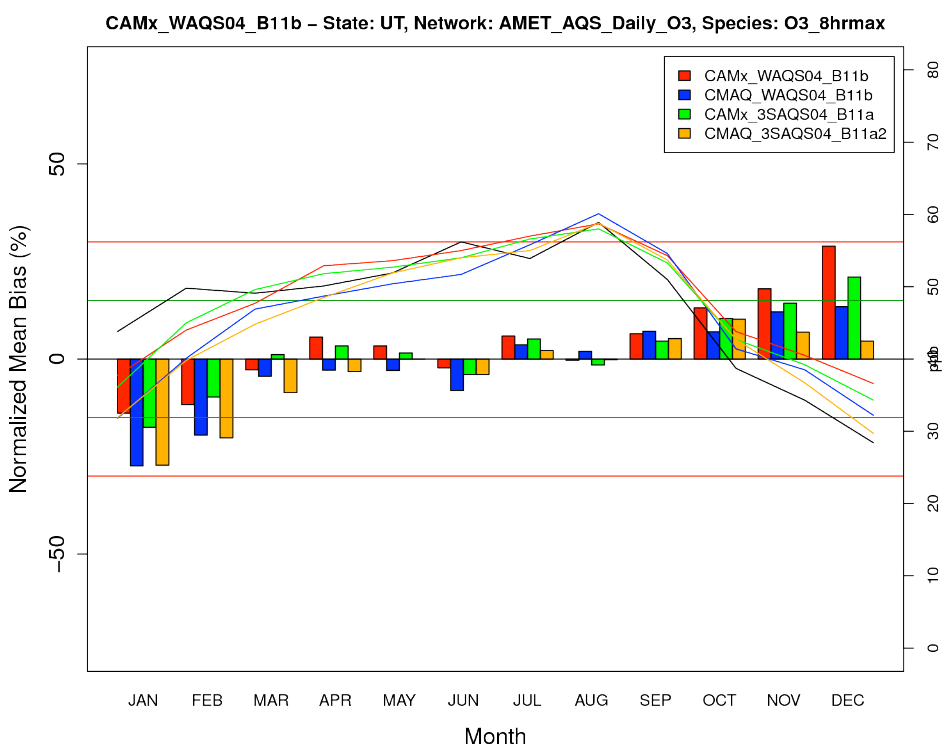


Figure 4-15. Bias-concentration plot for MDA8 predictions at AQS sites in Utah.

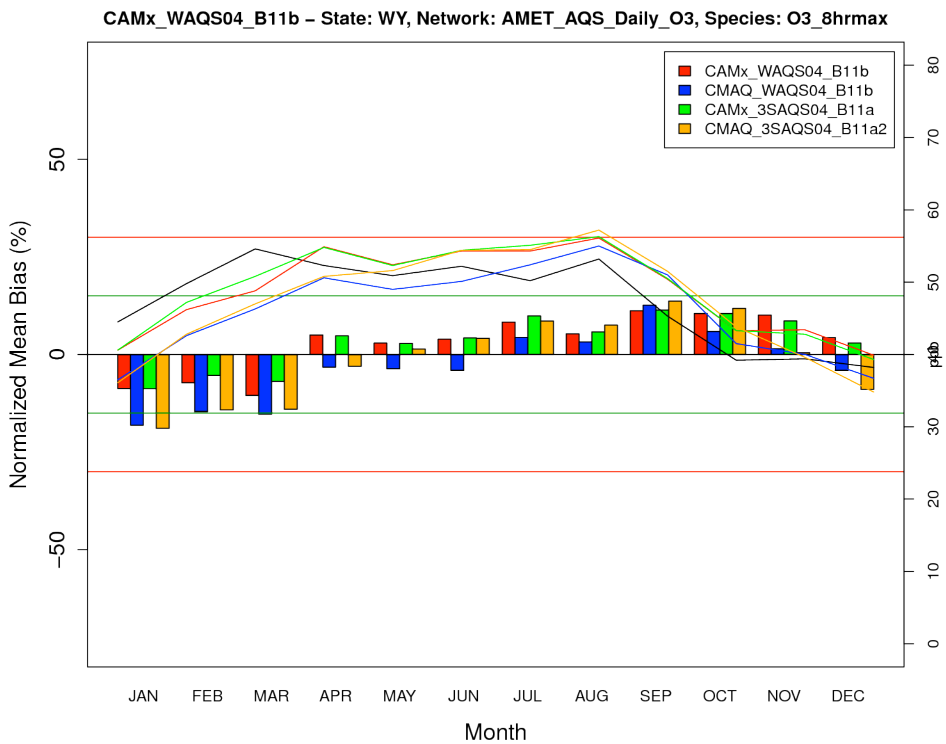


Figure 4-16. Bias-concentration plot for MDA8 predictions at AQS sites in Wyoming.

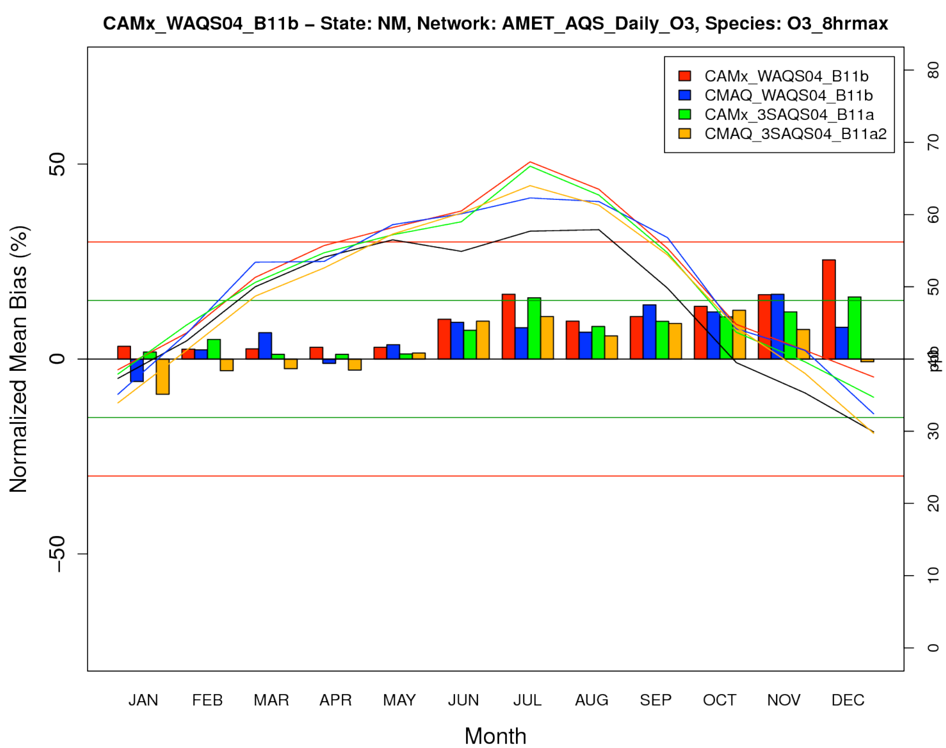


Figure 4-17. Bias-concentration plot for MDA8 predictions at AQS sites in New Mexico.

4.1.5 WAQS Base11b 4-km Model Performance at Key Monitoring Locations

This section presents the O_3 model performance at select sites within the 4-km modeling domain. We selected the sites to illustrate the model performance at regional indicator locations for different ground level O_3 formation conditions (e.g. urban, long-range transport, stratosphere-troposphere exchange). Table 4-6 shows annual average model performance statistics for MDA8 O_3 at the different sites. Along with the performance statistics, the table includes the site name, site ID, the type of ozone condition for which the site is an indicator. Both models easily meet the performance goals for all of the selected sites.

Figure 4-18 through Figure 4-32 show details of the model performance at the selected sites. Refer to the figure captions for each site to find the time period covered by the plot. The timeseries plots compare the daily MDA8 O_3 observations (black) to the CAMx (red) and CMAQ (blue) predictions. These plots include a 70 ppb reference line to highlight the level of the current National Ambient Air Quality Standard (NAAQS) for O_3.

The skill plots are modified versions of scatter plots, which compare the models (y-axis) to the observations (x-axis) for MDA8 O_3. These plots include cross hairs that indicate the current O_3 NAAQS levels and highlight in the upper right quadrant when the models correctly predict (hit) observed NAAQS exceedances. Along with the standard model performance statistics shown in the upper left quadrant of these plots, the skill plots show the number of points that fall in each quadrant. The upper left and bottom right quadrants indicate poor model performance. The upper left quadrant includes days in which the model falsely predicted exceedances. The bottom right quadrant includes days in which the model failed to predict observed exceedances. The skill plots are not shown for any of the background O_3 sites.

The box plots show period average hourly and day-of-week mean and 5^{th}-95^{th} percentile modeled and observed MDA8 O_3 concentrations. These plots highlight the general ability of the model to capture the diurnal and weekday-weekend trends in the observed O_3. The box plots are also not shown for any of the background O_3 sites.

Table 4-6. MDA8 O3 performance indicators at sites in the WAQS 4-km modeling domain

Site	Type	Model	NMB (%)	NME (%)	R^2	RMSE (ppb)	Mean Obs (ppb)	Mean Mod (ppb)
Gothic, CO CASTNet ID: GTH1	Background/ LR transport	CAMx	7.58	11.25	0.37	7.30	50.27	54.09
		CMAQ	-0.13	9.99	0.25	6.84	50.27	50.21
Mesa Verde, CO CASTNet ID: MEV405	Background	CAMx	4.87	10.31	0.59	6.45	50.41	52.87
		CMAQ	2.31	10.66	0.53	6.80	50.41	51.58
Rocky Flats N., CO AQS ID: 080590006	Rural/ High Ozone	CAMx	-1.20	11.53	0.60	7.97	53.01	52.37
		CMAQ	-6.55	12.65	0.60	8.60	53.01	49.54
Canyonlands, UT CASTNet ID: CAN407	Background	CAMx	1.92	9.01	0.54	5.88	51.08	52.05
		CMAQ	-1.37	9.77	0.49	6.54	51.08	50.38
Hawthorn, UT AQS ID: 490353006	Urban	CAMx	3.84	15.76	0.76	8.60	41.13	42.71
		CMAQ	-0.35	16.50	0.75	8.63	41.13	40.98
Navajo Lake, NM AQS ID: 350450018	Rural/ High Ozone	CAMx	2.25	11.92	0.72	7.26	48.74	49.83
		CMAQ	-0.62	14.34	0.64	8.78	48.74	48.43
Thunder Basin, WY AQS ID: 560050123	Background	CAMx	2.60	11.82	0.49	6.66	44.36	45.52
		CMAQ	0.75	13.86	0.39	7.98	44.36	44.70
Pinedale, WY AQS ID: 560350101	Rural/ Oil and Gas	CAMx	1.85	10.55	0.37	6.95	48.10	48.99
		CMAQ	-6.43	13.44	0.21	8.96	48.10	45.01

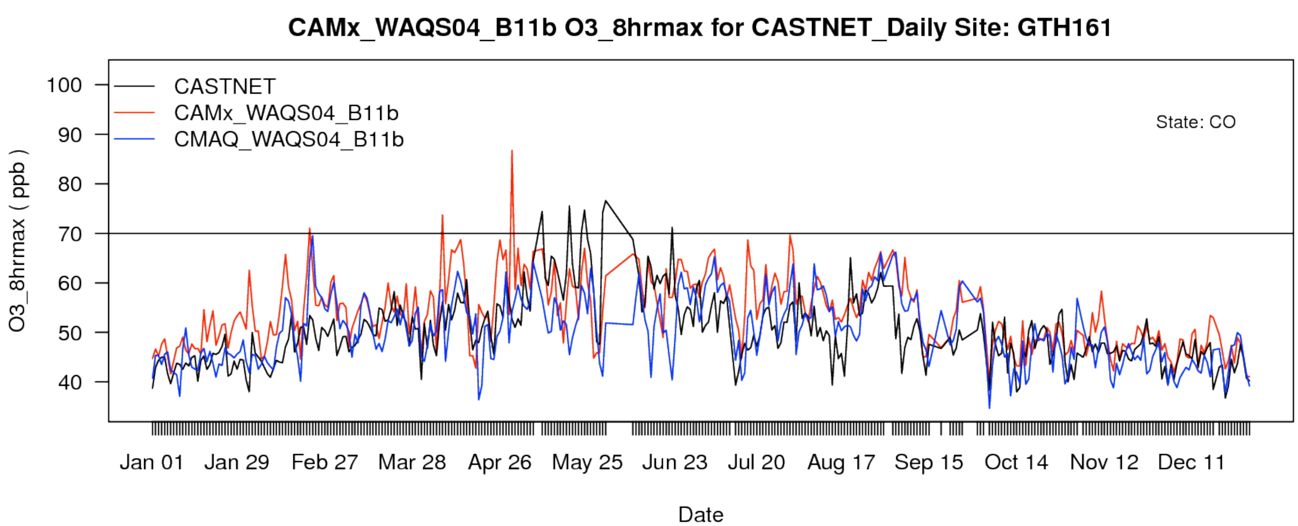


Figure 4-18. Annual 2011 MDA8 timeseries at the Gothic, Colorado CASTNet monitor.

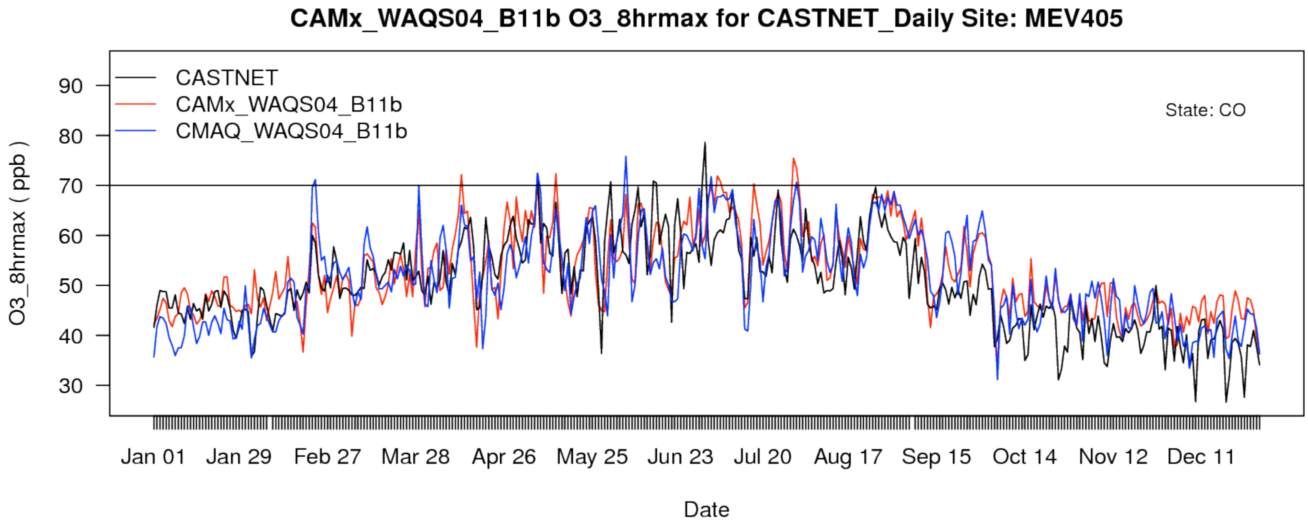


Figure 4-19. Annual 2011 MDA8 timeseries at the Mesa Verde, Colorado CASTNet monitor

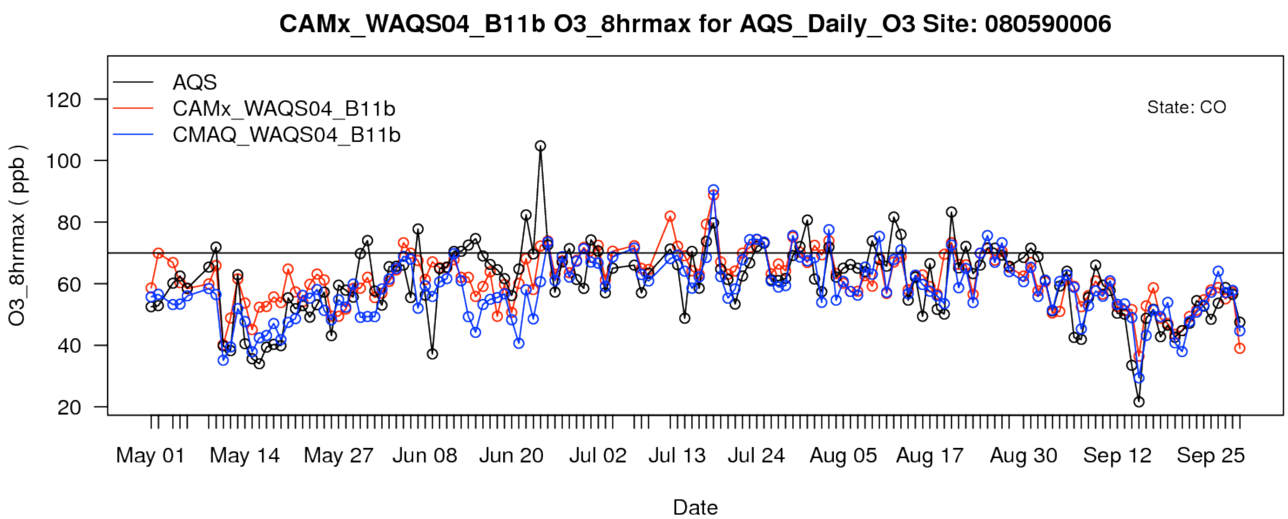


Figure 4-20. May-Sept 2011 MDA8 timeseries at the Rocky Flats N, Colorado AQS monitor

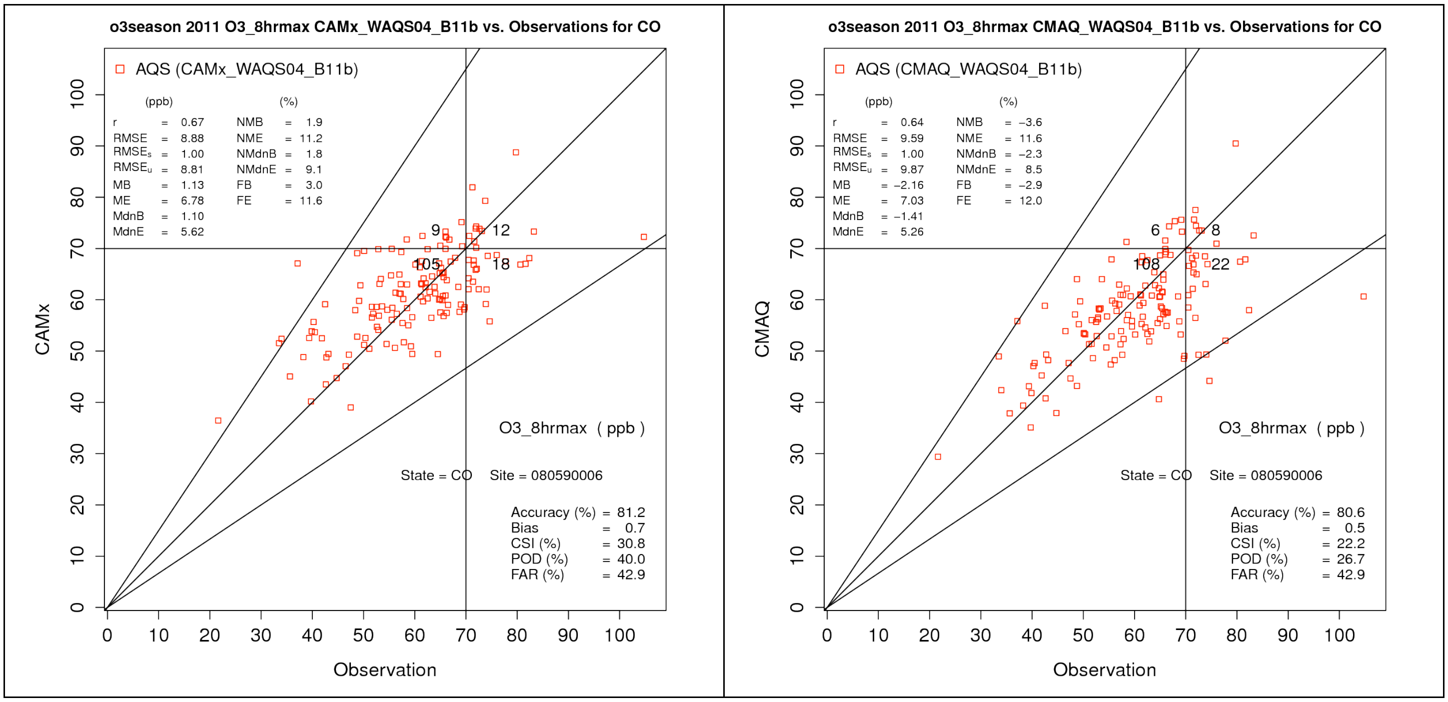


Figure 4-21. CAMx (L) and CMAQ (R) skill plots for May-Sept 2011 MDA8 at Rocky Flats N, Colorado AQS monitor

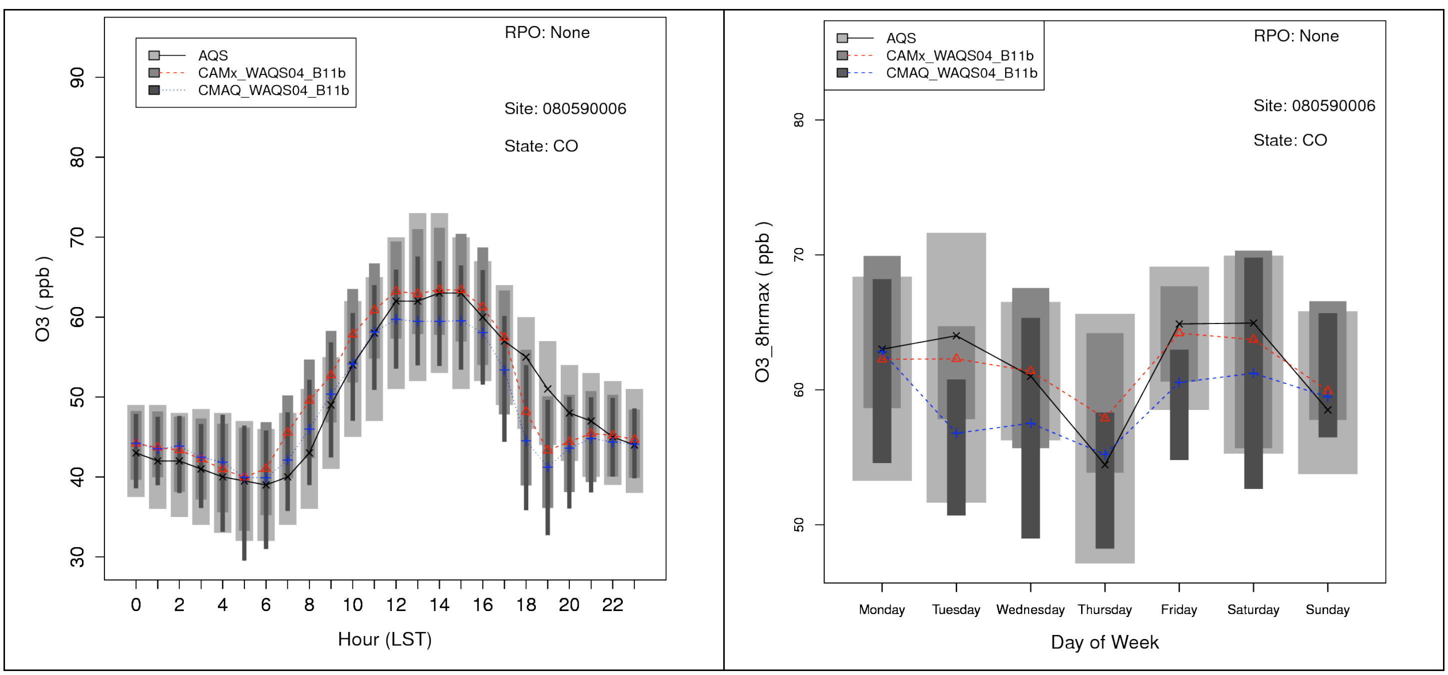


Figure 4-22. May-Sept 2011 hourly O3 diurnal plot and MDA8 day of week plot at the Rocky Flats N, Colorado AQS monitor

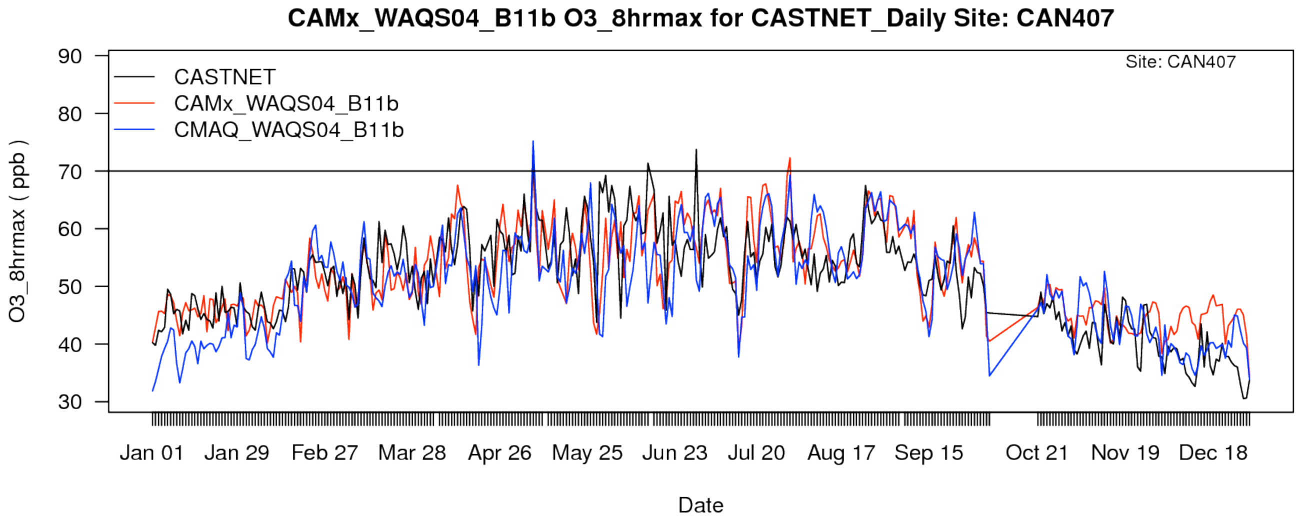


Figure 4-23. Annual 2011 MDA8 timeseries at the Canyonlands, Utah CASTNet monito

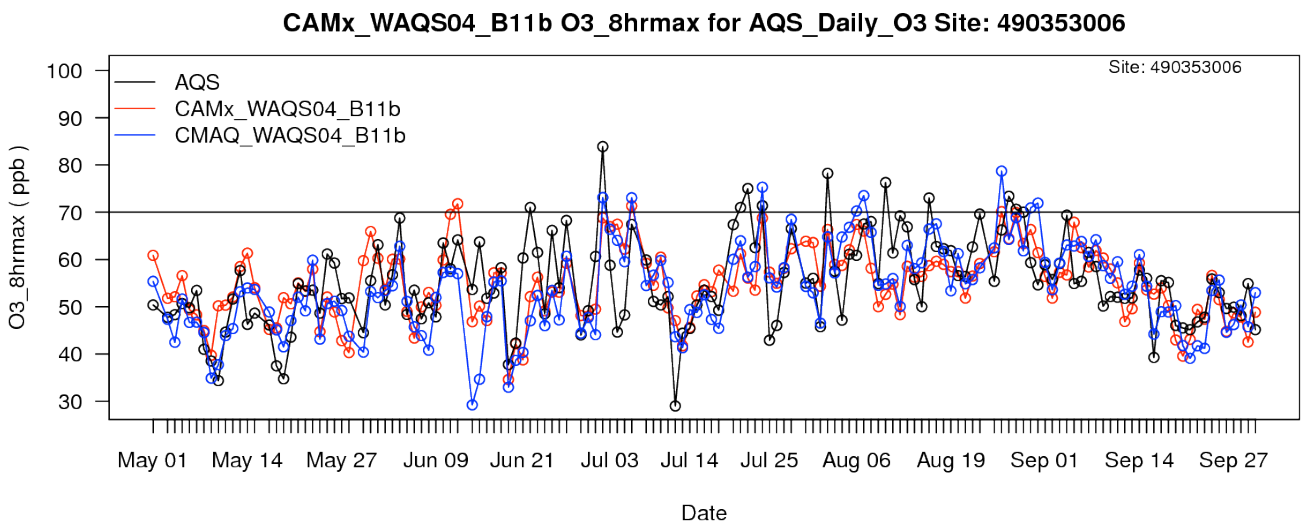


Figure 4-24. May-Sept 2011 MDA8 timeseries at the Hawthorn, UT AQS monitor

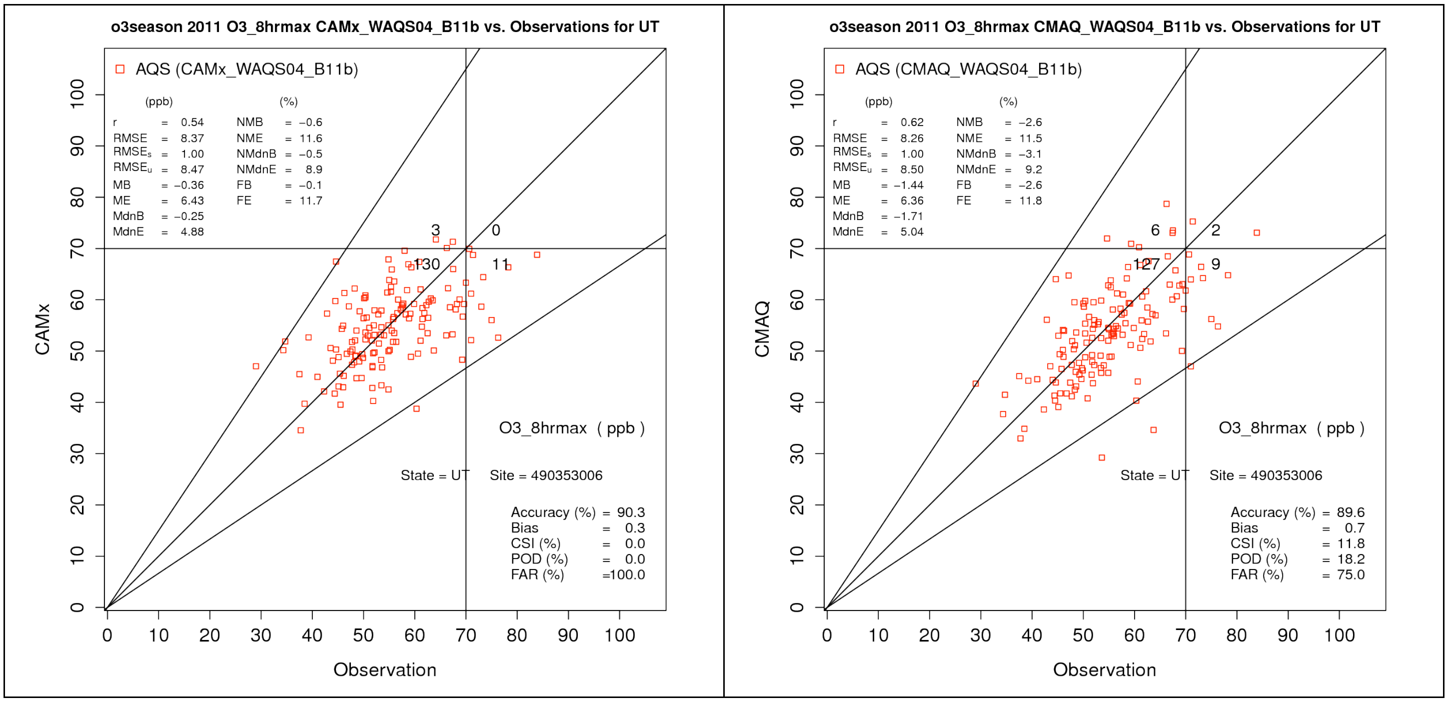


Figure 4-25. CAMx (L) and CMAQ (R) skill plots for May-Sept 2011 MDA8 at Hawthorn, UT AQS monitor

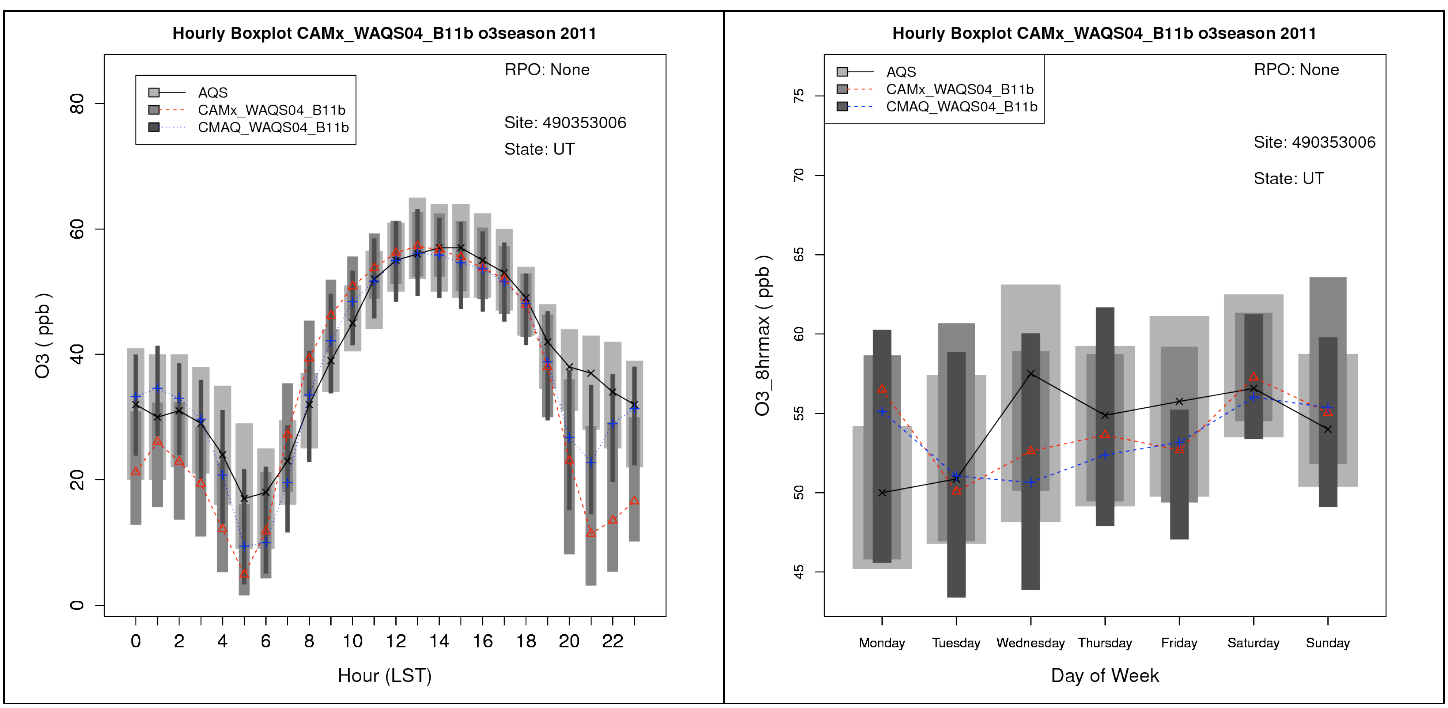


Figure 4-26. May-Sept 2011 hourly O3 diurnal plot and MDA8 day of week plot at the Hawthorn, UT AQS monitor

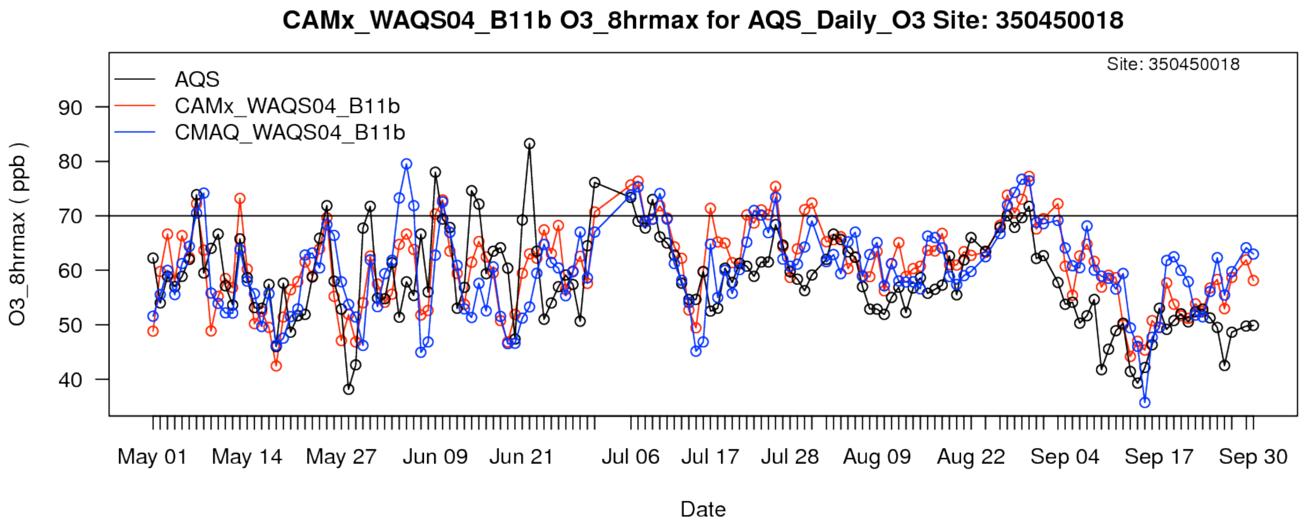


Figure 4-27. May-Sept 2011 MDA8 timeseries at the Navajo Lake, NM AQS monitor

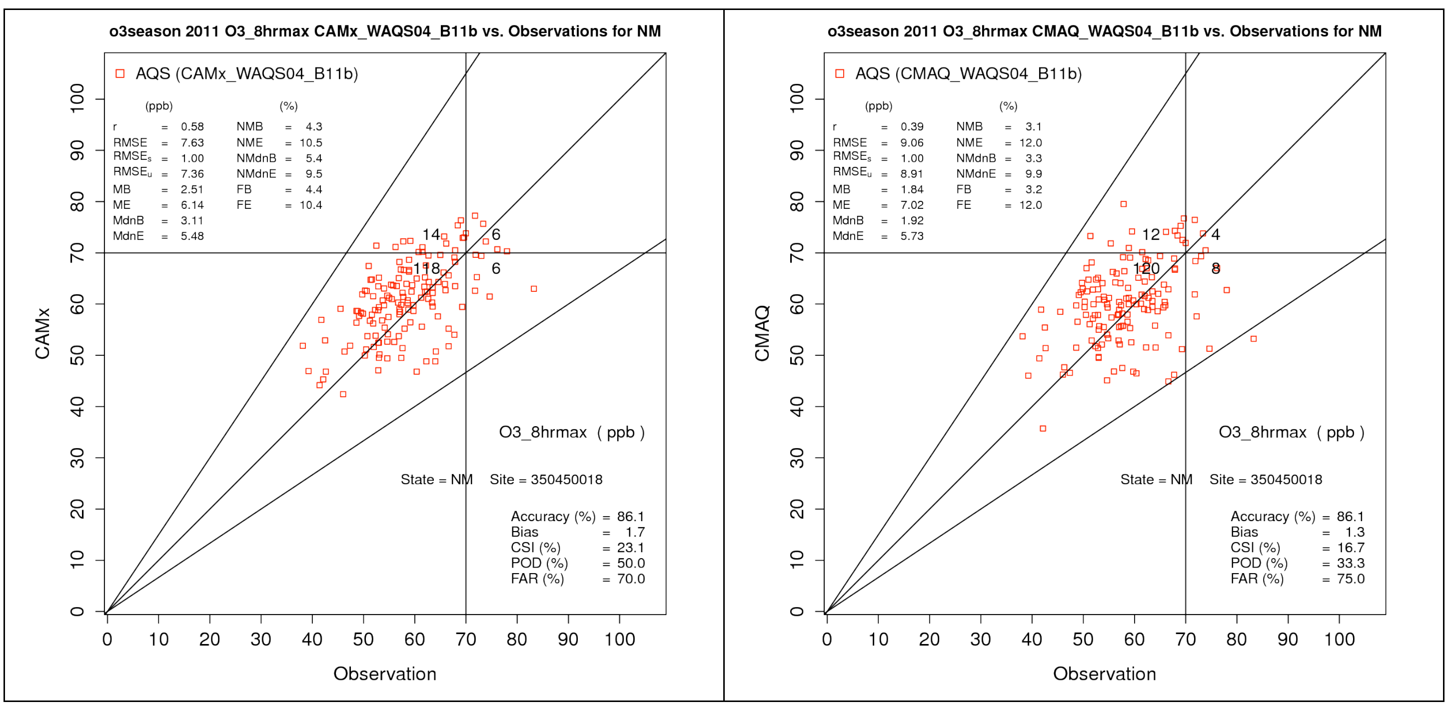


Figure 4-28. CAMx (L) and CMAQ (R) skill plots for May-Sept 2011 MDA8 at Navajo Lake, NM AQS monitor

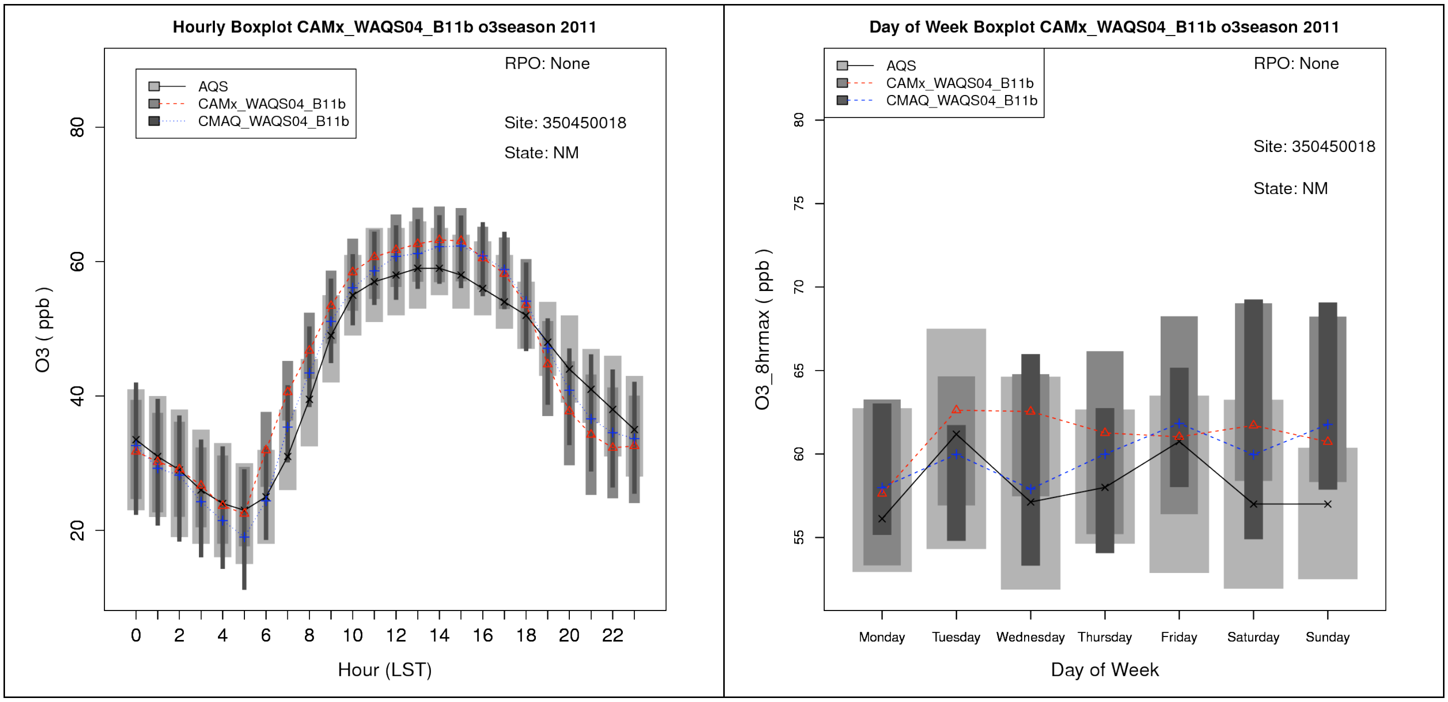


Figure 4-29. May-Sept 2011 hourly O3 diurnal plot and MDA8 day of week plot at the Navajo Lake, NM AQS monitor

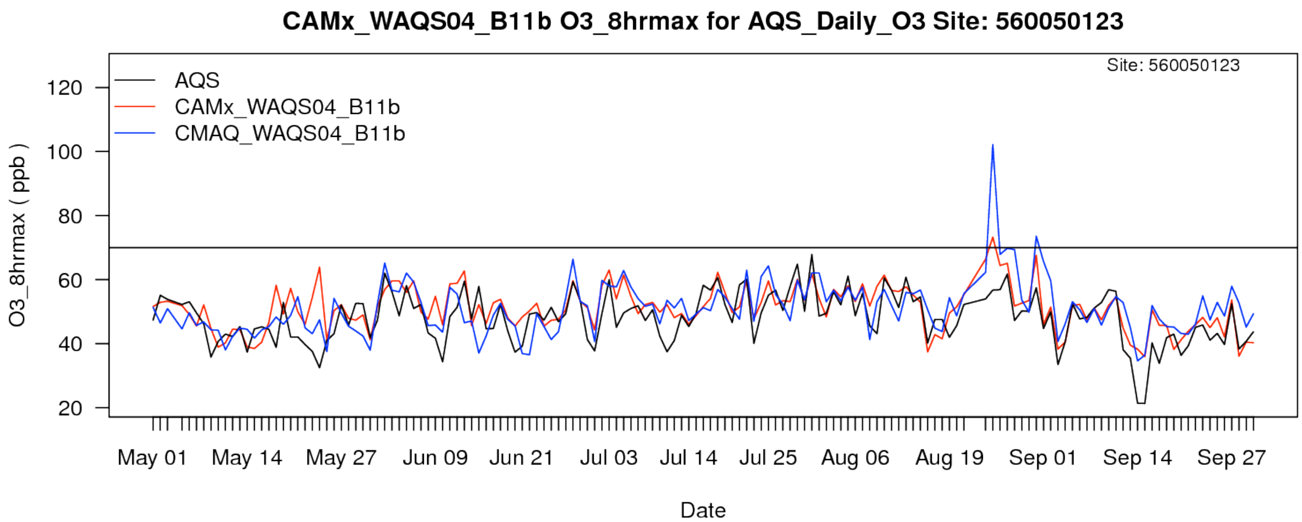


Figure 4-30. May-Sept 2011 MDA8 timeseries at the Thunder Basin, WY AQS monitor

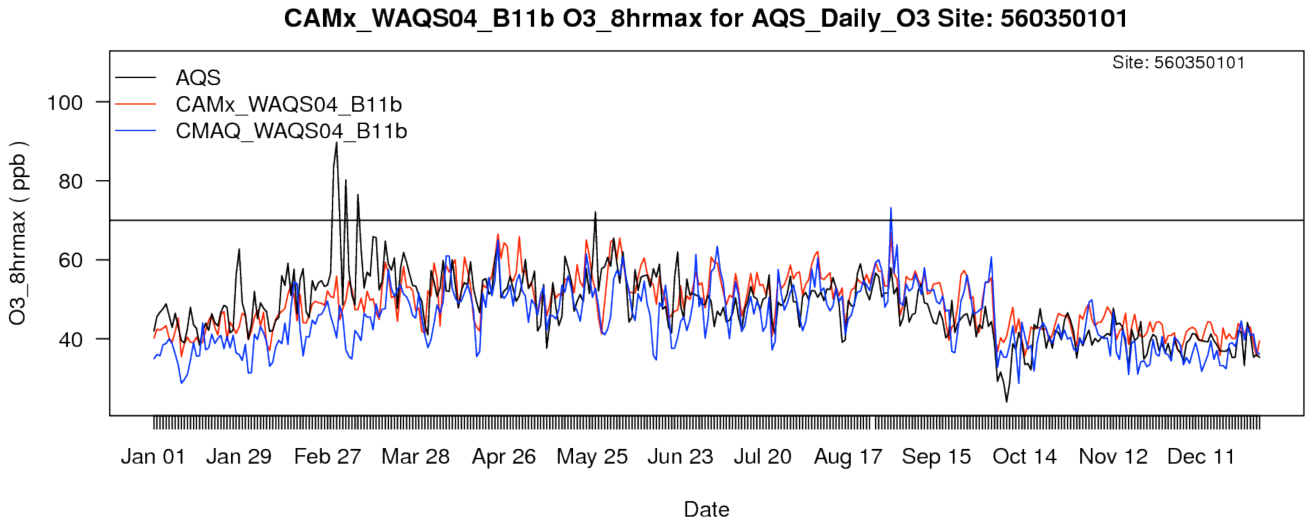


Figure 4-31. Annual 2011 MDA8 timeseries at the Pinedale, WY AQS monitor

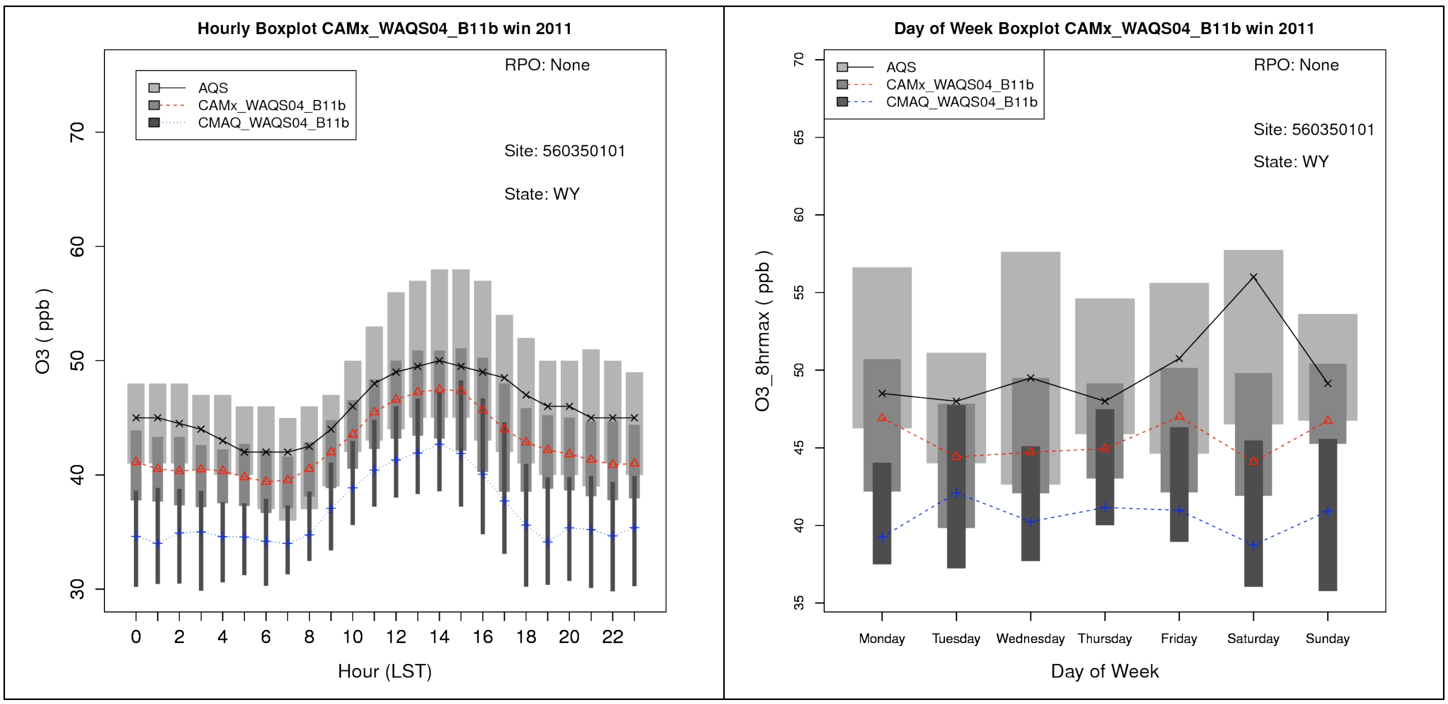


Figure 4-32. Jan-Mar 2011 hourly O3 diurnal plot and MDA8 day of week plot at the Pinedale, WY AQS monitor

4.1.6 WAQS Base11b NO_2 Model Performance

This section shows the annual average, statewide CAMx and CMAQ model performance for simulating nitrogen dioxide (NO_2). The model performance is evaluated through comparison to AQS network NO_2 observations. In general, the models both tend to overestimate NO_2, although the positive biases have been reduced in simulation Base11b relative to Base11a. CAMx estimates higher NO_2 concentrations than CMAQ, leading to higher biases in most months.

Table 4-7. State-level NO_2 performance indicators for 4-km WAQS simulation 2011b

Species		Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod
		Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)	(ppb)	(ppb)
AQS Hourly NO_2	CO	CAMx	17.2	57.0	2.7	5.5	31.2	63.3	8.6	11.3
AQS Hourly NO_2	CO	CMAQ	-7.5	65.6	1.7	4.9	19.6	57.3	8.6	10.3
AQS Hourly NO_2	UT	CAMx	8.3	57.5	0.2	5.7	1.6	56.6	10.1	10.3
AQS Hourly NO_2	UT	CMAQ	-15.2	66.2	-1.2	5.7	-11.4	56.3	10.1	9.0
AQS Hourly NO_2	WY	CAMx	8.3	63.3	0.7	2.5	25.5	85.6	2.9	3.6
AQS Hourly NO_2	WY	CMAQ	-27.9	83.0	0.5	2.6	15.7	89.0	2.9	3.4
AQS Hourly NO_2	NM	CAMx	-1.9	66.3	1.3	6.6	12.6	62.0	10.7	12.1
AQS Hourly NO_2	NM	CMAQ	-15.3	72.8	0.3	6.6	2.9	61.6	10.7	11.0

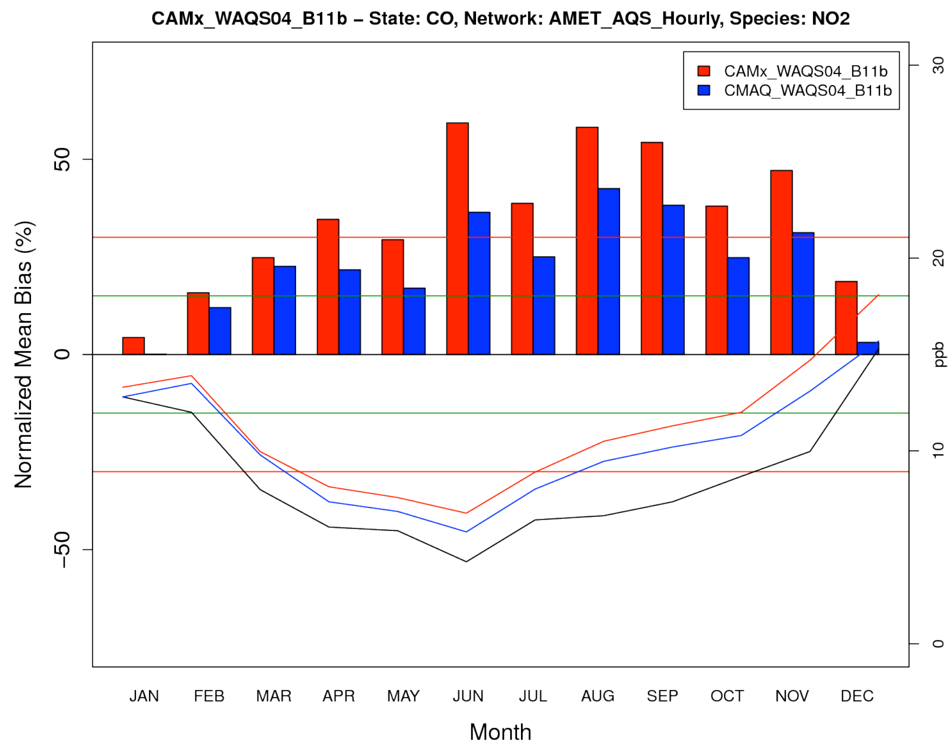


Figure 4-33. Bias-concentration plot for NO_2 predictions at AQS sites in Colorado.

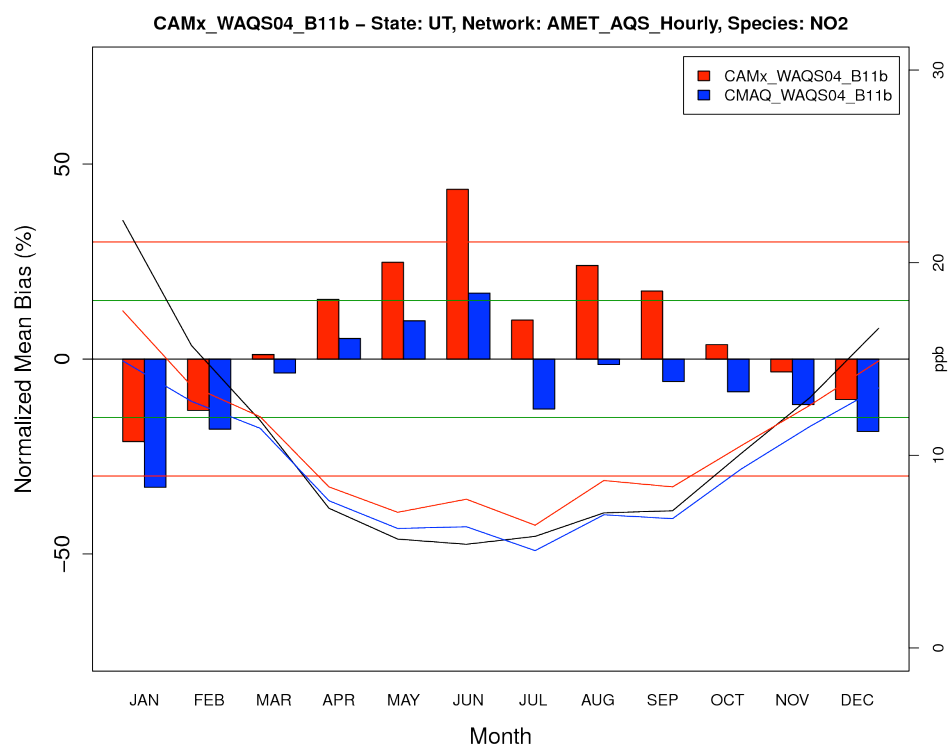


Figure 4-34. Bias-concentration plot for NO_2 predictions at AQS sites in Utah.

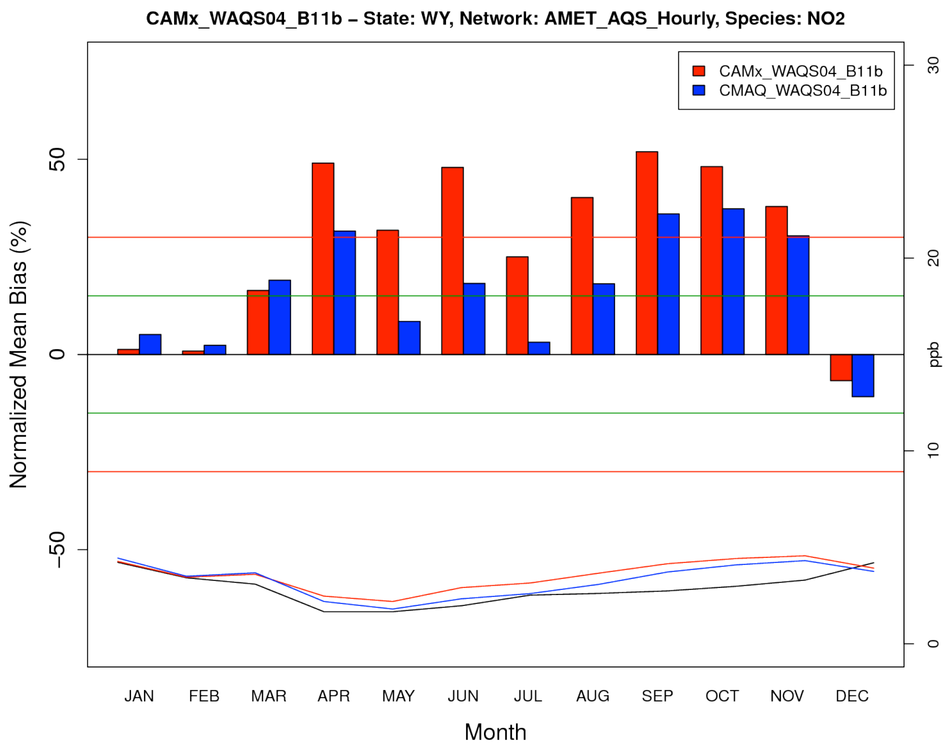


Figure 4-35. Bias-concentration plot for NO_2 predictions at AQS sites in Wyoming.

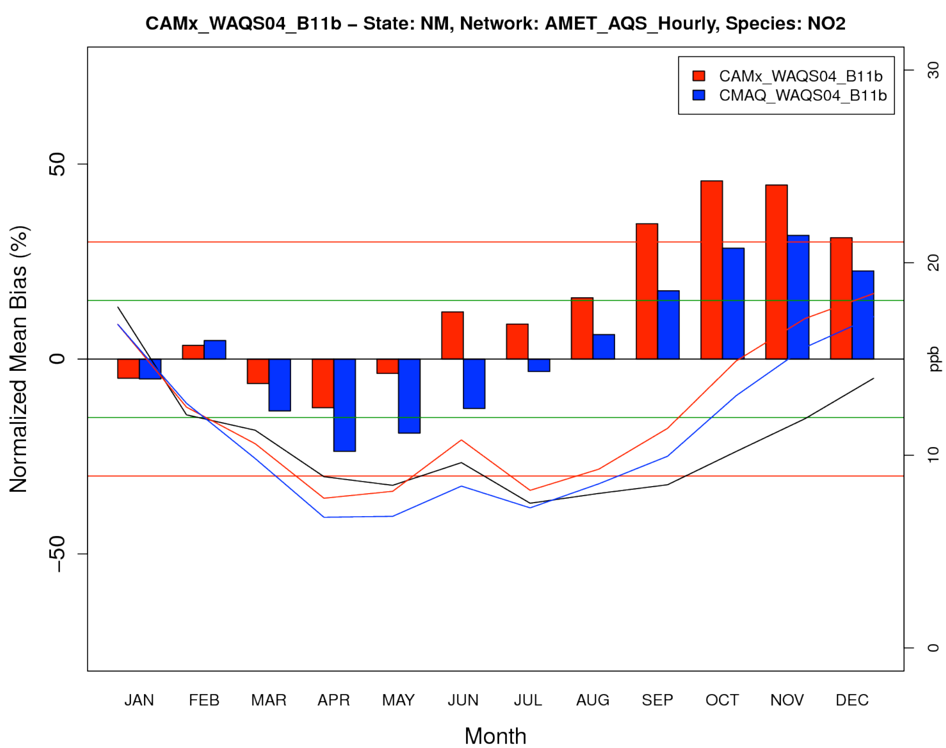


Figure 4-36. Bias-concentration plot for NO_2 predictions at AQS sites in New Mexico.

4.1.7 WAQS Base11b CO Model Performance

This section shows the annual average, statewide CAMx and CMAQ model performance for simulating carbon monoxide (CO). The model performance is evaluated through comparison to AQS network CO observations. In general, the models both tend to underestimate CO, although the performance is mixed when looking at the monthly performance in each state. CAMx exhibits high positive biases at the Colorado sites during the winter months. The magnitudes of the biases in the CMAQ simulation during the same months are much lower. Both CMAQ and CAMx exhibit similar performance in the other states, with negative biases in all months except for positive biases in January through July at the Wyoming sites.

Table 4-8. State-level CO performance indicators for 4-km WAQS simulation 2011b

Species		Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod
		Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)	(ppb)	(ppb)
AQS Hourly CO	CO	CAMx	-6.6	53.6	41.2	233.0	12.0	67.9	344.0	385.0
		CMAQ	-14.6	53.3	-23.6	195.0	-6.9	56.7	344.0	320.0
	UT	CAMx	-25.4	56.7	-107.0	242.0	-24.6	56.1	432.0	326.0
		CMAQ	-31.8	58.3	-143.0	240.0	-33.0	55.4	432.0	290.0
	WY	CAMx	27.5	93.2	-22.6	149.0	-13.5	89.2	167.0	145.0
		CMAQ	22.2	94.5	-31.5	149.0	-18.8	89.2	167.0	136.0
	NM	CAMx	-24.0	61.4	-131.0	223.0	-32.1	54.9	407.0	276.0
		CMAQ	-32.6	64.9	-166.0	232.0	-40.9	56.9	407.0	240.0

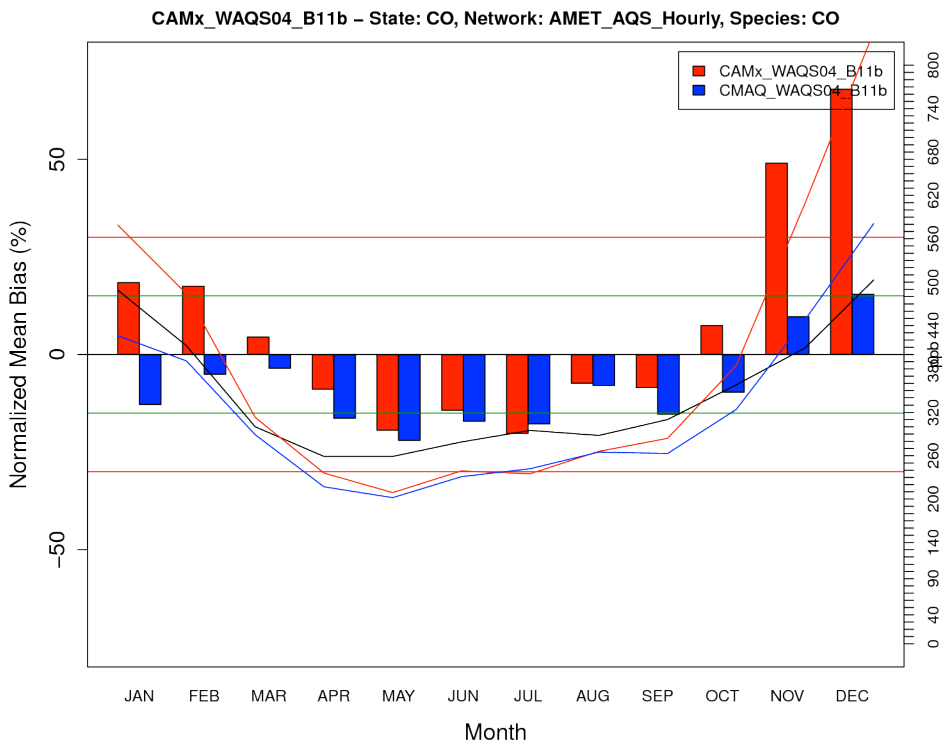


Figure 4-37. Bias-concentration plot for CO predictions at AQS sites in Colorado.

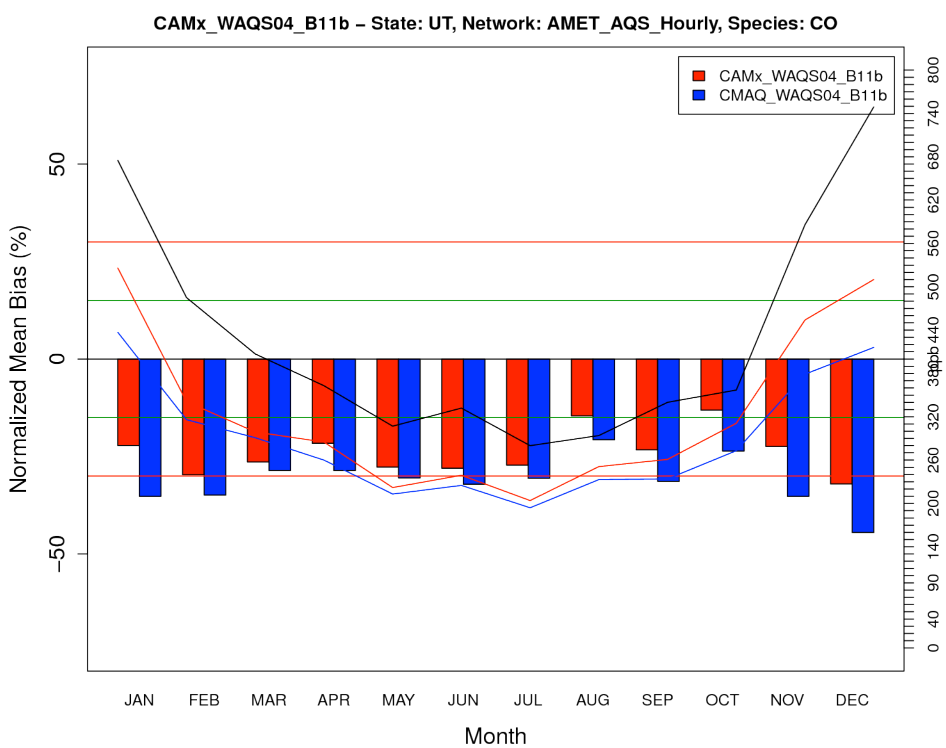


Figure 4-38. Bias-concentration plot for CO predictions at AQS sites in Utah.

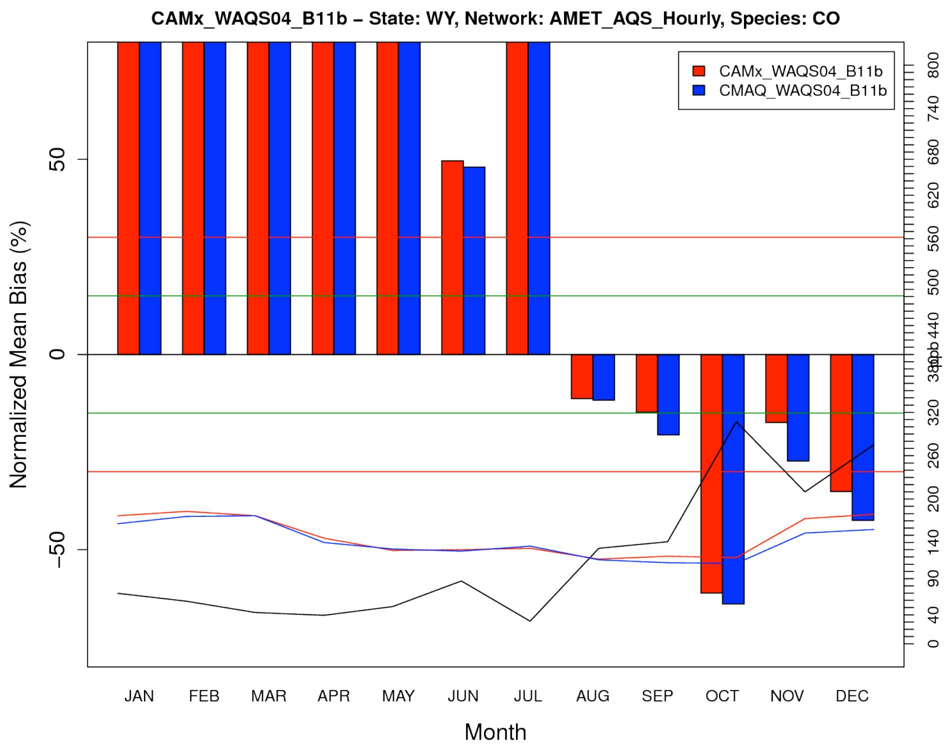


Figure 4-39. Bias-concentration plot for CO predictions at AQS sites in Wyoming.

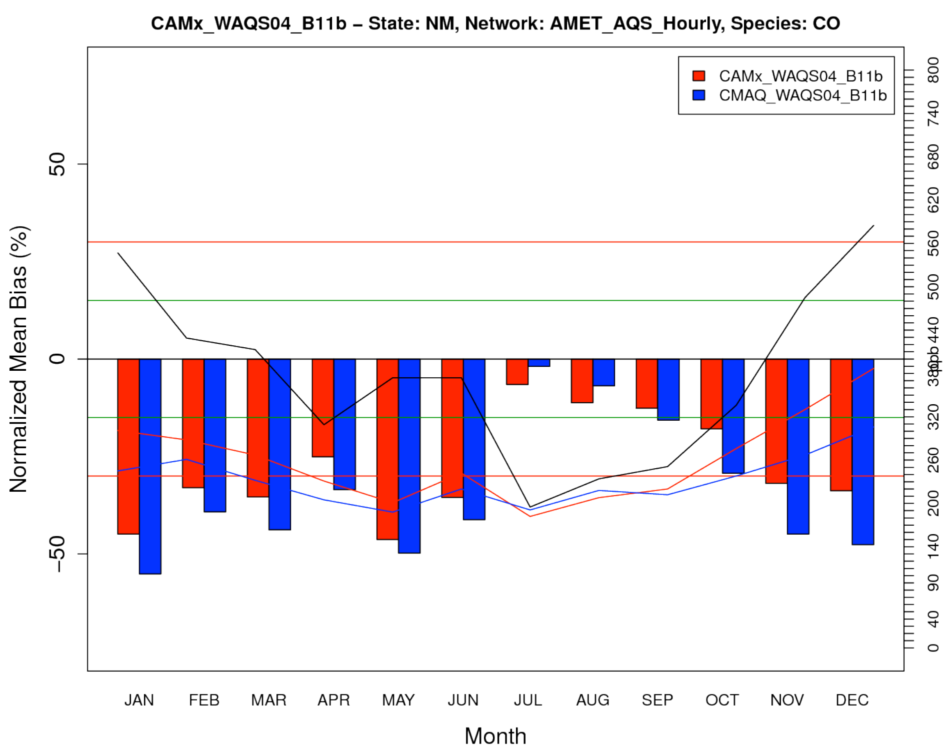


Figure 4-40. Bias-concentration plot for CO predictions at AQS sites in New Mexico.

4.1.8 WAQS Base11b SO_2 Model Performance

This section shows the annual average, statewide CAMx and CMAQ model performance for simulating sulfur dioxide (SO_2). The model performance is evaluated through comparison to AQS network SO_2 observations. In Utah, Wyoming, New Mexico the models both tend to underestimate SO_2; the models overestimate SO_2 in Colorado. The simulated SO_2 trends outside of Colorado are relatively flat across the months and consistent in both CAMx and CMAQ. The profile of the simulated SO_2 concentrations at the Colorado sites shows elevated concentrations in June through October in both models that are not present in the observations. CMAQ also estimates elevated SO_2 in March at the Colorado AQS sites that exists in neither the observations nor the CAMx simulation.

Table 4-9. State-level SO_2 performance indicators for 4-km WAQS simulation 2011b

Species		Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod
		Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)	(ppb)	(ppb)
AQS Hourly SO2	CO	CAMx	15.7	80.4	0.8	2.7	31.0	105.0	2.6	3.4
		CMAQ	8.3	85.8	1.1	3.2	41.2	121.0	2.6	3.7
	UT	CAMx	-71.8	96.6	-0.8	1.1	-50.1	71.1	1.6	0.8
		CMAQ	-81.6	102.0	-0.9	1.1	-55.3	72.1	1.6	0.7
	WY	CAMx	-21.2	103.0	-1.5	2.4	-60.7	97.0	2.4	1.0
		CMAQ	-27.9	102.0	-1.3	2.5	-52.7	103.0	2.4	1.2
	NM	CAMx	-32.3	90.0	-0.2	1.0	-17.3	86.2	1.1	0.9
		CMAQ	-45.0	93.8	-0.3	1.0	-27.3	84.8	1.1	0.8

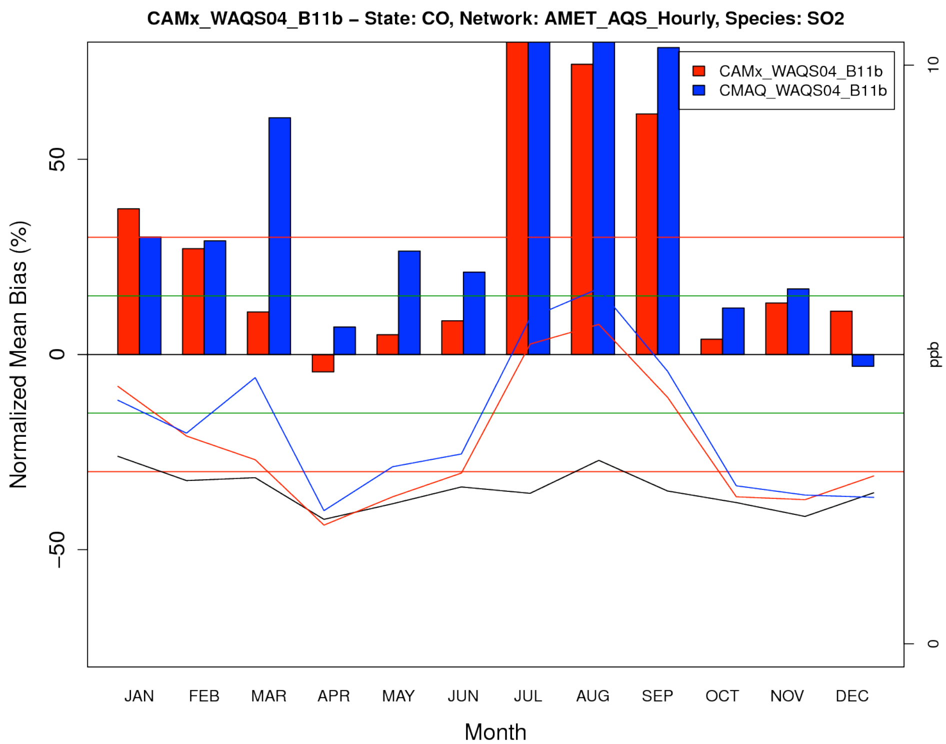


Figure 4-41. Bias-concentration plot for SO_2 predictions at AQS sites in Colorado.

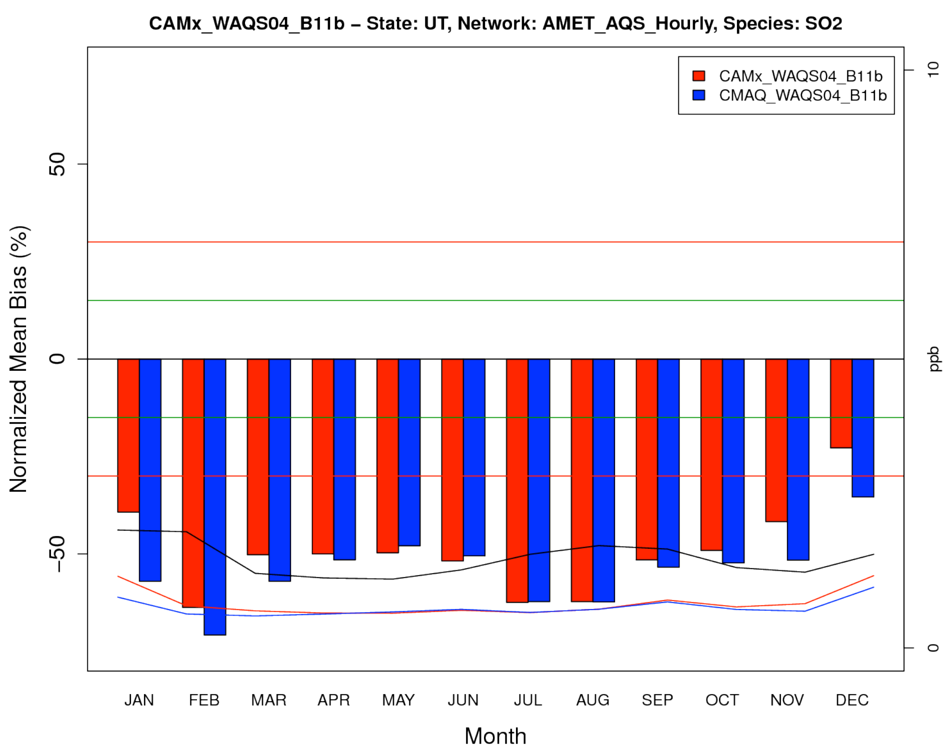


Figure 4-42. Bias-concentration plot for SO_2 predictions at AQS sites in Utah.

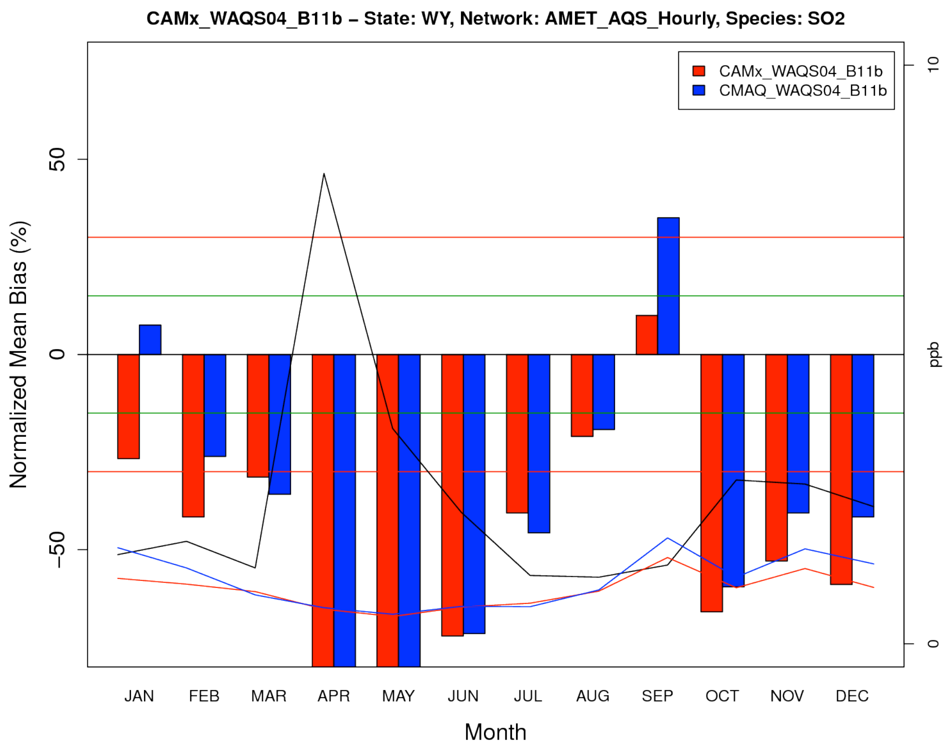


Figure 4-43. Bias-concentration plot for SO_2 predictions at AQS sites in Wyoming.

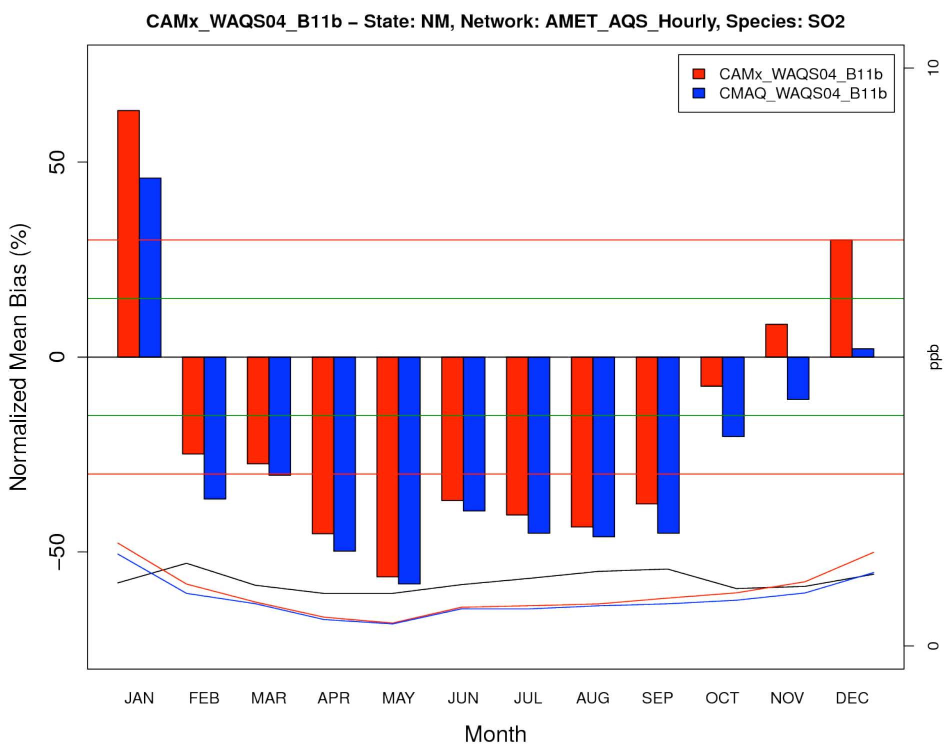


Figure 4-44. Bias-concentration plot for SO_2 predictions at AQS sites in New Mexico.

4.1.9 WAQS Base11b Winter Model Performance

As one of the focus points of the WAQS is to simulate winter season high O_3 concentrations in western oil and gas basins, this section presents the model performance at monitors located near a few oil and gas development areas that were active in 2011. The analysis periods presented here include periods of high observed ozone. Three monitoring sites that measured both ozone and NO_2 in 2011 include:

- Rangely, CO; Rio Blanco County; Piceance Basin
- Myton, UT; Uintah County; Uintah Basin
- Pinedale, WY; Sublette County; Southwest Wyoming Basin

Figure 4-45 through Figure 4-50 present Q-Q and timeseries plots for hourly O_3 and NO_2 at each monitoring site. These figures show that neither models simulate the high O_3 concentrations observed at these sites. As CAMx systematically simulates higher O_3 than CMAQ, it provides a slightly better model of winter O_3, although it still does not capture the peak O_3 concentrations. CMAQ simulates higher NO_2 than CAMx at Rangely, CO and Pinedale, WY, but lower NO_2 at Myton, UT.

Simulation Base11b estimates higher winter O_3 concentrations at these sites than Base11a, particularly for CAMx. This is a notable trend because simulation Base11b includes meteorology adjustments designed to improve the simulation of conditions that contribute to high ozone (Bowden et al., 2015). Despite these meteorology improvements, the WAQS winter O_3 model still does not adequately simulate the dynamical and chemical conditions that produced very high O_3 concentrations in these basins during the winter of 2011.

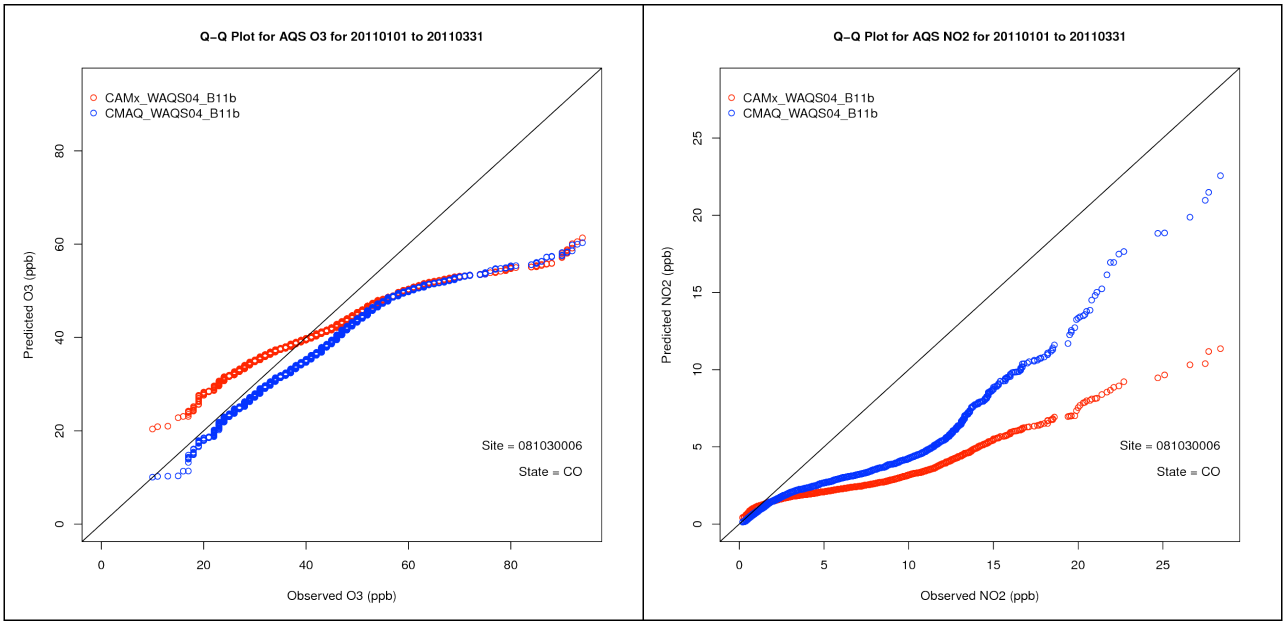
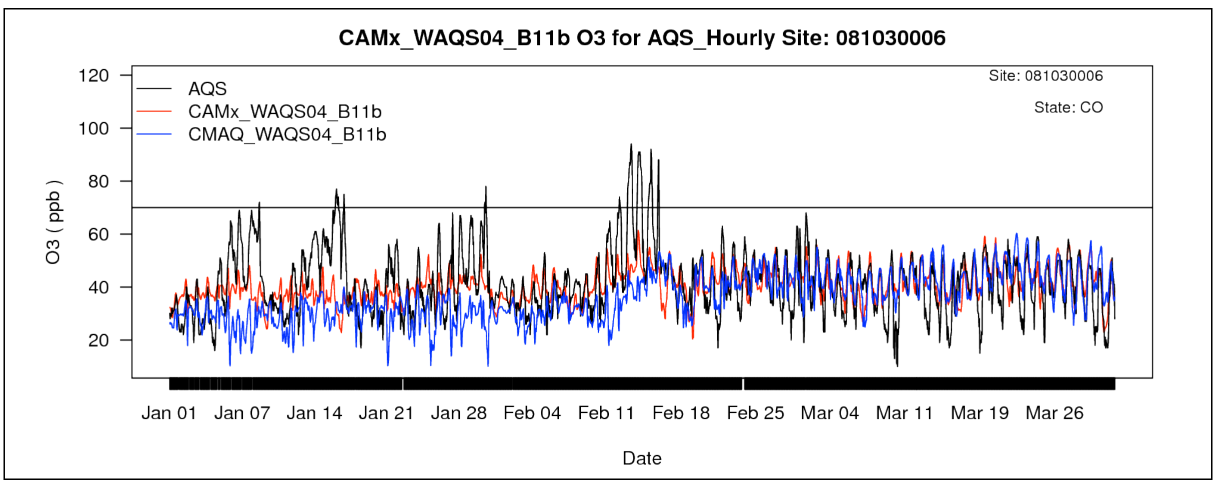


Figure 4-45. Rangely, Colorado AQS Hourly O_3 and NO_2 Q-Q plot for Jan-Feb 2011



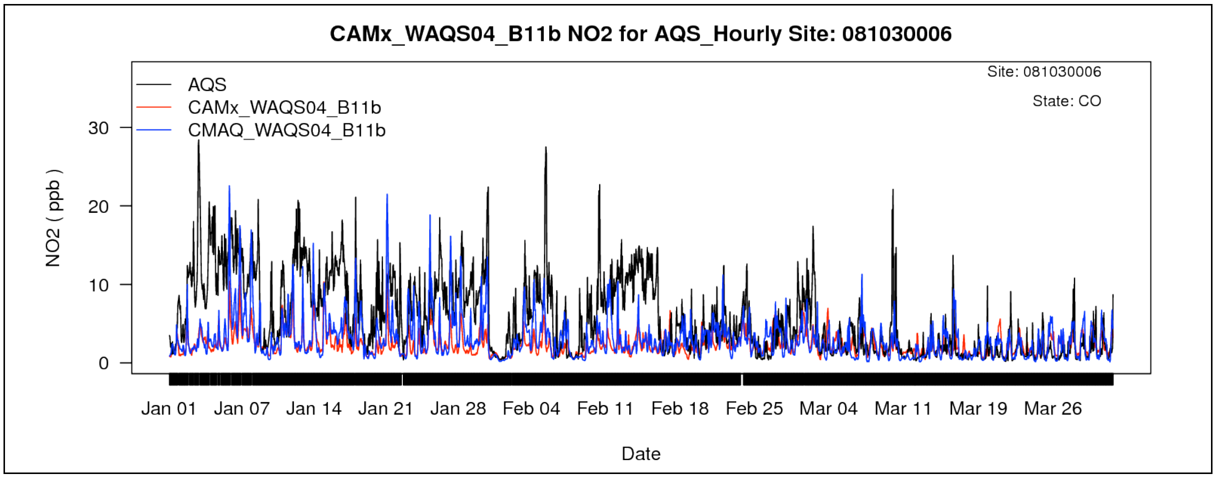


Figure 4-46. Rangely, Colorado AQS Hourly O_3 and NO_2 for Jan-Mar 2011

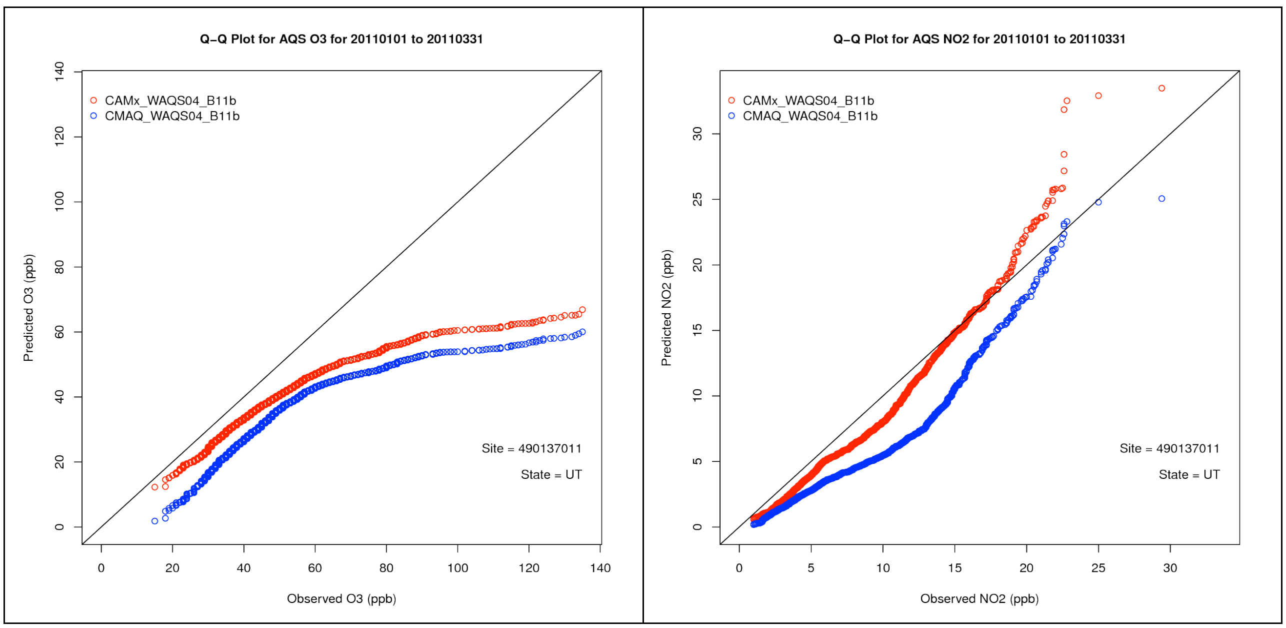


Figure 4-47. Myton, Utah AQS Hourly O_3 and NO_2 Q-Q plot for Jan-Mar 2011

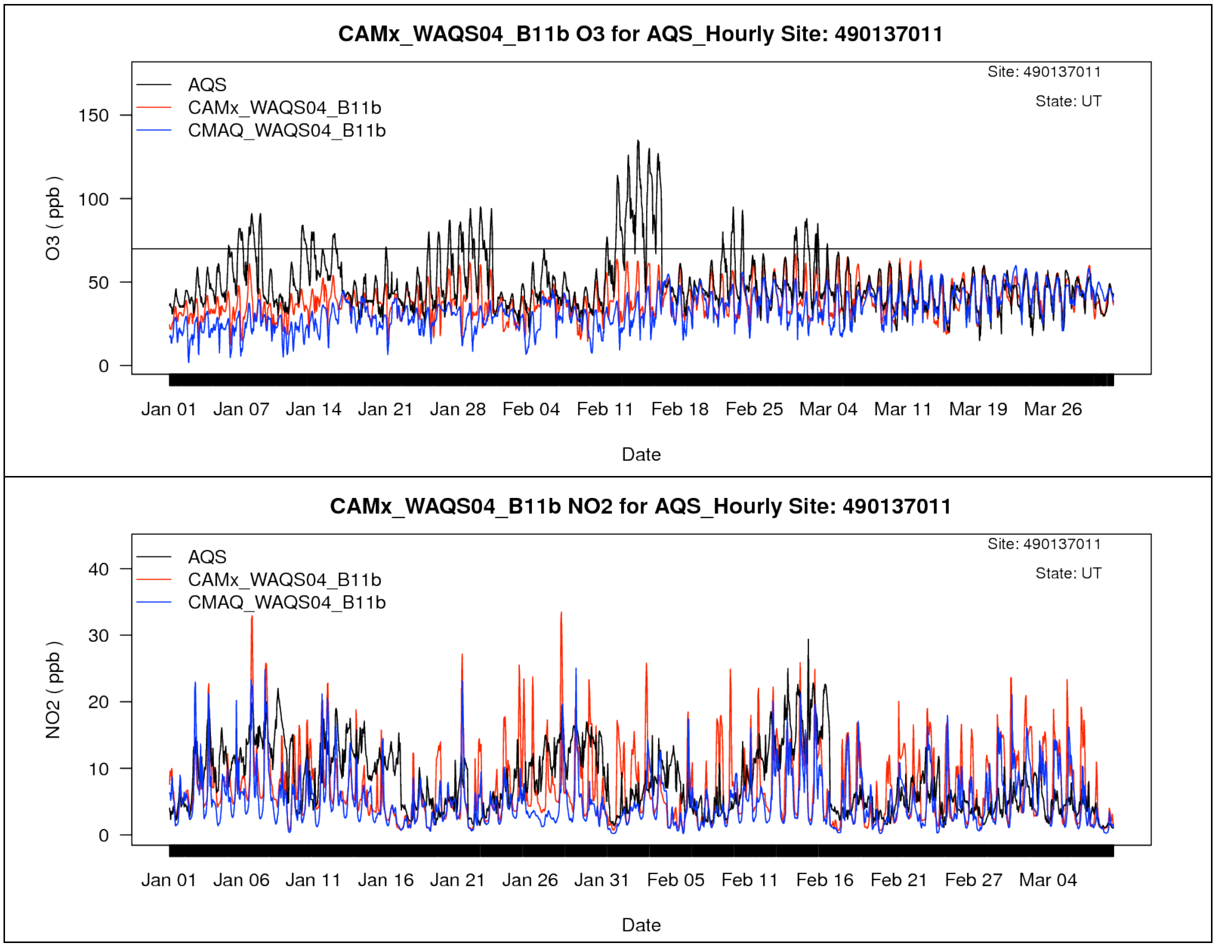


Figure 4-48. Myton, Utah AQS Hourly O_3 and NO_2 for Jan-Mar 2011

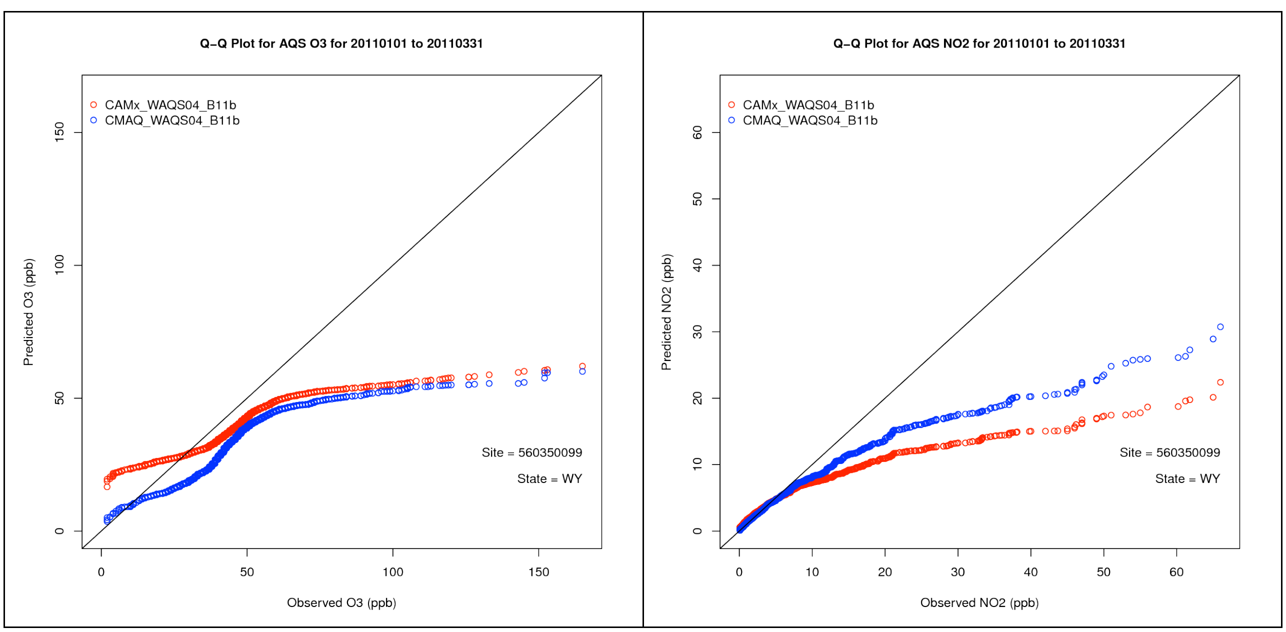


Figure 4-49. Boulder, Wyoming AQS Hourly O_3 and NO_2 Q-Q plot for Jan-Mar 2011

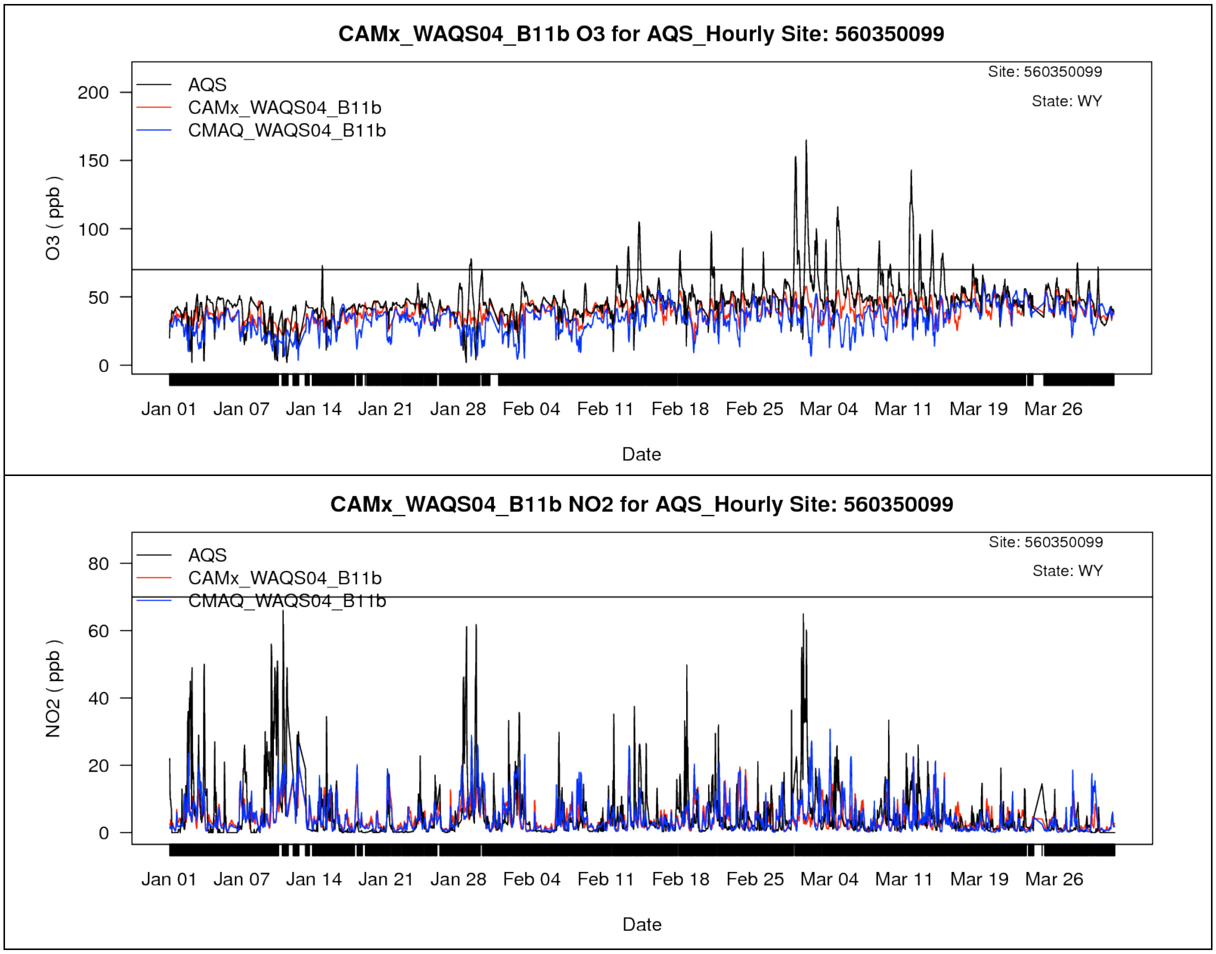


Figure 4-50. Boulder, Wyoming AQS Hourly O_3 and NO_2 for Jan-Mar 2011

4.2 PARTICULATE MATTER MODEL PERFORMANCE

This section presents the regional and statewide model performance for $PM_{2.5}$ and its constituents across the 12-km and 4-km modeling domains. Detailed performance evaluation metrics for the Base11b simulation are available through the IWDW.

4.2.1 Section Summary

- On an annual domain-wide basis, CAMx simulation Base11b has moved closer to the PM performance criteria for bias and error for total $PM_{2.5,}$ elemental carbon (EC), and sulfate (SO_4) relative to simulation Base11a. Urban OC performance also improved with lower positive biases in simulation Base11b at the CSN sites. The model performance for nitrate (NO_3), ammonium (NH_4) and rural OC (IMPROVE) degraded compared to the Base11a.
- Both models generally overestimate total $PM_{2.5}$ at the CSN sites and underestimate $PM_{2.5}$ at the IMPROVE sites, although some variability in these trends exist on a seasonal and monthly basis. For example, the IMPROVE $PM_{2.5}$ is overestimated in the winter.

- The residential wood combustion emissions reduction included in simulation Base11b improved winter OC performance at the CSN sites.
- EC is overestimated at all monitor locations in the mid-to-high sections of the observed concentration range.
- SO_4 is underestimated by CMAQ at rural (IMPROVE) sites, but otherwise shows an increasing tendency to overestimate at all locations as the concentration increases.
- SO_4 at the CSN sites is predicted well in the spring and fall, but moderately underestimated in the summer, and significantly overestimated in the winter.
- NO_3 performance improves in simulation Base11b relative to Base11a on an annual basis. Summer season NO_3 is severely underestimated in simulation Base11b.
- The boundary condition dust corrections in simulation Base11b reduced the overestimates of total $PM_{2.5}$ on an annual basis. This correction degrades spring season PM performance when dust entering the domain from the boundary impacts the observations. The boundary corrections for dust need to be re-examined, particularly in the spring and summer, when their contributions to total $PM_{2.5}$ mass are the greatest.
- Emission sources of NH_3 should be evaluated to correct underestimates in NH_4, which would also reduce nitrate formation, particularly in seasons and locations where there are overestimates of SO_4.

4.2.2 WAQS Base11b Domain-Wide $PM_{2.5}$ Model Performance

Table 4-10 and Table 4-11 summarize annual total fine particulate matter ($PM_{2.5}$) performance by monitoring network at all sites in the and 4-km modeling domains for CAMx and CMAQ, respectively. These results show that on an annual domain-wide basis, CAMx has moved closer to the PM performance criteria for bias (≤±60%) and error (≤±75%) for total $PM_{2.5,}$ elemental carbon (EC), and sulfate (SO_4). Urban OC performance also improved with lower positive biases in simulation Base11b at the CSN sites. The model performance for nitrate (NO_3), ammonium (NH_4) and rural OC (IMPROVE) degraded compared to the Base11a. The Base11b model simulation included updates to the fire emission inventory involving significant increases in VOC emissions from fires, particularly in Colorado and Wyoming; reductions in residential wood combustion (RWC) emissions by 50%; and the removal of boundary condition dust. While the net result of these changes was a significant reduction in the overbias in the CAMx performance for OC, it may have also been an overcorrection of the bias in SO_2 and SO_4. This section presents analyses of the annual, seasonal, and compositional CAMx $PM_{2.5}$ model performance for the WAQS base 2011b simulations.

The scatter plots in Figure 4-51 compare the 12-km and 4-km model predictions to observations and display the error and bias statistics of CAMx and CMAQ for total $PM_{2.5}$ for the annual Base 2011b simulation. The bias statistics are somewhat better in the 12-km simulation possibly because of the larger number of data points available for comparison. Both simulations show a significant overestimate at the urban (CSN) network sites, and a comparable level of underestimate at the rural (IMPROVE) sites on an annual basis. The CAMx to CMAQ comparison reveals similar performance between the models except for the simulation of total $PM_{2.5}$ at

IMPROVE sites in the 12-km domain. CMAQ severely overestimates several days of observations, offsetting the negative bias trend seen in the CAMx results.

Figure 4-52 and Figure 4-53 are scatterplots of the CAMx and CMAQ Base11b 12-km domain $PM_{2.5}$ model performance in each of the four seasons at the IMPROVE and CSN sites. Both models overestimate total $PM_{2.5}$ at the CSN sites in all seasons except in the summer. The results at the IMPROVE sites are more varied, with significant (> 15%) underestimation of $PM_{2.5}$ by both models in the spring and summer. Both models also produce significant overestimation of IMPROVE total $PM_{2.5}$ in the fall and winter. Figure 4-53 illustrates that the excessive CMAQ $PM_{2.5}$ predictions seen in the annual plots occur during the fall. The net annual results for both models is an underestimation at the IMPROVE sites, as seen in **Error! Reference source not found.**.

The IWDW includes additional seasonal scatter plots for the 4-km domain and by state. Findings of the seasonal total $PM_{2.5}$ scatterplots for CO, UT, WY and NM are as follows:

- All four states show significant overestimates of $PM_{2.5}$ at IMPROVE sites in winter.
- Except for NM, which shows a slight overprediction in the fall, all states show underestimates of $PM_{2.5}$ at the IMPROVE sites in the remaining seasons.
- At the CSN sites,
  - $PM_{2.5}$ is underestimated in the summer in all monitored states (CO, UT and NM).
  - Moderate to significant overpredictions in fall and spring in all monitored states.
  - More varied performance among the monitored states during the winter: overestimates in CO and NM, and underestimates in UT.

Table 4-10. 4-km domain PM species performance indicators for WAQS CAMx Base 2011b

Species	Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod
	Units	(%)	(%)	(µg/m^3)	(µg/m^3)	(%)	(%)	(µg/m^3)	(µg/m^3)
SO4	IMPROVE	19.20	46.10	0.00	0.23	-0.63	48.30	0.48	0.48
	CASTNET	2.20	35.40	-0.04	0.19	-7.00	34.80	0.53	0.50
	CSN	10.40	44.10	0.06	0.36	7.63	50.00	0.73	0.78
NO3	IMPROVE	-127.00	154.00	-0.10	0.15	-60.10	88.60	0.16	0.07
	CASTNET	-107.00	132.00	-0.13	0.16	-62.60	78.90	0.20	0.07
	CSN	-119.00	129.00	-0.83	1.04	-55.40	69.90	1.49	0.67
EC	IMPROVE	11.90	52.80	0.02	0.07	20.00	81.40	0.09	0.11
	CSN	40.40	57.60	0.52	0.63	78.70	96.50	0.66	1.17
OC	IMPROVE	-27.10	58.20	-0.19	0.33	-34.30	60.50	0.54	0.36
	CSN	64.00	78.70	1.99	2.30	146.00	168.00	1.37	3.35
NH4	IMPROVE	-22.00	44.90	-0.07	0.11	-31.10	46.20	0.23	0.16
	CASTNET	-16.30	32.60	-0.04	0.06	-19.20	30.60	0.20	0.16
	CSN	2.48	53.90	-0.15	0.38	-25.00	64.30	0.59	0.44
PM2.5	IMPROVE	-25.90	50.10	-1.03	1.54	-35.70	53.40	2.88	1.85
	CSN	19.20	46.10	0.00	0.23	-0.63	48.30	8.31	0.48

Table 4-11. 4-km domain PM species performance indicators for WAQS CMAQ Base 2011b

Species	Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod
	Units	(%)	(%)	(µg/m^3)	(µg/m^3)	(%)	(%)	(µg/m^3)	(µg/m^3)
SO4	IMPROVE	4.42	43.90	-0.03	0.21	-7.16	43.20	0.48	0.45
	CASTNET	-14.40	35.70	-0.11	0.19	-19.80	34.30	0.54	0.44
	CSN	1.29	45.10	0.01	0.36	0.98	49.60	0.73	0.74
NO3	IMPROVE	-52.40	105.00	-0.02	0.14	-14.20	87.00	0.16	0.14
	CASTNET	-59.10	101.00	-0.07	0.15	-33.80	74.10	0.20	0.13
	CSN	-65.10	94.70	-0.57	1.00	-38.10	66.90	1.50	0.93
EC	IMPROVE	7.85	54.90	0.02	0.07	18.50	75.60	0.09	0.11
	CSN	29.80	52.90	0.31	0.46	47.20	70.10	0.66	0.97
OC	IMPROVE	-18.20	63.00	-0.13	0.35	-23.50	64.70	0.54	0.42
	CSN	82.80	93.30	2.71	2.94	198.00	215.00	1.37	4.07
NH4	IMPROVE	-23.50	48.30	-0.05	0.10	-23.80	45.60	0.23	0.17
	CASTNET	-18.50	36.20	-0.04	0.07	-18.60	33.40	0.21	0.17
	CSN	14.80	58.90	-0.08	0.41	-12.80	68.70	0.60	0.52
PM2.5	IMPROVE	-23.10	55.80	-0.75	1.64	-26.00	57.10	2.88	2.13
	CSN	20.40	57.90	2.57	6.07	30.90	73.10	8.31	10.90

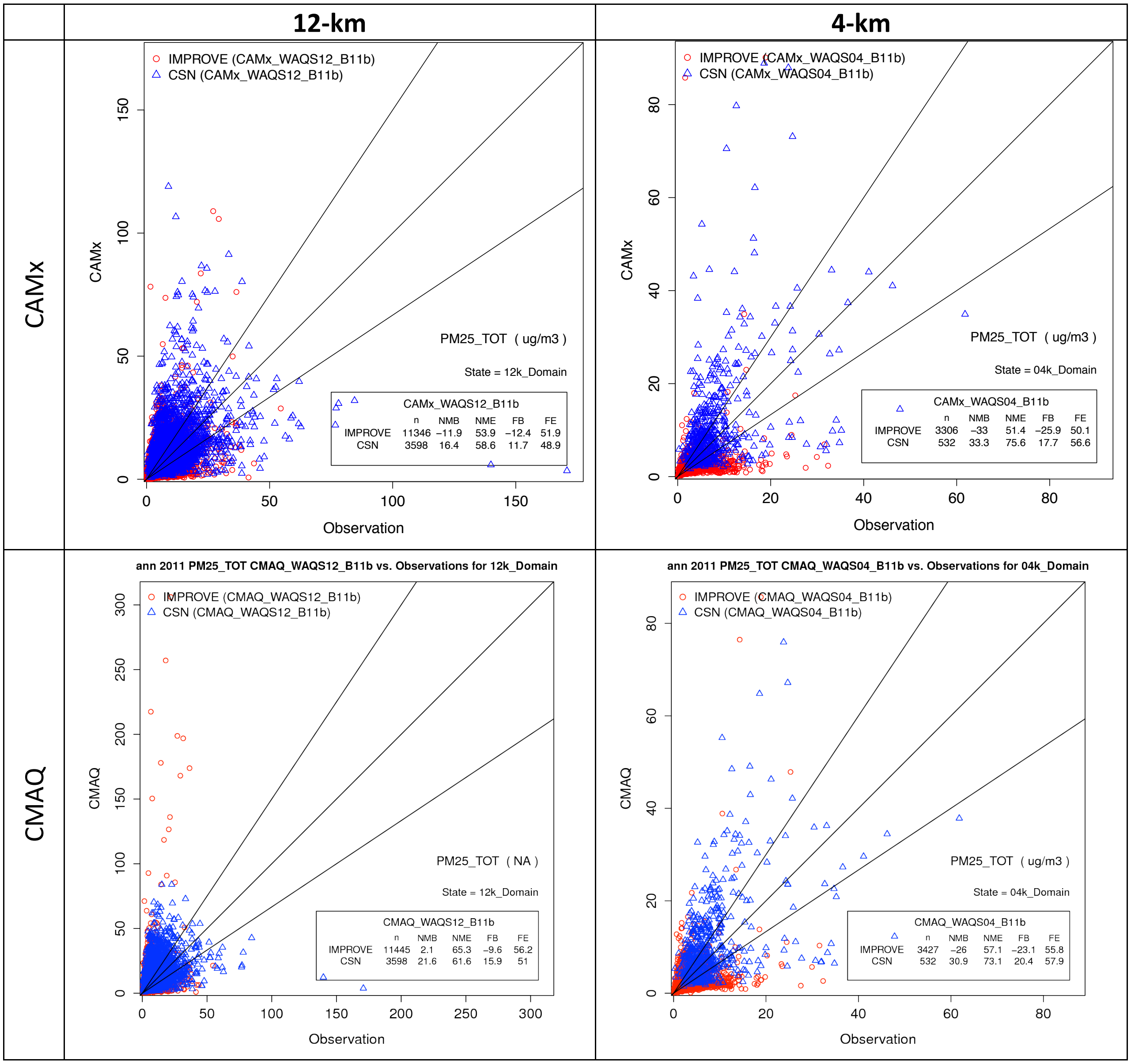


Figure 4-51. CAMx and CMAQ Base11b total $PM_{2.5}$ 12-km and 4-km domain performance.

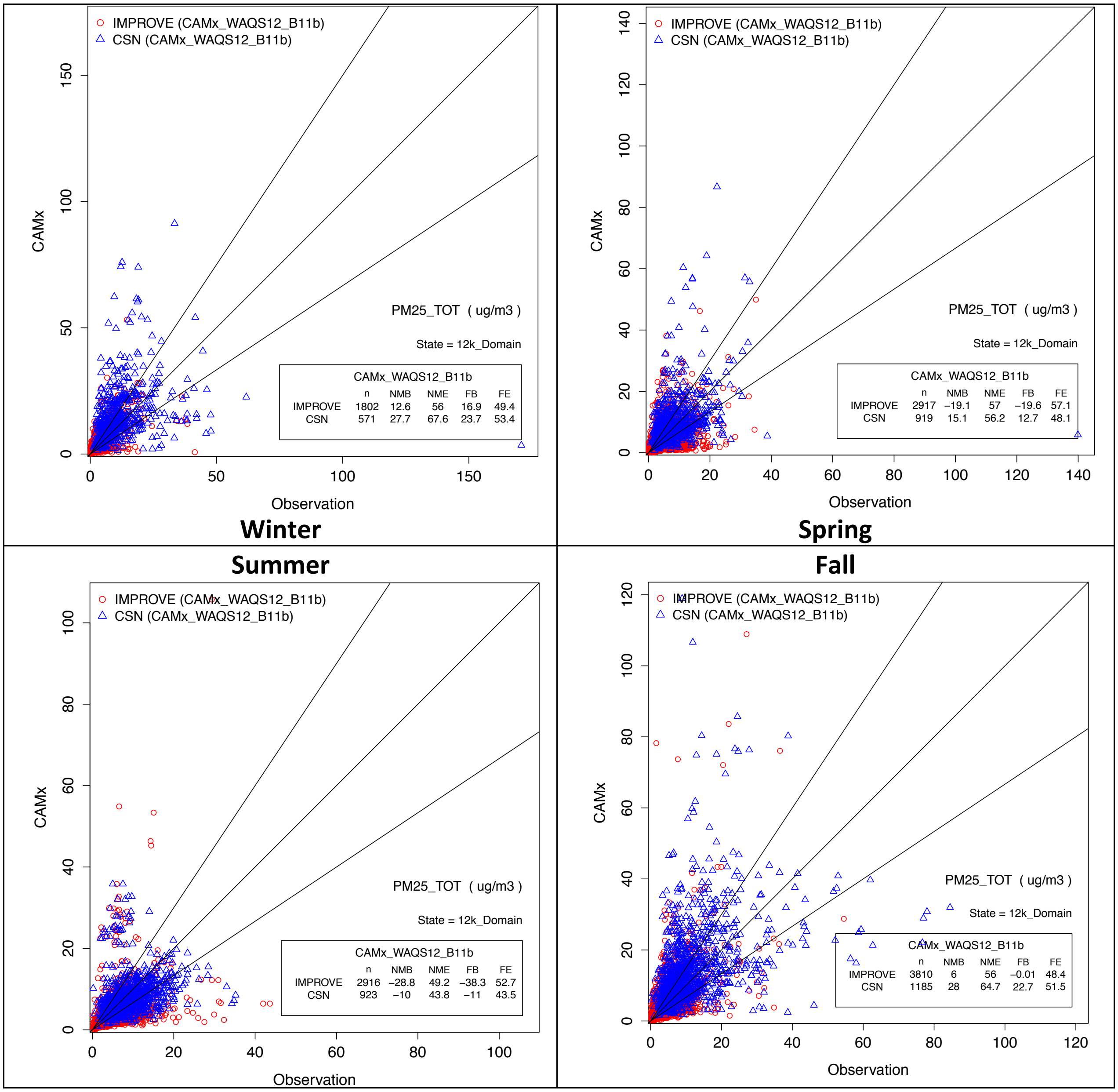


Figure 4-52. Scatterplot of WAQS Base11b CAMx 12-km seasonal total $PM_{2.5}$

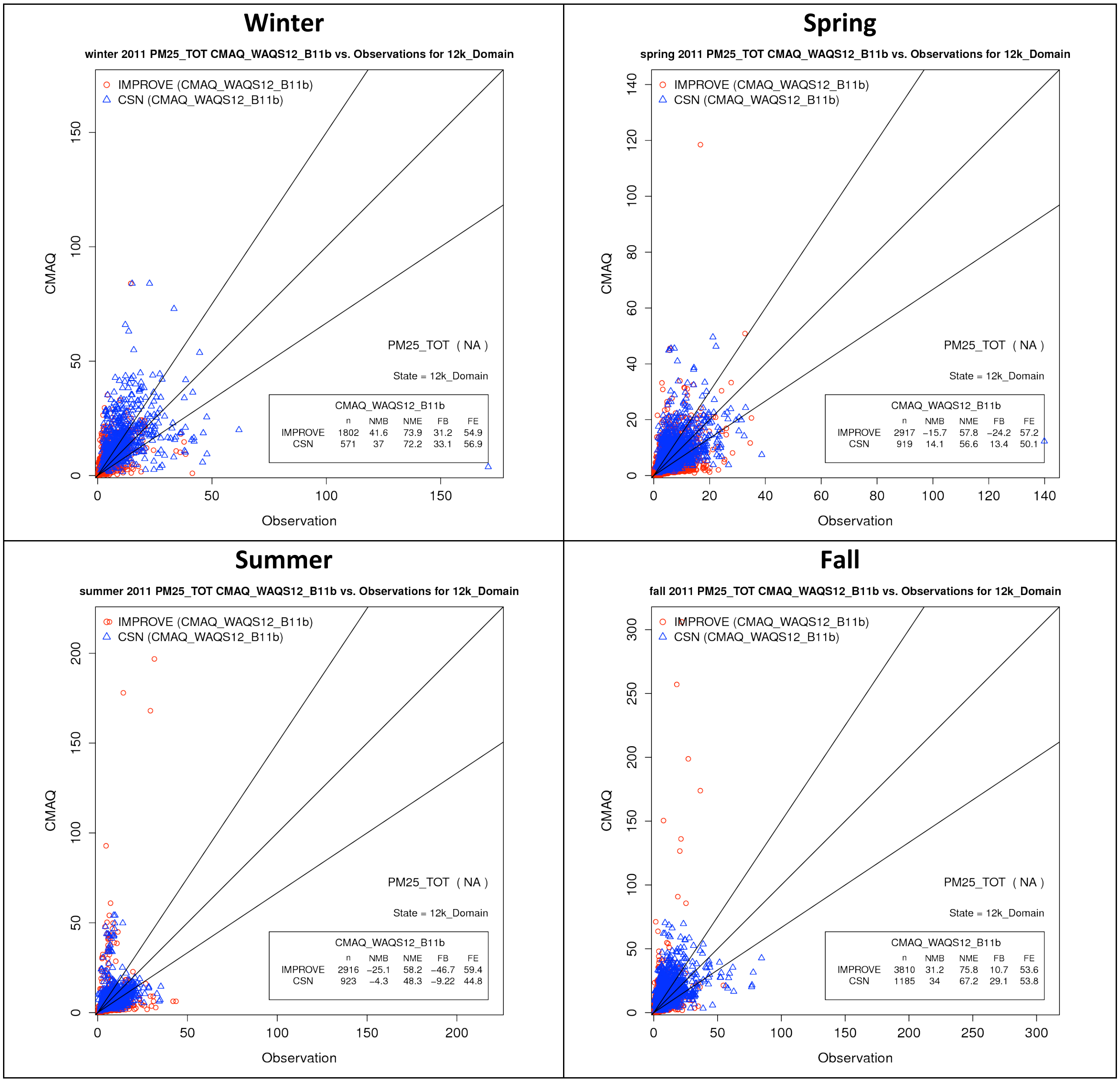


Figure 4-53. Scatterplot of WAQS Base11b CMAQ 12-km seasonal total $PM_{2.5}$.

4.2.3 WAQS Base11b Annual Speciated $PM_{2.5}$ Model Performance

The annual PM component contributions to the total $PM_{2.5}$ biases in the CAMx and CMAQ Base11b simulations are displayed in the Q-Q plots in Figure 4-54 and Figure 4-55 for the IMPROVE and CSN sites, respectively. The effect of reductions in the RWC emissions is clearly seen in the reduced OC concentrations in CAMx Base11b compared to CAMx Base11a, particularly at urban CSN locations. The Base11b CMAQ simulation still shows large positive biases in the upper end of the concentration range for OC at the IMPROVE sites. Further, there is a consistent overestimate of EC in the upper end of the range in all models. This is most likely due to increased emissions of EC during the fire season; the updated fire inventory resulted in increases in emissions of this component in the Base11b case. To better understand the EC annual trend, the seasonality of the EC overestimates is explored in the seasonal stacked-bar plots in Figure 4-56 and Figure 4-57.

The plots in Figure 4-54 show that at the IMPROVE sites there is also a tendency in both the CAMx and CMAQ Base11b simulations to increasingly underestimate the inorganic constituents as their concentrations increase. As there is an overestimate of SO_4 over the whole year in the upper end of the concentration range in CAMx Base11b, but the opposite trend in the semivolatile inorganic constituents (NO_3 and NH_4), there is likely to be a compensating influence that accounts for the underestimate of these latter semivolatile inorganics on an annual basis at the higher concentrations. This is explored further in the seasonal stacked-bar plots in Figure 4-56 and Figure 4-57.

The Q-Q plots in Figure 4-55 compare the PM constituents to the CSN network observations. They show much better agreement with observations in total $PM_{2.5}$ in the Base11b simulations than at the IMPROVE sites, although there is still a tendency for overestimation of the higher concentrations. This improved agreement, however, is the result of offsetting over-and-underestimates of various PM constituents, especially in the mid-to-high concentrations. While the reduced RWC emissions significantly improve the OC predictions in CAMx Base11b relative to Base11a, the higher OC values are still overestimated at the CSN sites, and contribute to the total $PM_{2.5}$ overestimates. In comparison to OC, and in comparison to EC at the IMPROVE sites, EC overestimates at the high end of the observed concentration range are much smaller at CSN monitor locations. SO_4 is also overestimated significantly in all model simulations in the mid-to-high concentrations, and to a greater degree at the CSN sites than at the IMPROVE sites. The changes in SO_2 emissions due to updates to the wildfire and the RWC emission sectors do not appear to have contributed significantly to reducing the Base11b SO_4 model overpredictions that were seen in the Base11a simulation. The underestimates in the semivolatile inorganic species at the CSN sites are equally as large, particularly for NO_3, and offset the overestimates in the aforementioned constituents. Seasonal trends that may explain these biases are further investigated in Figure 4-56 and Figure 4-57.

To summarize the findings based on the annual Q-Q plots:

- EC is overestimated at all monitor locations in the mid-to-high sections of the concentration range.

- OC performance is improved in CAMx Base11b compared to the CMAQ Base11b and the previous CAMx Base11a model simulations, but urban sites still show an overprediction tendency that increases with increasing concentrations. This suggests an overestimation of OC primary and precursor emissions from sectors other than were significantly updated in Base11b, namely, RWC and wildfires.
- SO_4 is underestimated by CMAQ at rural (IMPROVE) sites, but otherwise shows an increasing tendency to overestimate at all locations as the concentration increases.
- There is a lack of correlation of the SO_4 trends with those of the semivolatile inorganic species (NO_3 and NH_4), which are increasingly *under*estimated in Base11b as their concentrations increase.
- Seasonal analyses could help identify the different source sectors that may contribute to these annual trends.

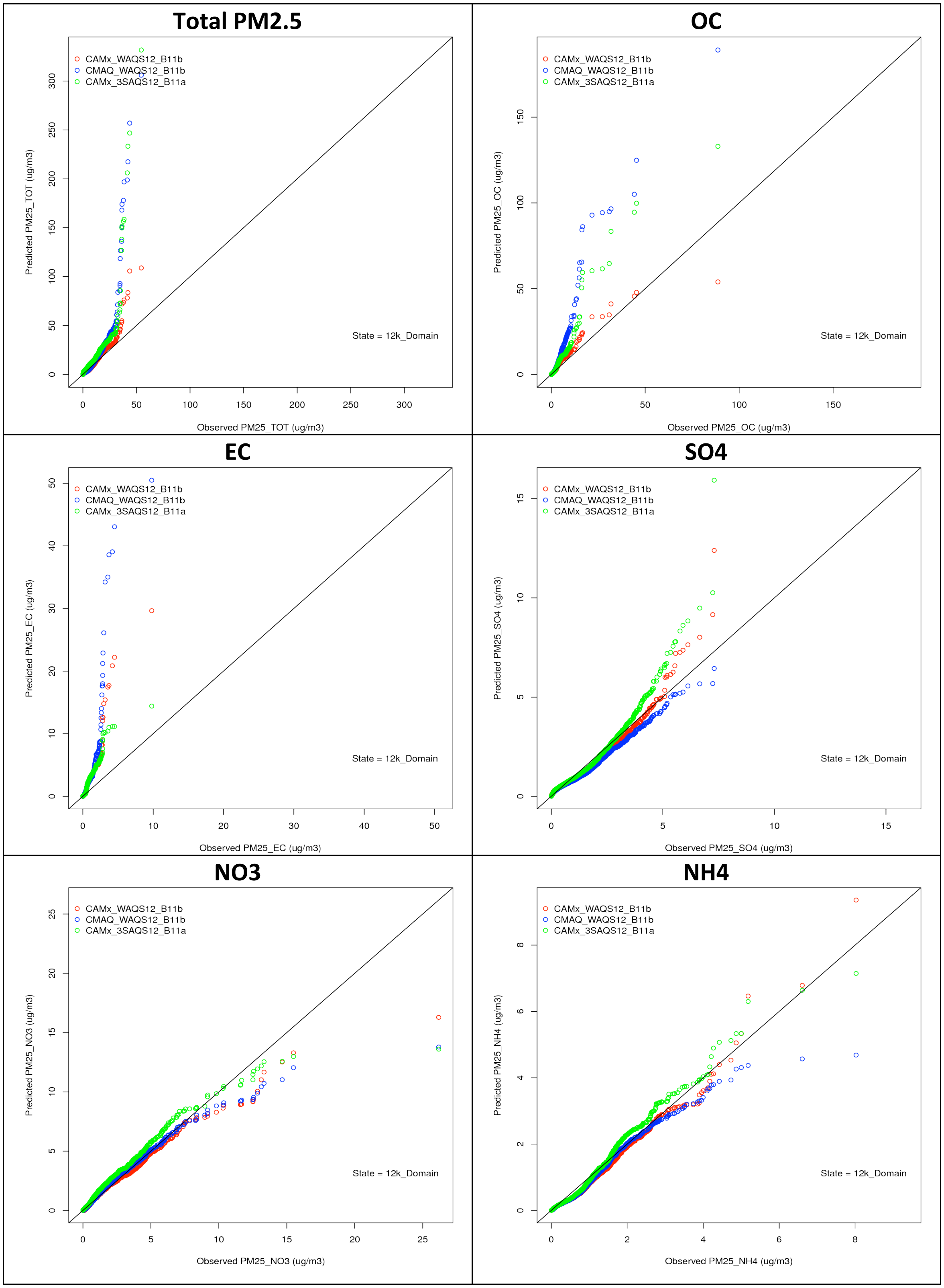


Figure 4-54. WAQS 12-km speciated PM performance at IMPROVE sites for CAMx and CMAQ.

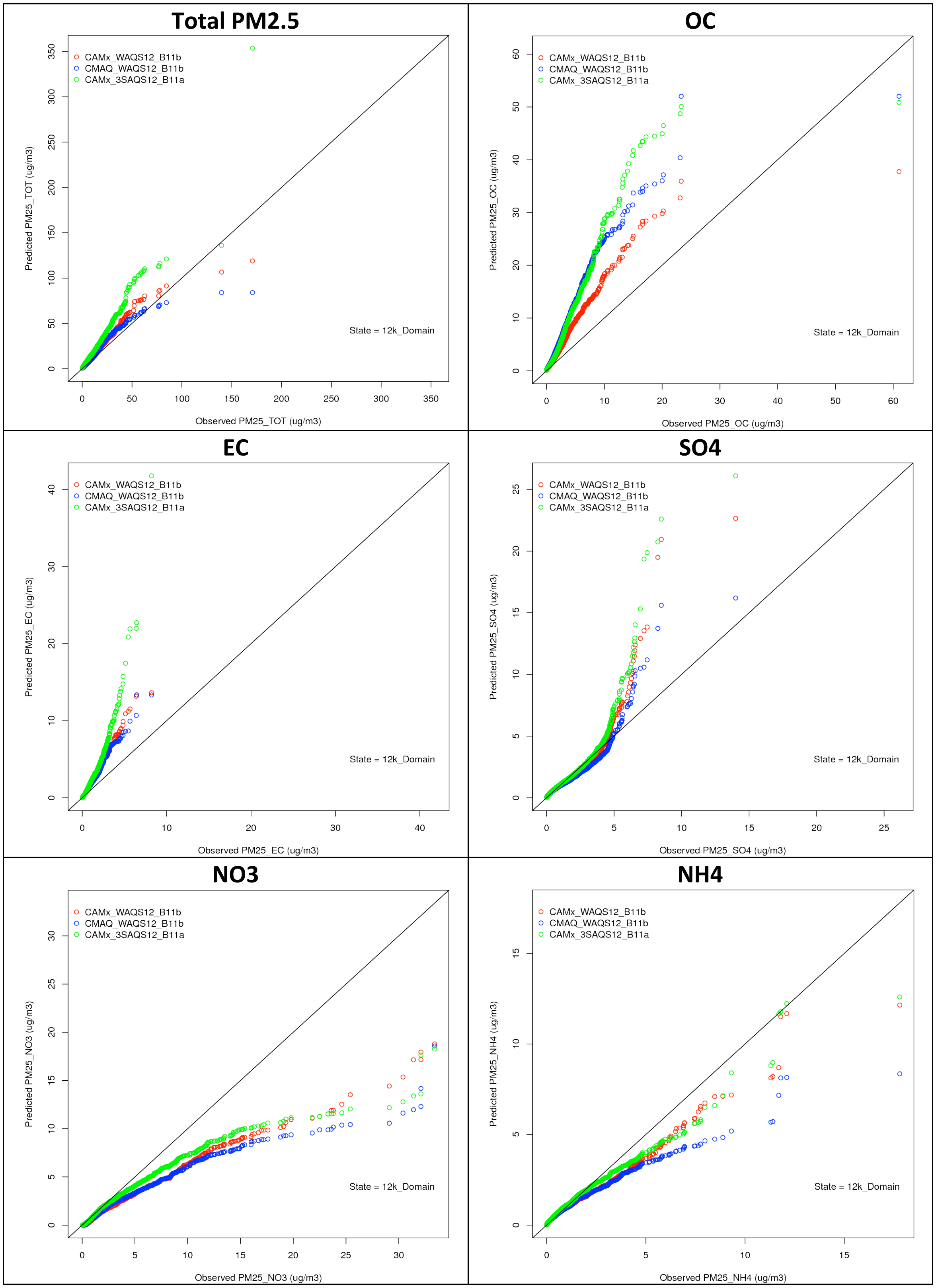


Figure 4-55. WAQS 12-km speciated PM performance at CSN sites for CAMx and CMAQ.

4.2.4 WAQS Base11b Seasonal Speciated $PM_{2.5}$ Model Performance

In the stacked bar plots of $PM_{2.5}$ mass composition in Figure 4-56 comparing the models to IMPROVE over the 12-km domain in each season, the effect of reducing boundary concentrations of dust and sea salt is immediately obvious in the Base11b model results. The Other-PM positive bias in Base11a is dramatically reduced, and the agreement with observations, significantly better, in the winter. This agreement is somewhat degraded with an Other-PM underestimate in the spring, which gets dramatically worse in the summer, and improves somewhat in the fall. Reducing the boundary inputs of fugitive dust may have overcorrected the model during the spring for transported dust plumes from Asia and the Sahel, but there may also be a contribution to the underestimate from the windblown dust model in the summer months.

The next most apparent performance improvement in CAMx Base11b is in OC. Spring and summer OC concentrations in CAMx Base11b are slightly lower than observations compared to Base11a, and slightly higher in winter and fall, but overall OC performance at the IMPROVE sites is significantly better in all seasons. On the other hand, EC in the CAMx Base11b simulation shows significant overestimates relative to IMPROVE in all seasons, with the worst agreement in the spring and fall. The Base11b EC performance in the summer and fall is actually worse than that of Base11a, suggesting that the fire inventory updates may need to include additional corrections to the speciation, i.e., the OC/EC ratio. The aggregate of these results over the four seasons is consistent with the findings of Figure 4-54 for OC and EC.

Also consistent with Figure 4-54, NO_3 performance in CAMx Base11b, while improved in comparison to Base11a at the IMPROVE sites, shows moderate to slight underestimates in winter and spring, and a severe underestimate in summer. NH_4 is also significantly underestimated in summer. These biases are consistent with the significant SO_4 underestimates in the summer compared to IMPROVE observations. Thus, the annual SO_4 overestimate shown in Figure 4-54 in CAMx Base11b compared to IMPROVE comes mainly from the wintertime overestimate seen in Figure 4-56. Possible sources of the wintertime overestimate could be the power generation sector and prescribed or agricultural burning in the updated fire inventory.

In contrast to the IMPROVE sites, Other-PM is somewhat overestimated in Base11b at the CSN sites as shown in Figure 4-57. The Other-PM agreement is better in the summer and very good in the spring, with underestimates in both of these seasons. Overall, the boundary condition corrections have greatly improved the results for dust and other primary fine PM compared to the Base11a simulation. OC, however, is significantly overestimated in every season, consistent with the findings in Figure 4-55, albeit to a lesser degree than in the Base11a simulations. Thus the corrections made in Base11b inputs to the RWC and open biomass combustion emissions do not seem to address all of the CAMx and CMAQ OC overestimates at the CSN sites. Similar to the IMPROVE sites, the modeled EC concentrations at the CSN sites are overestimated in every season, particularly in the winter and spring; taken together with the OC overestimates, this argues for further corrections to the RWC sector and/or the PM emissions speciation.

Figure 4-57 shows that SO_4 at the CSN sites is predicted well in the spring and fall, but moderately underestimated in the summer, and significantly overestimated in the winter. The wintertime NH_4 is slightly underestimated, and in combination with the SO_4 overestimate, may account for less winter nitrate formation in the model than observed. However, the modeled NO_3 is not always consistent with that of the other inorganic species. For example, NO_3 is significantly underestimated in the fall in CAMx Base11b at the CSN sites, even though the predicted NH_4 and SO_4 are not significantly different. In the summer, there is considerably less NO_3 formed than would be expected for the given SO_4 underestimate, as evidenced by the large underestimate in total fine inorganic PM. This result suggests an underestimation of urban NO_x emissions in the summer and fall.

Figure 4-58 and Figure 4-59 show the $PM_{2.5}$ composition and model performance domain-wide by season over the 4-km domain compared to the IMPROVE and CSN observations, respectively. The total $PM_{2.5}$ mass (Figure 4-58) at the IMPROVE sites is considerably lower in the winter and spring than that for the 12-km domain, mainly due to smaller contributions from Other-PM, OC and NO_3. The CAMx Base11b predictions show good agreement in total $PM_{2.5}$ with IMPROVE observations in the winter, with the exception of moderate underestimates in OC, NO_3 and NH_4, somewhat offset by overestimates in Other-PM and SO_4. However, the total mass is underestimated significantly in the remainder of the year, and largely due to an underestimate of Other-PM. This result confirms the conclusion from Figure 4-56 that the boundary corrections for dust need to be re-examined, particularly in the spring and summer, when their contributions to total $PM_{2.5}$ mass are the greatest. Other constituents contributing to the underestimates are (a) OC, NO_3 and SO_4 in spring and summer, and (b) OC, and NO_3 in the fall. The speciation in the fire sector may be a contributor to the underestimate seen in OC in all seasons, particularly since the worst agreement is seen in the summer, and since EC appears to be in good agreement overall, and even overestimated in the fall.

Figure 4-59 compares the 4-km mass composition of predicted $PM_{2.5}$ against CSN observations domain-wide. At these sites, the CAMx Base11b agreement is best in the spring, followed by summer, due to improved agreement in Other-PM and OC; Other-PM however, is still overestimated in all seasons except summer. The source of this bias could be different from that at the IMPROVE sites, which showed an overall underestimate in this component except in winter. While OC shows good agreement in the summer, in contrast with the performance at the IMPROVE sites for that season, it is overestimated in all other seasons, and EC shows positive biases in all seasons. These results indicate a different source for the discrepancies in carbonaceous PM at CSN sites, as compared to the rural sites. NO_3 shows moderate to severe underestimates in all seasons, with the worst agreement in winter and summer. The summertime under bias could be in part due to an underestimate in SO_4, which in general shows acceptable performance in the other seasons. Overestimation of the deposition of NO_3

could be a source of the negative bias, but a more likely source would be urban NO_x emissions, as was discussed in the 12-km domain results of Figure 4-57.

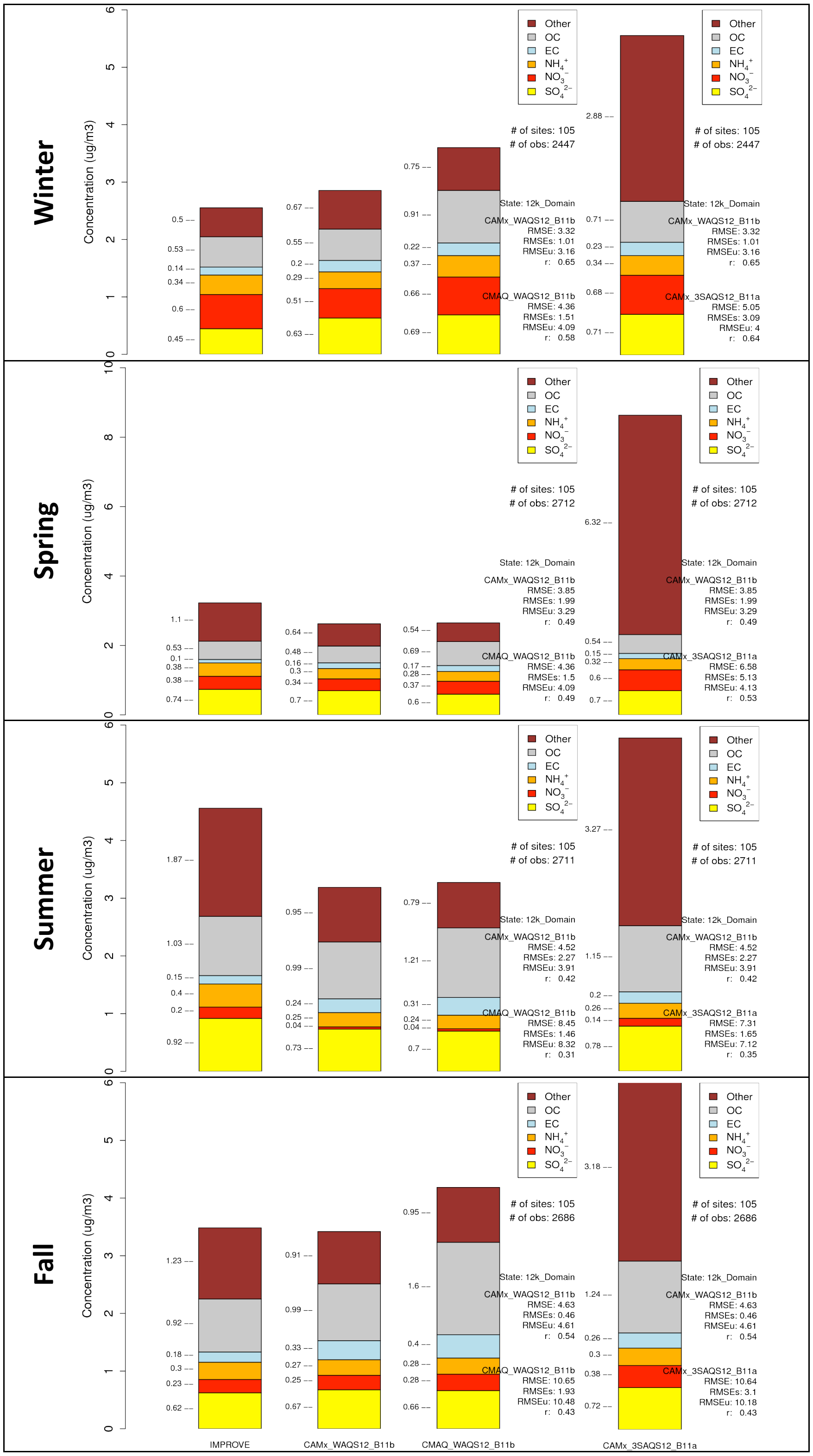


Figure 4-56. WAQS 12-km domain seasonal IMPROVE $PM_{2.5}$ composition stacked bar charts.

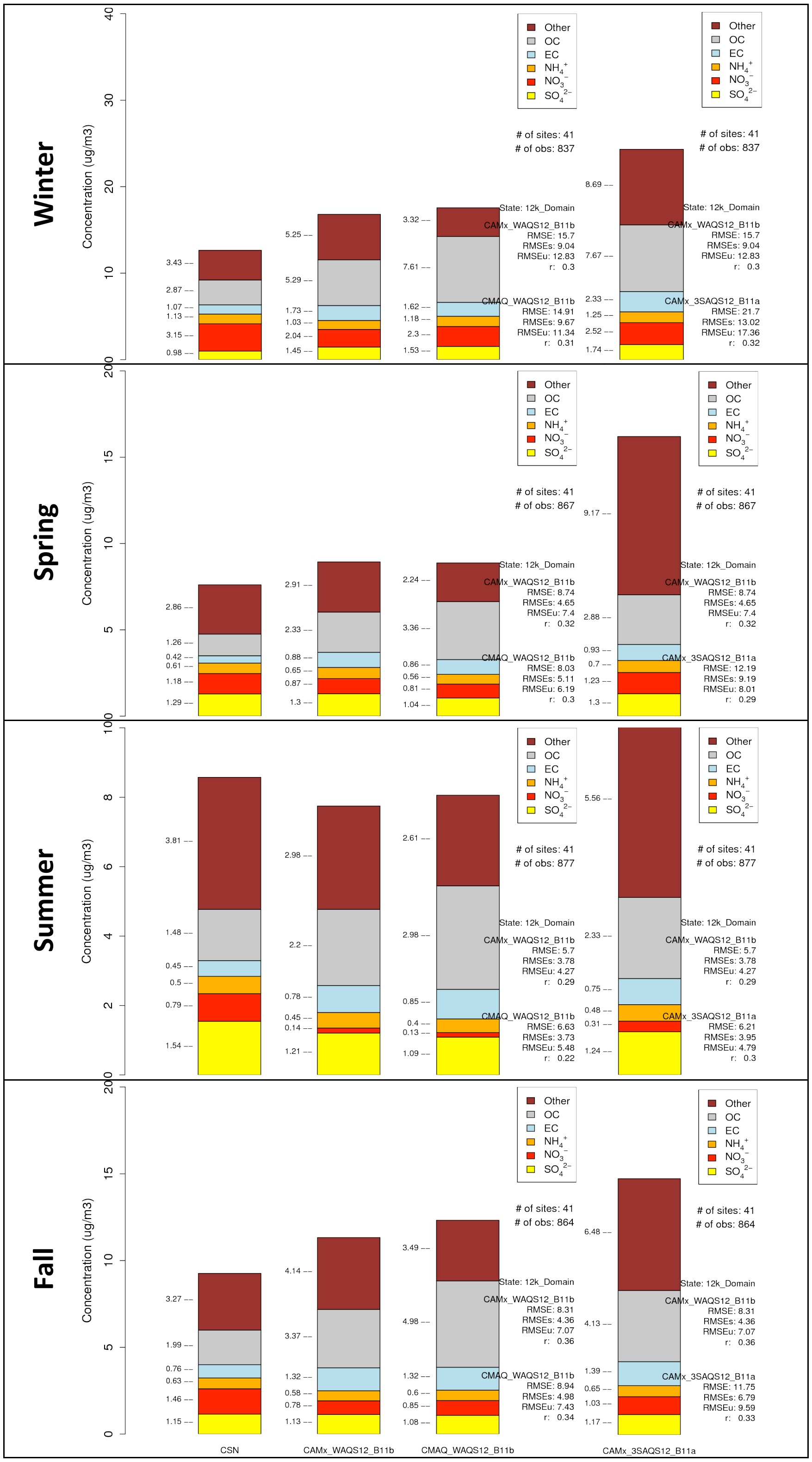


Figure 4-57. WAQS 12-km domain seasonal CSN $PM_{2.5}$ composition stacked bar charts.

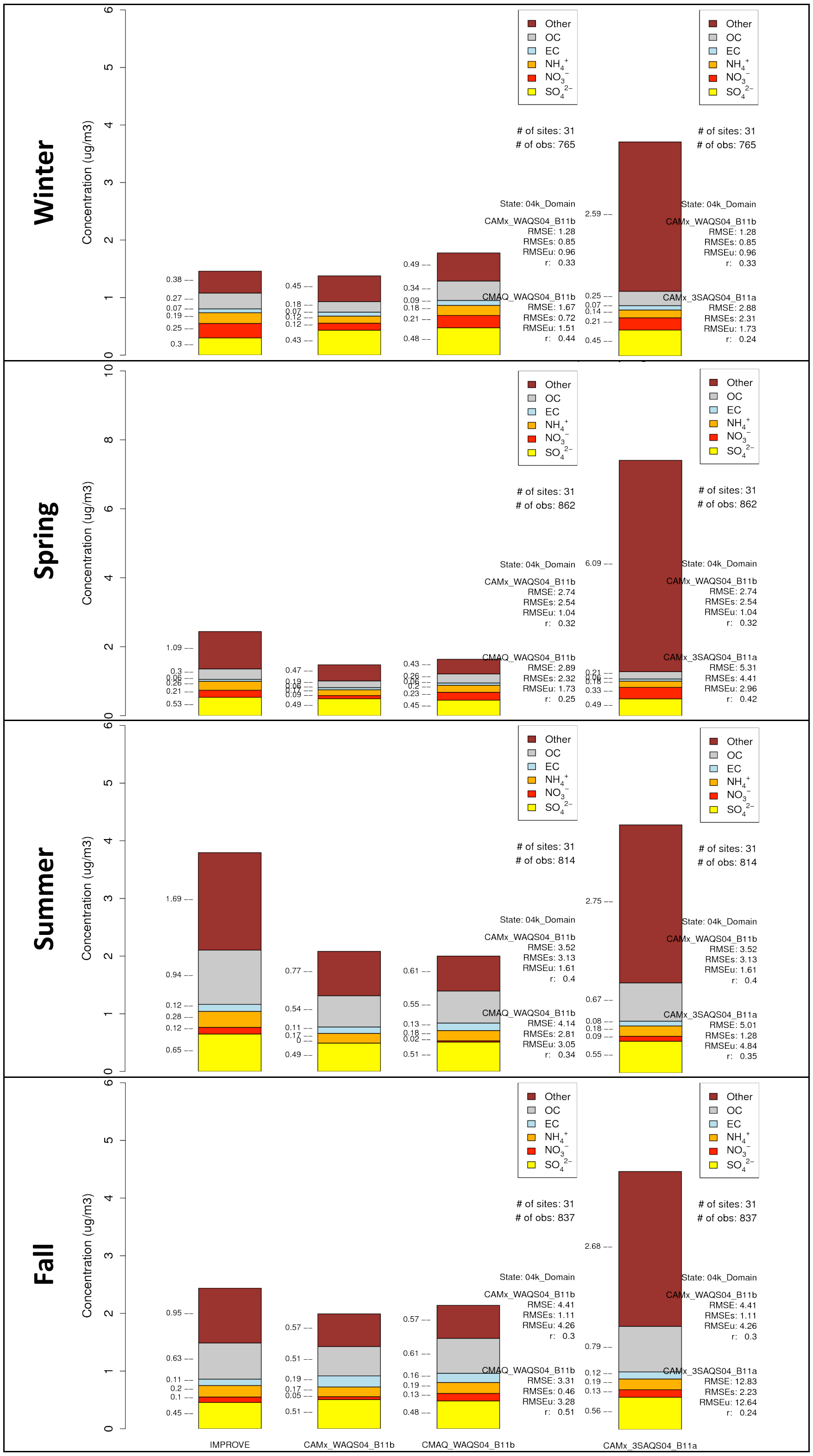


Figure 4-58. WAQS 4-km domain seasonal IMPROVE $PM_{2.5}$ composition stacked bar charts.

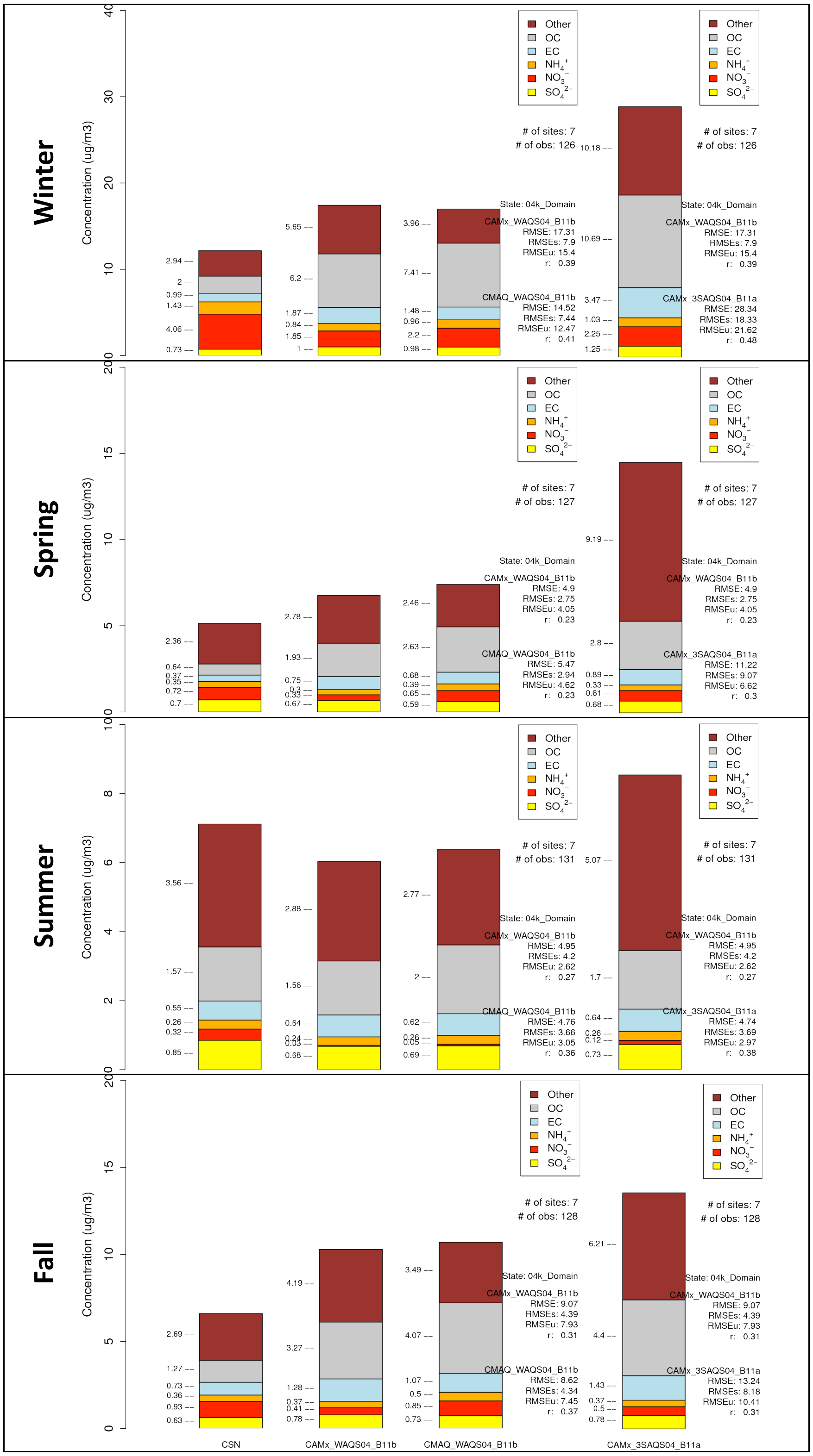


Figure 4-59. WAQS 4-km domain seasonal CSN $PM_{2.5}$ composition stacked bar charts.

4.2.5 WAQS Base11b Performance for $PM_{2.5}$ Composition by Season and by State

The PM composition variability and model performance against observations at the IMPROVE and CSN networks within each of the four states of interest, CO, UT, WY and NM, are shown for each season in Figure 4-60 through Figure 4-63. Figure 4-60 shows the best model performance for total $PM_{2.5}$ and for constituent concentrations at IMPROVE sites in CO. OC performance is somewhat degraded compared to the Base11a simulations in CO and UT, suggesting a possible overcorrection of the RWC emissions in these states. While UT shows good agreement for total $PM_{2.5}$ mass, the compositional differences relative to IMPROVE observations state-wide are greatest in UT due to underestimates in OC, NH_4 and NO_3, and overestimates in Other PM and SO_4. Overestimates of these last two constituents in the rural sites in WY and NM largely accounts for the wintertime overestimate of total PM in those sites.

Figure 4-61 shows that at the IMPROVE sites in the spring there is an overcorrection of the Other-PM due to reducing the boundary inputs for dust and sea salt. CAMx predicts SO_4 in good agreement with IMPROVE in all four states, but NO_3 is predicted well only in the WY IMPROVE sites, and significantly underestimated in the other states. OC is underestimated to a moderate-to-significant degree in CO, UT and WY.

Similar to the spring, the summer concentrations of Other-PM are underestimated at the IMPROVE sites in all four states. In addition, there is significant underestimation of an appreciably high OC component of total $PM_{2.5}$ for this season. The likely source of the high summertime OC is open biomass combustion, rather than RWC. Thus the 50% reduction of RWC is not likely to be the source of the underestimation. The inventory updates for wildfires should be examined as to the speciated emissions of OC and EC, because EC performance is acceptable to good in all four states. In contrast to these results, the fall OC predictions are more in line with observations. Fall values of Other PM are significantly underestimated in CO, UT, and WY, but show moderately good agreement in the NM IMPROVE sites, which also show good performance for all other species except NO_3. There is an underestimation of NO_3 in CO, UT and NM that seems to also correlate with an underestimation of NH_4. In sulfate-rich environments, this would inhibit nitrate formation, and provides an explanation for nitrate underestimations in seasons when SO_4 is overestimated, or when NH_3 emissions are underestimated.

In summary, these seasonal four-state results for rural sites suggest that

- The boundary conditions for dust may need to be further adjusted in all seasons over the 12-km domain, along with an evaluation of local dust source contributions to the $PM_{2.5}$ in the three-state region (CO, UT and WY);
- The RWC emission speciation (OC vs. EC) should be examined from CO and UT sectors, and its seasonal variability should be updated;
- SO_2 emissions should be examined for possible overestimates from the power generation sector in the fall (CO and WY) and winter (all states), and for underestimates from the power generation and biomass combustion sectors in the summer;

- Emission sources of NH_3 should be evaluated to correct underestimates in NH_4, which would also reduce nitrate formation, particularly in seasons and locations where there are overestimates of SO_4.

Figure 4-60 through Figure 4-63 compare seasonal $PM_{2.5}$ compositions between the models and observations at the CSN sites in each of the three states, CO, UT and NM. Note that there are no comparisons available for WY, as there are no CSN sites in that state. Figure 4-60 shows Other-PM and OC are both overestimated in CAMx Base11b in all three states in winter. Wintertime EC is also significantly overestimated in CO and UT. Among the inorganic constituents, NO_3 and NH_4 somewhat overestimated at the CSN sites in CO, possibly as a result of a significant SO_4 overestimate; these species are severely underestimated in UT and NM. There is reasonably good agreement of SO_4 at CSN sites in UT and NM, which suggests that the NH_4 and NO_3 underestimations in these states may be due to missing NH_3 sources there, or an overestimation of deposited amounts.

In the spring comparisons shown in Figure 4-61, there is better agreement seen in Other-PM in all three states, but OC and EC show significant overestimates. SO_4 as well as NH_4 show reasonably good agreement, but NO_3 is underestimated in all three states. The performance for Other-PM degrades somewhat in the summer, with CAMx Base11b showing underestimation in CO and UT. OC is underestimated in NM, although EC shows reasonable agreement. SO_4 is underestimated in all three states, and possibly as a result, NH_4 is moderately underestimated, and NO_3 to a greater extent.

Other-PM is overestimated in both CO and NM in the fall. This trend is possibly due to local influences rather than boundary conditions. There is, however, an underestimation of Other-PM for UT. OC is significantly overestimated, and EC less so in all states. SO_4 is moderately overestimated in CO, and slightly overestimated elsewhere; NO_3 continues to be significantly underestimated with the exception of CO CSN sites, perhaps due to an overestimate in NH_4.

In summary, these trends at the CSN sites for the CAMx Base11b performance suggest that:

- Boundary input corrections of dust have improved the model performance at urban, as well as rural sites, but local sources of overestimate of Other-PM cannot be ruled out in the winter;
- The RWC and urban VOC sources should be re-examined in regard to emission magnitudes and speciation profiles
- Emissions of urban NO_x sources may be underestimated in all seasons.

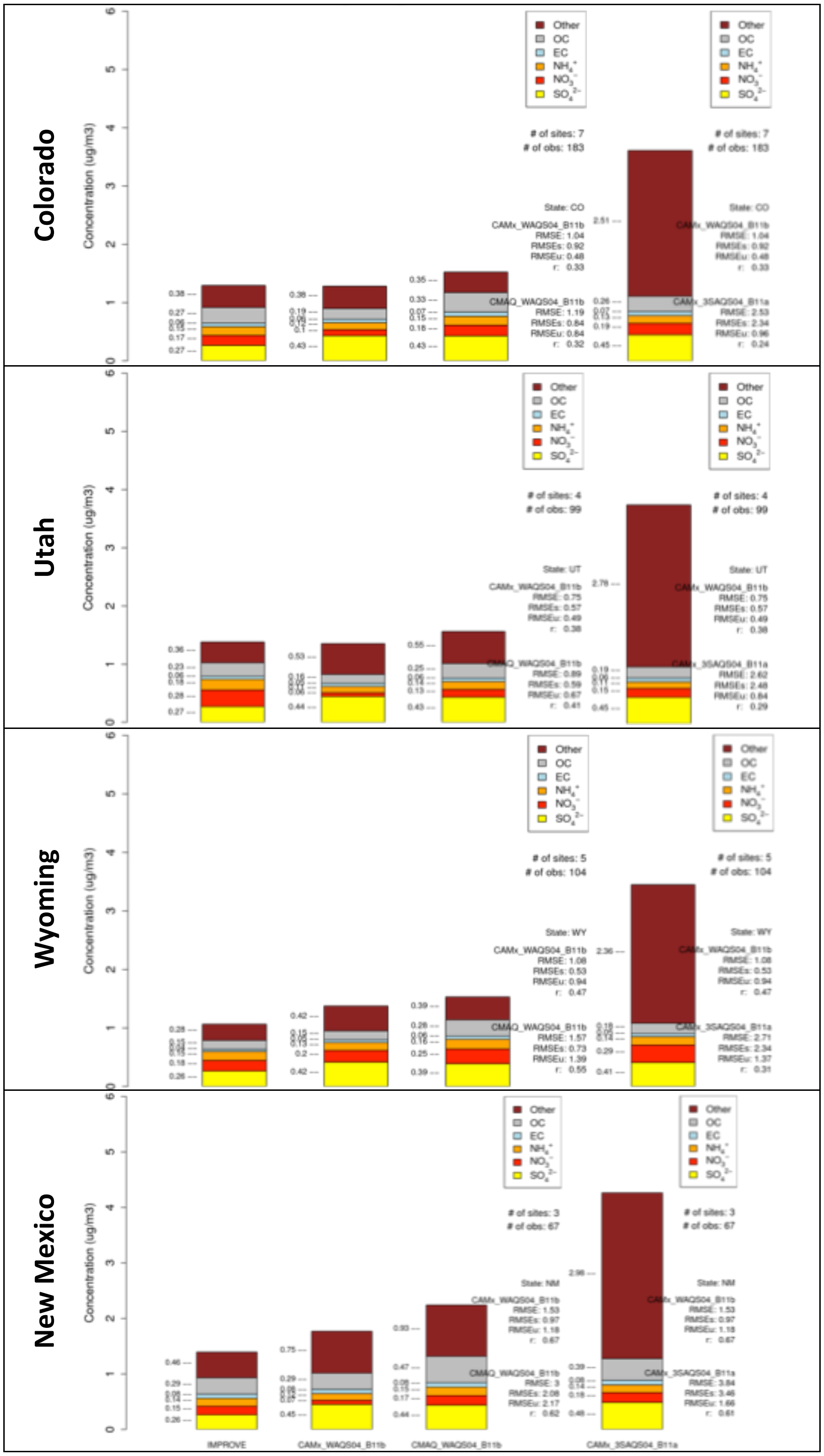


Figure 4-60. Winter CAMx and CMAQ $PM_{2.5}$ mass composition vs. IMPROVE observations.

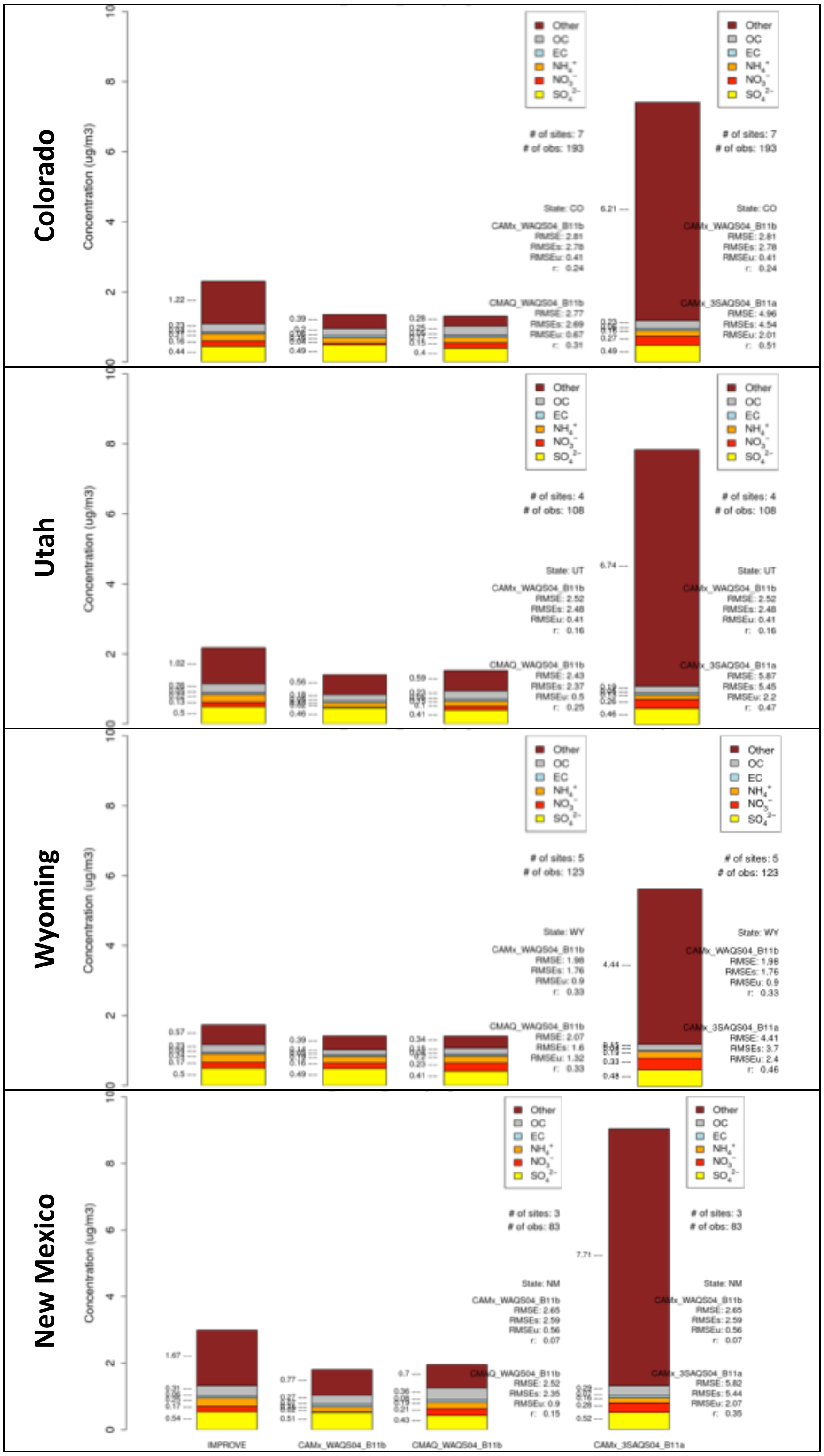


Figure 4-61. Spring CAMx and CMAQ $PM_{2.5}$ mass composition vs. IMPROVE observations.

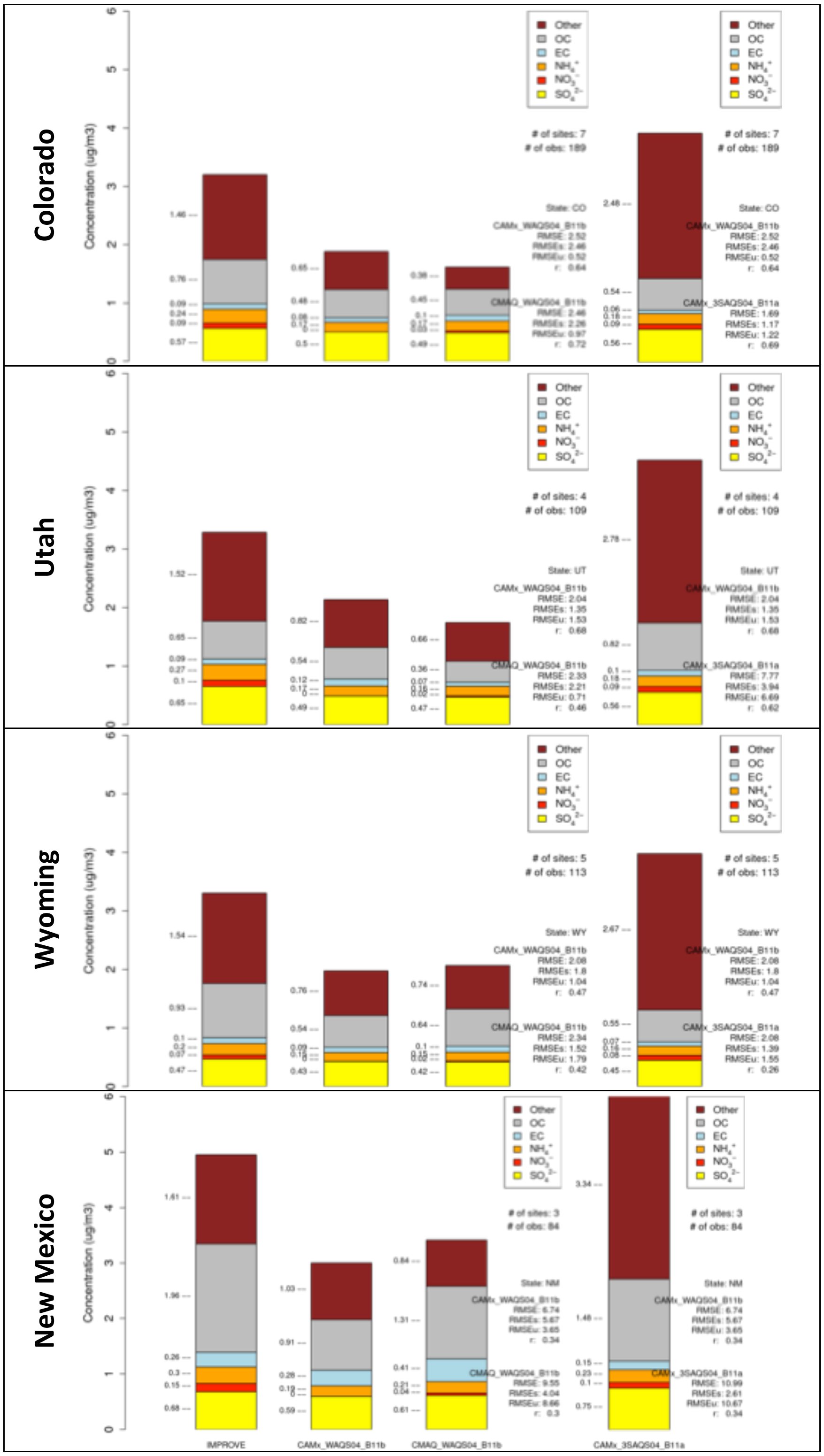


Figure 4-62. Summer CAMx and CMAQ $PM_{2.5}$ mass composition vs. IMPROVE observations.

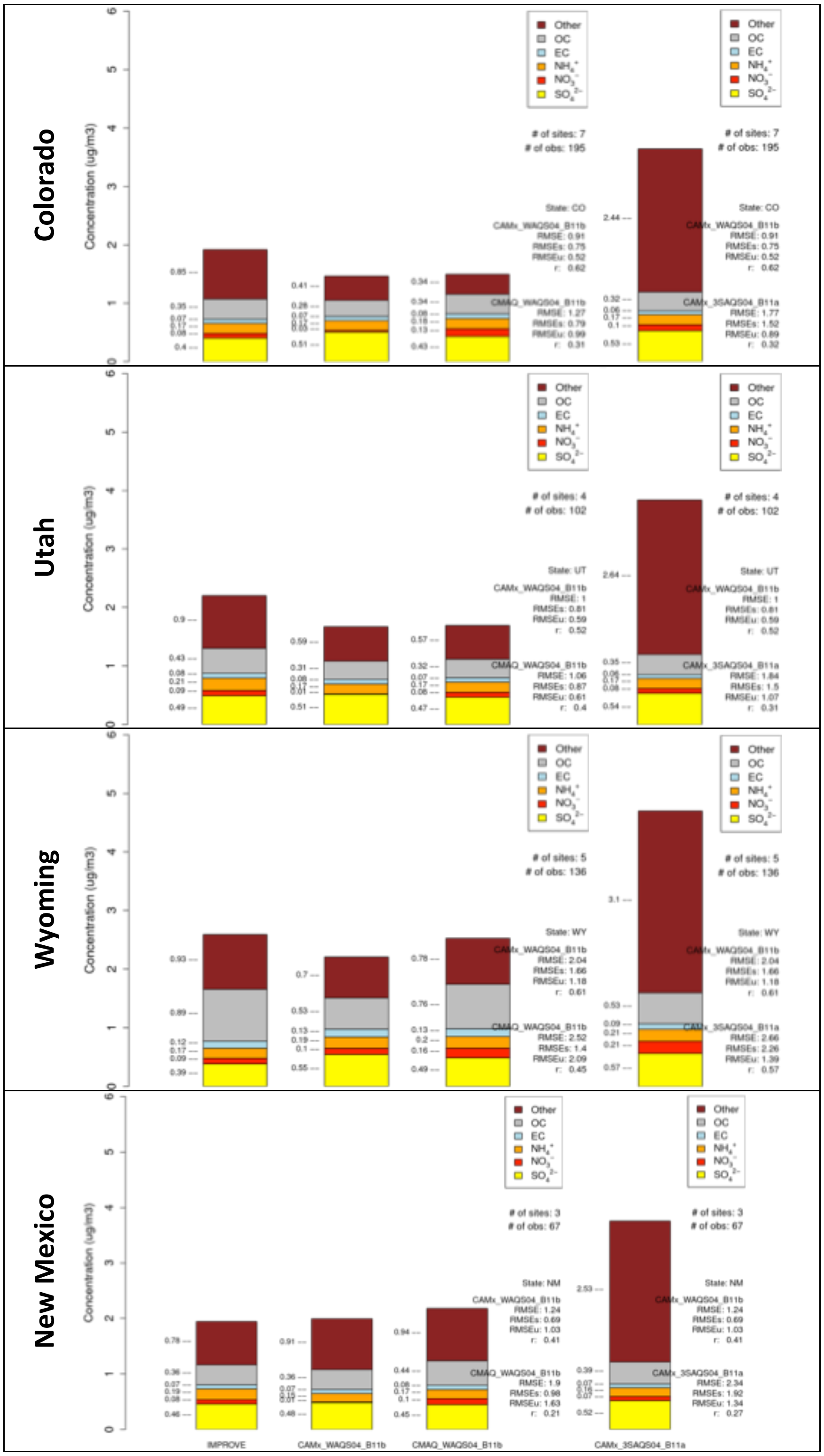


Figure 4-63. Fall CAMx and CMAQ $PM_{2.5}$ mass composition vs. IMPROVE observations.

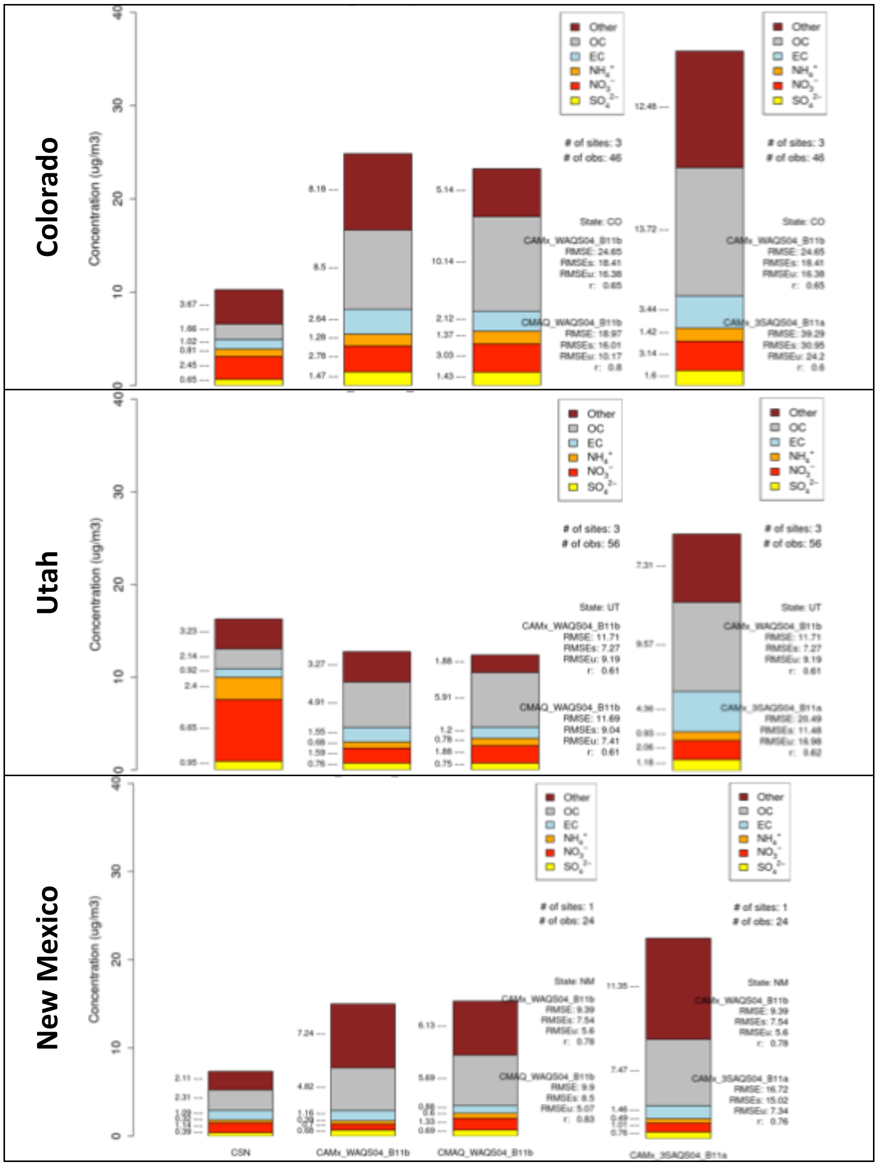


Figure 4-64. Winter CAMx and CMAQ $PM_{2.5}$ mass composition vs. CSN observations.

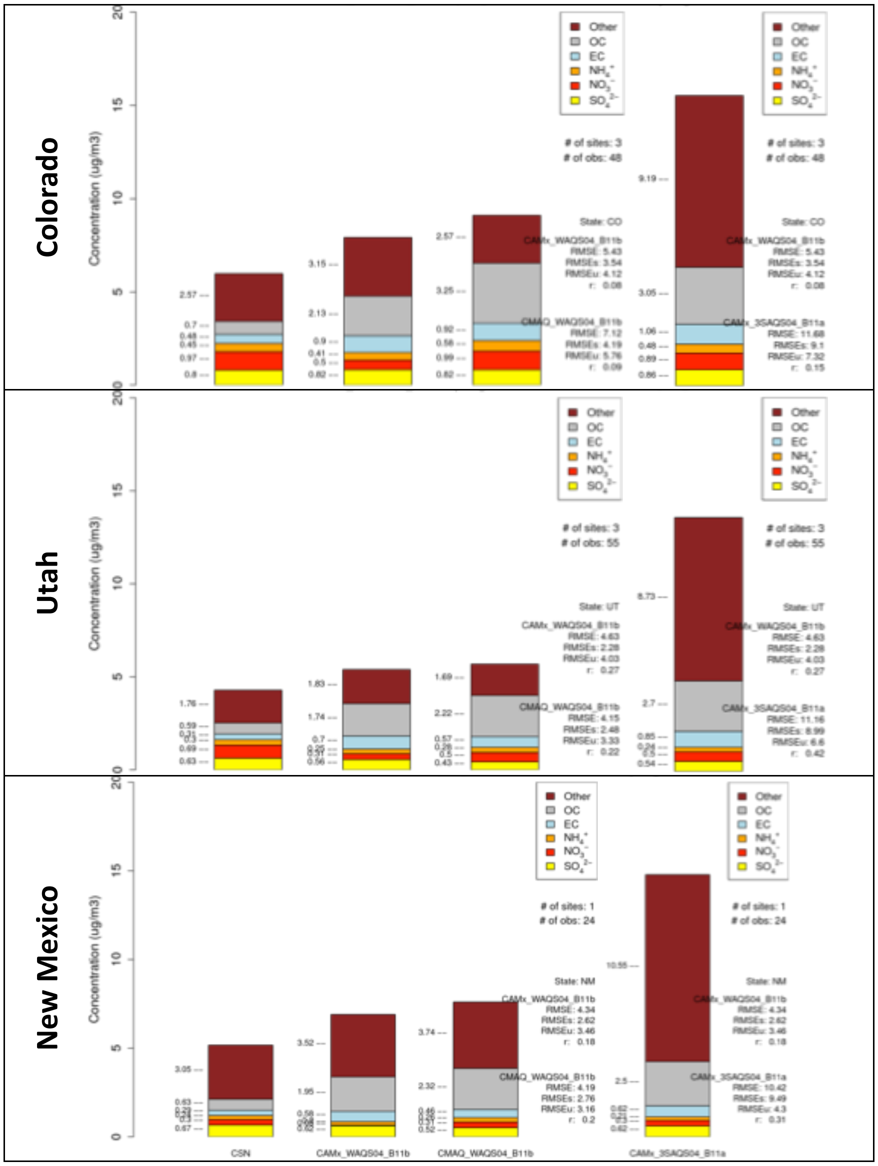


Figure 4-65. Spring CAMx and CMAQ $PM_{2.5}$ mass composition vs. CSN observations.

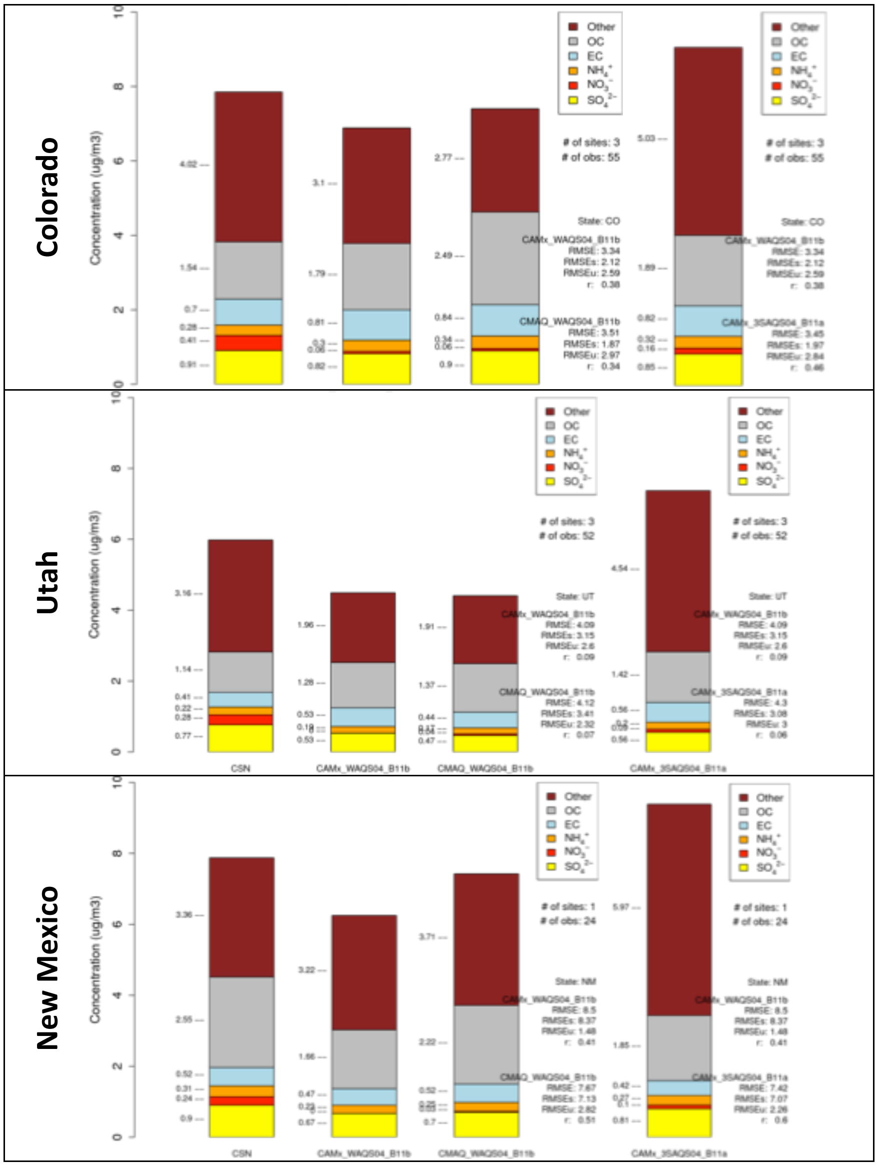


Figure 4-66. Summer CAMx and CMAQ $PM_{2.5}$ mass composition vs. CSN observations.

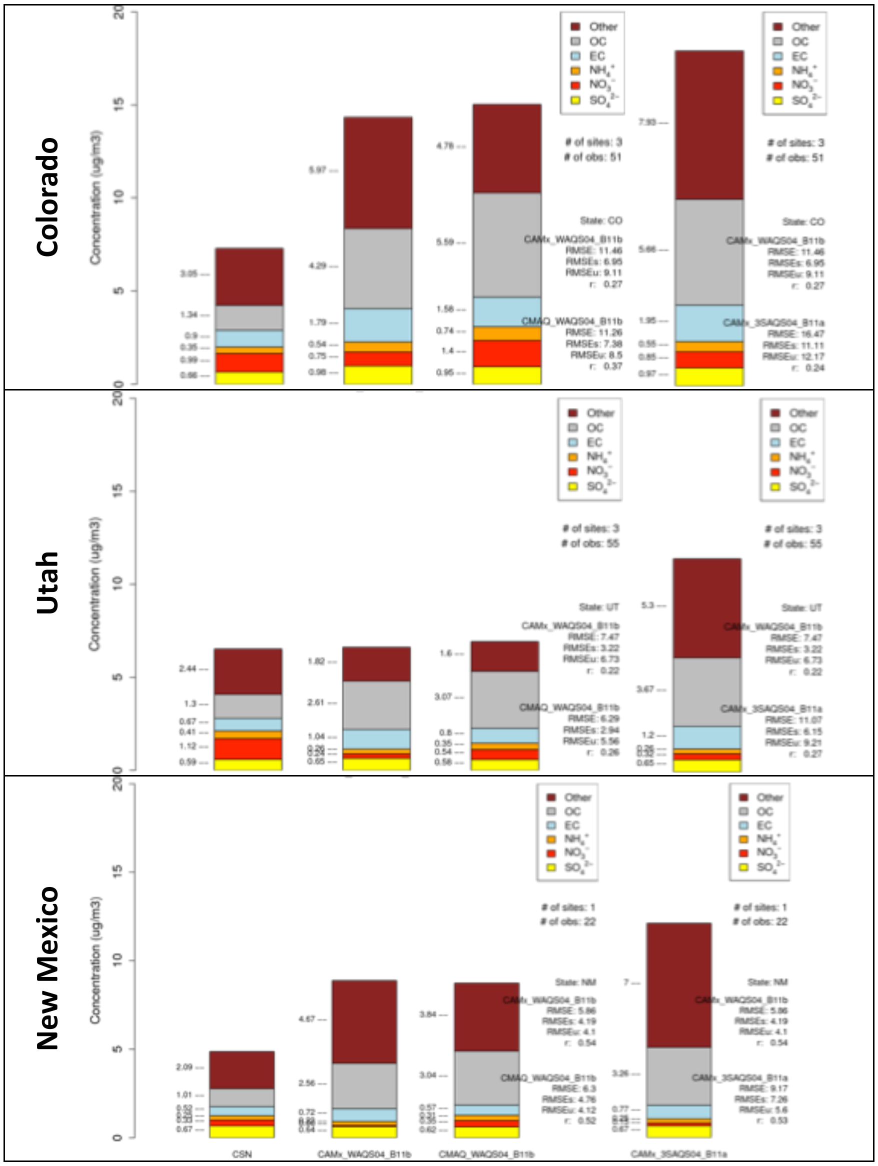


Figure 4-67. Fall CAMx and CMAQ $PM_{2.5}$ mass composition vs. CSN observations.

4.2.1 Site-specific Annual Performance Trends

In this section we further examine the temporal variability of $PM_{2.5}$ and its constituents at five Class I areas compared to IMPROVE. The sites that we selected for analysis include:

- Canyonlands National Park, UT
- Bridger National Forest, WY
- Rocky Mountain Nation Park, CO
- Mesa Verde National Park, CO and
- Bandolier National Park, NM

In addition to the temporal trends shown in Figure 4-68 through Figure 4-72, we also present CAMx vs CMAQ scatter plots, and seasonal average $PM_{2.5}$ speciated component stacked bar charts. We discuss each of these sites below.

Canyonlands National Park, UT (Figure 4-68): The overestimates in CAMx Base11a $PM_{2.5}$ have been greatly reduced due to the improvements to the boundary condition dust. However, CAMx Base11b shows a slight low bias through the spring and summer for $PM_{2.5,}$ with severe underestimates (> 5 $\mu g/m^3$) during April and June; the seasonal underestimate of total $PM_{2.5}$ at Canyonlands are due to the underestimation of fine dust during episodic dust events. While both models underestimate wintertime NO_3, the largest source of model bias in simulating the Canyonlands monitor is from Other-PM (dust).

Bridger National Forest, WY (Figure 4-69): Similar underestimates are seen in the spring and summer as in Canyonlands, indicating synoptic scale long-range dust transport events that are being missed by the models. Wintertime NO_3 is overestimated by both models at Bridger and the Other-PM underestimates persist through spring, summer, and fall. Underestimates of summer season OC indicates deficiencies in the skill of the models in capturing the impacts of wildfires.

Rocky Mountain National Park, CO (Figure 4-70): This site also measures spring, summer, and fall dust concentrations that are missed by both models. There are large negative biases in $PM_{2.5}$ for much of the spring and somewhat lower biases in the summer as well; the model misses a spike in June in the observations, most likely from a fire event. The stacked bar charts shows underestimation of summer season OC, also pointing to missing fires as a source of the model underbias in the summer. While CMAQ overestimates OC in the winter and fall, CAMx tends to underestimate this species during these seasons. As with the other sites, the model biases in simulating the Rocky Mountain National Park monitor are driven by dust underestimates through most of the year.

Mesa Verde National Park, CO (Figure 4-71): The negative biases in the spring and summer are larger at this site than at Rocky Mountain National Park with the models missing several peaks in the $PM_{2.5}$ observations from dust events. Along with dust, underestimation of NO_3 during these seasons lead to the large negative biases in the models.

Bandolier National Park, NM (Figure 4-72): Both models show fairly low biases with respect to IMPROVE observations except for the overestimate of two $PM_{2.5}$ peaks in June and July, likely from large fire events. The stacked bar charts confirm that both models estimate relatively large signals from OC during the summer, indicating an abundance of PM from fires in the models. Significant overestimates of winter and fall season PM-Other in both models point to deficiencies in local dust emissions sources, such as the windblown dust model and the fugitive dust inventory.

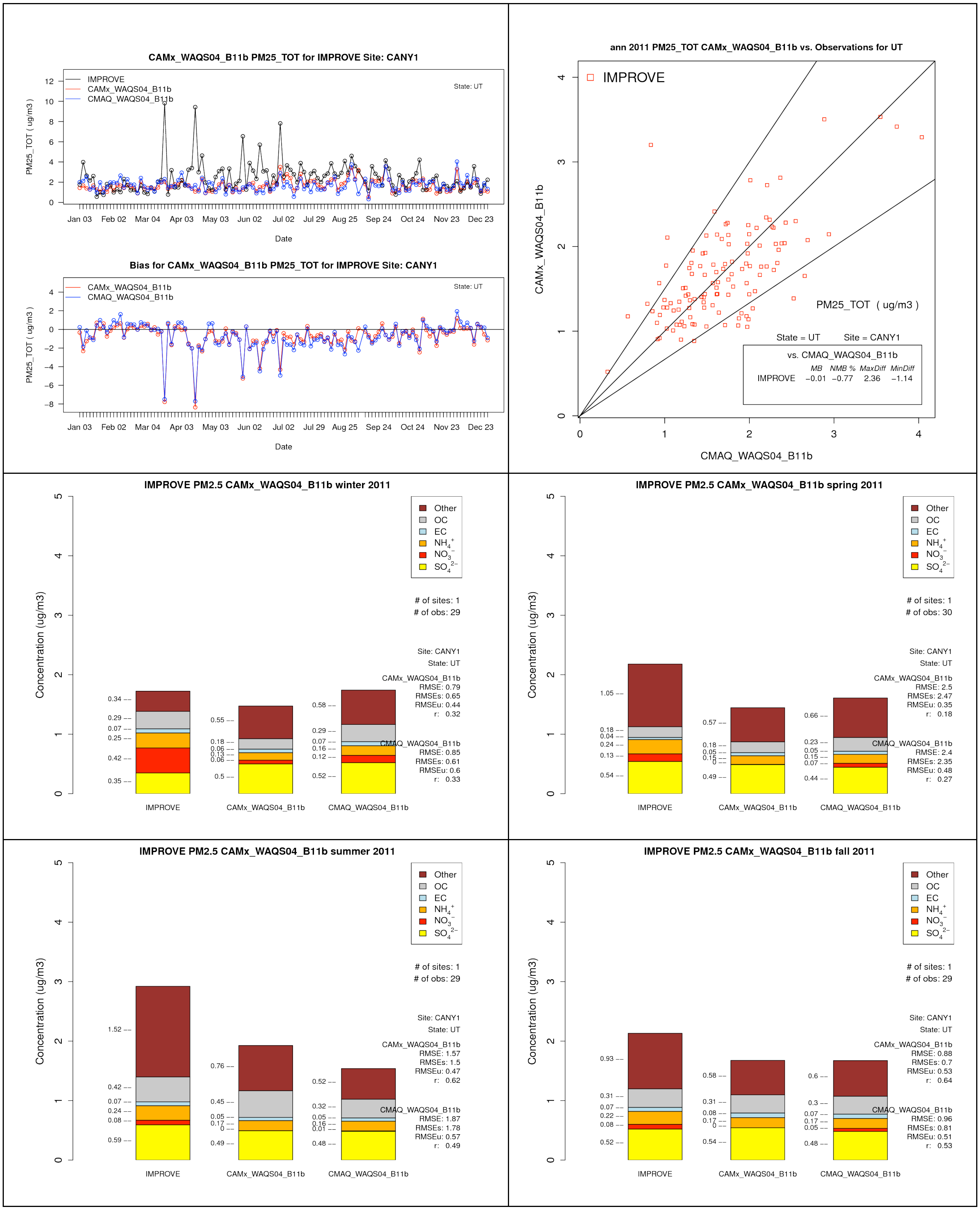


Figure 4-68. Canyonlands National Park, UT $PM_{2.5}$ model performance plots.

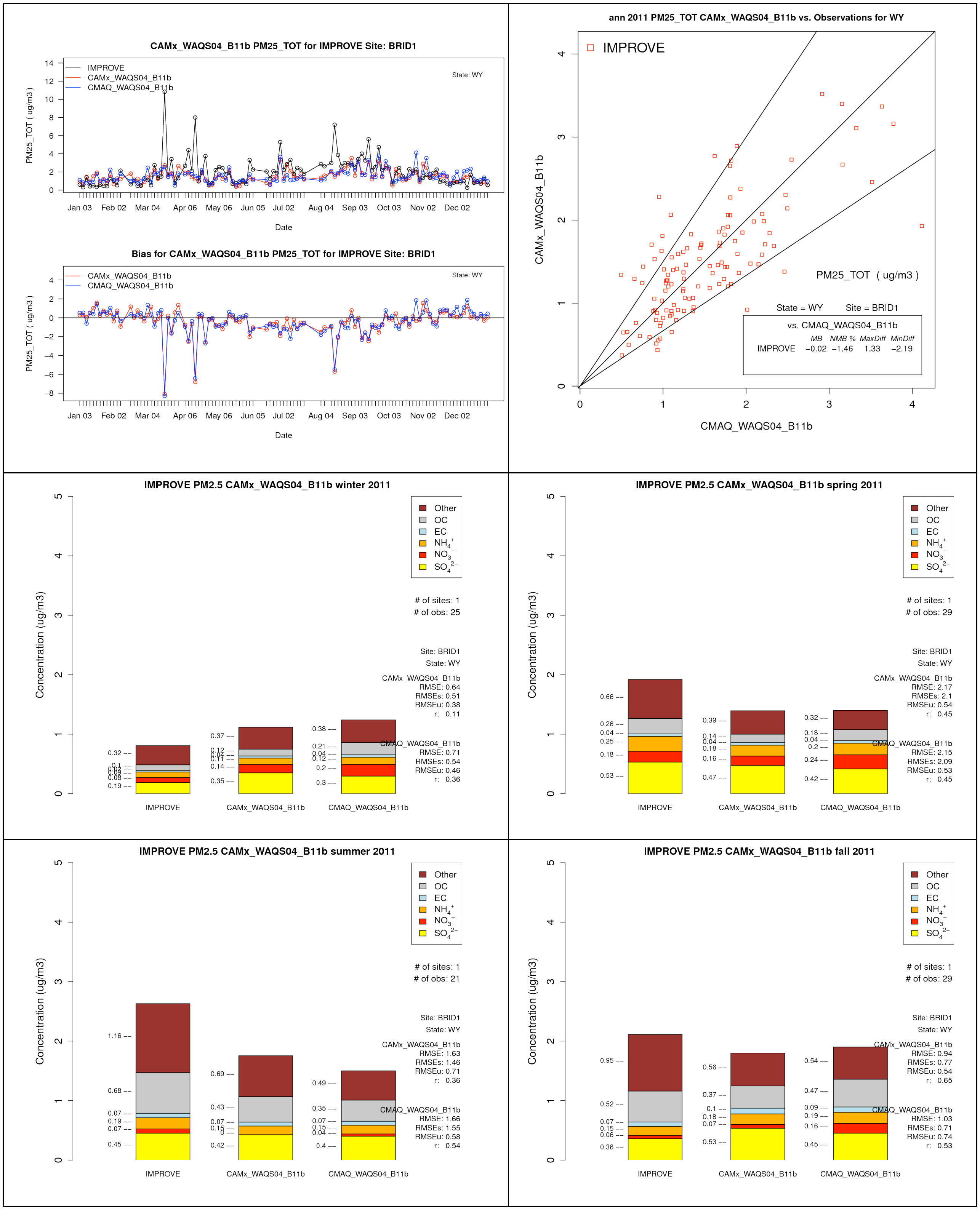


Figure 4-69. Bridger National Forest, WY $PM_{2.5}$ model performance plots.

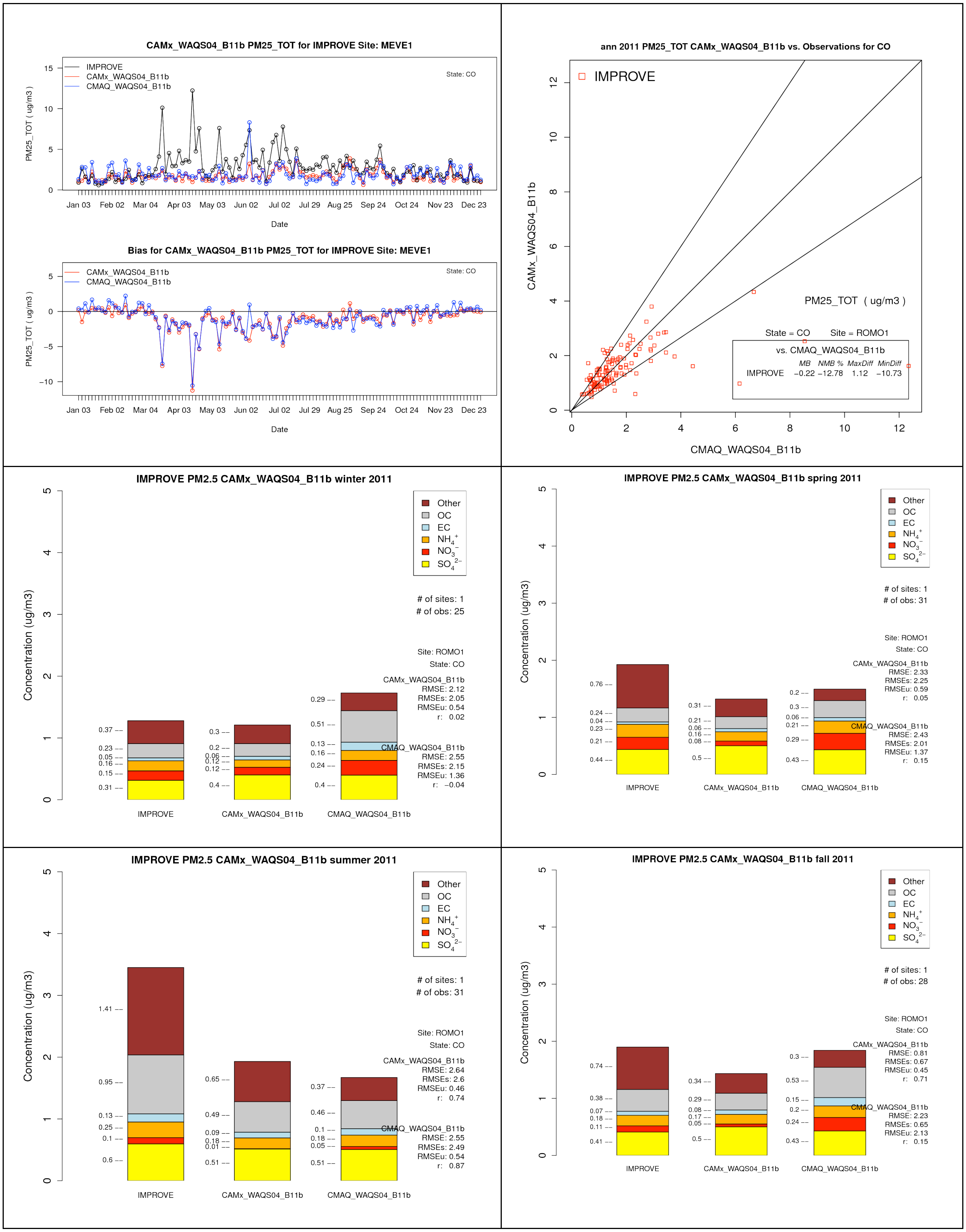


Figure 4-70. Rocky Mountain National Park, CO $PM_{2.5}$ model performance plots.

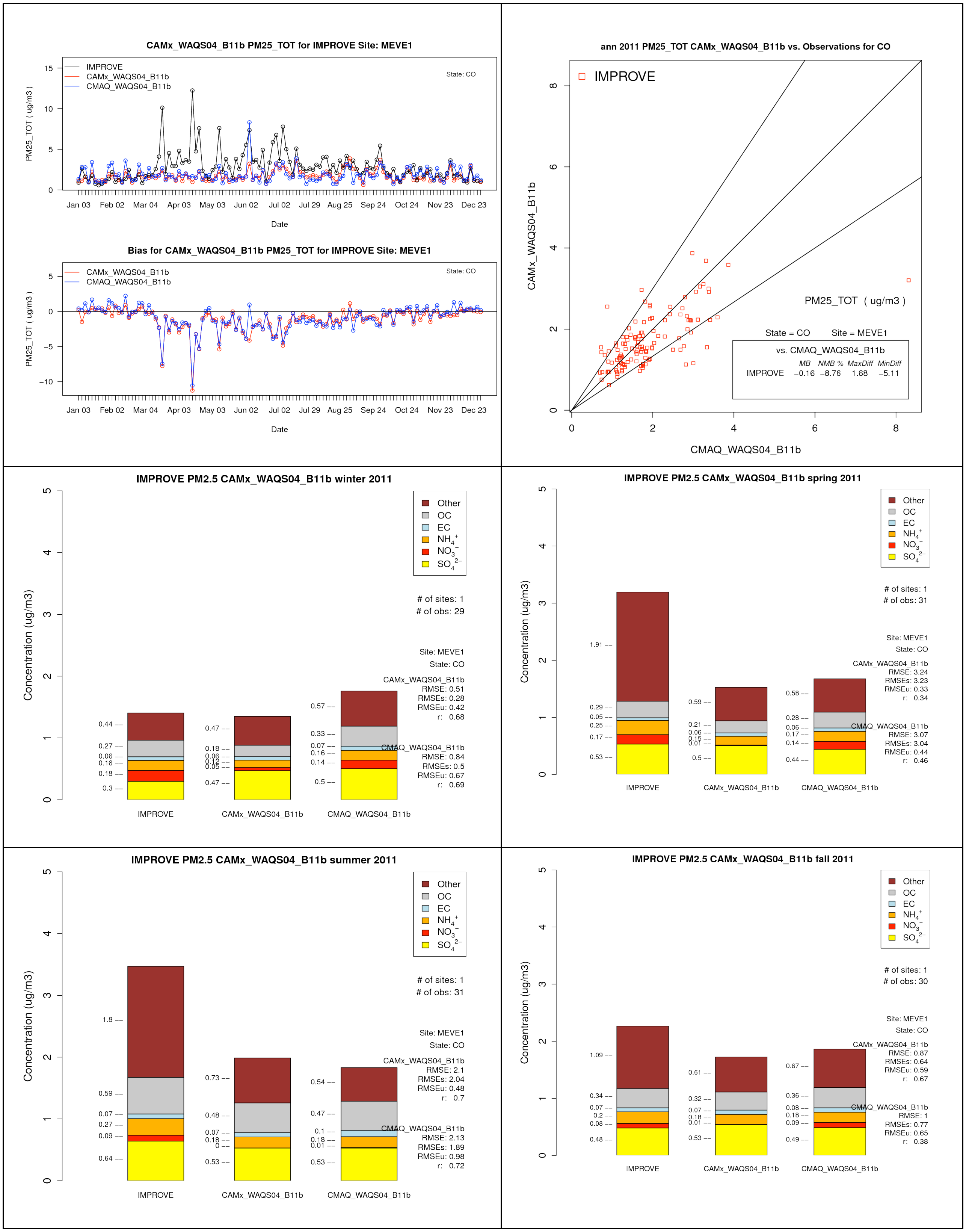


Figure 4-71. Mesa Verde National Park, CO $PM_{2.5}$ model performance plots.

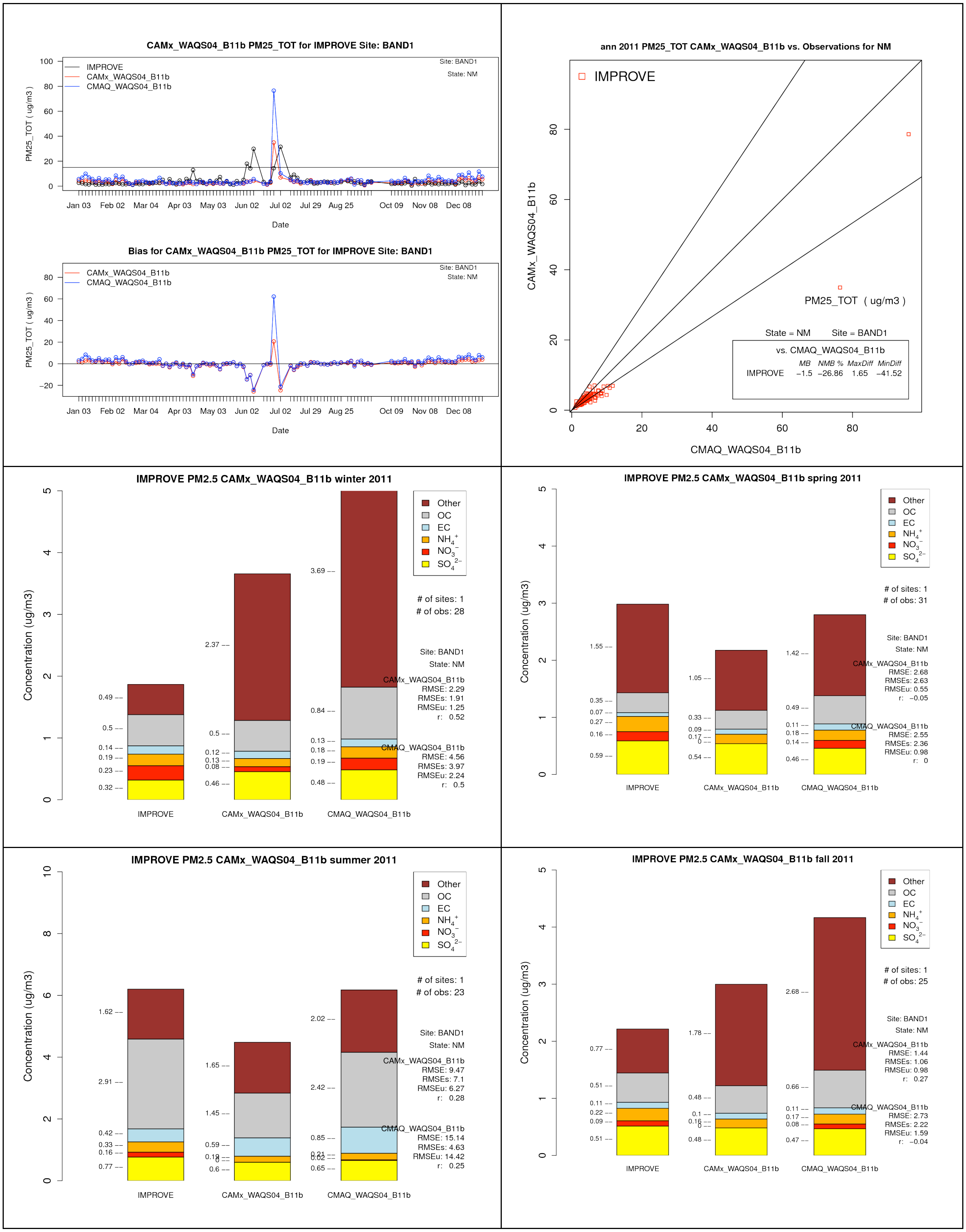


Figure 4-72. Bandolier National Park, NM $PM_{2.5}$ model performance plots.

4.3 AMMONIA MODEL PERFORMANCE

We examined the model performance for gas-phase ammonia (NH_3) through comparison to the Ammonia Modeling Network (AMoN) measurements. We followed the same approach and used the same sites for the Base11b evaluation as was used for the Base11a evaluation (UNC and Environ, 2015). We used the actual 2011 AMON observations for the sites listed in Table 4-12 to evaluate the performance of CAMx in simulating NH_3 surface concentrations in the 4-km WAQS modeling domain. As the Gothic, CO and Brooklyn Lake, WY monitors were not operating in 2011, these data are not used for the 2011 NH_3 model performance evaluation.

Table 4-13 and Figure 4-73 show that CAMx and CMAQ are both systematically underestimating NH_3. Table 4-13 shows model performance averaged across all sites in the 4-km modeling domain. As with simulation Base11a, the negative normalized mean biases (CAMx: -70.3%; CMAQ: -62.2%) indicate that the models are not accurately capturing at least one key parameter needed to estimate ambient NH_3. The biases are highest in the winter and summer months and lowest in October and November. Site-specific evaluation plots for the AMON NH_3 observations are available on the IWDW.

Table 4-12. AMoN NH_3 monitors in the 3SAQS 4-km domain

Site ID	Name	Start Date
CO10	Gothic	9/11/2012
CO13	Fort Collins	11/27/2007
CO88	Rocky Mountain Nat'l Park – Longs Peak	5/10/2011
CO98	Rocky Mountain Nat'l Park – Loch Vale	5/10/2011
ID03	Craters of the Moon Nat'l Monument	6/7/2010
NM98	Navajo Lake	1/11/2008
NM99	Farmington	1/9/2008
UT01	Logan	11/8/2011
UT09	Canyonlands Nat'l Monument – Islands in the Sky	5/6/2014
UT97	Salt Lake City	11/8/2011
WY94	Grand Teton Nat'l Park	9/22/2011
WY95	Brooklyn Lake	6/19/2012

Table 4-13. AMON NH_3 model performance indicators for all sites in the 4-km domain.

Location	R^2	NMB	NME	FB	FE	Mean Obs	Mean Mod
Units		%	%	%	%	ppb	ppb
CAMx	0.67	-70.3	73.0	-109.0	120.0	1.22	0.36
CMAQ	0.59	-62.2	70.0	-65.2	97.0	1.22	0.46

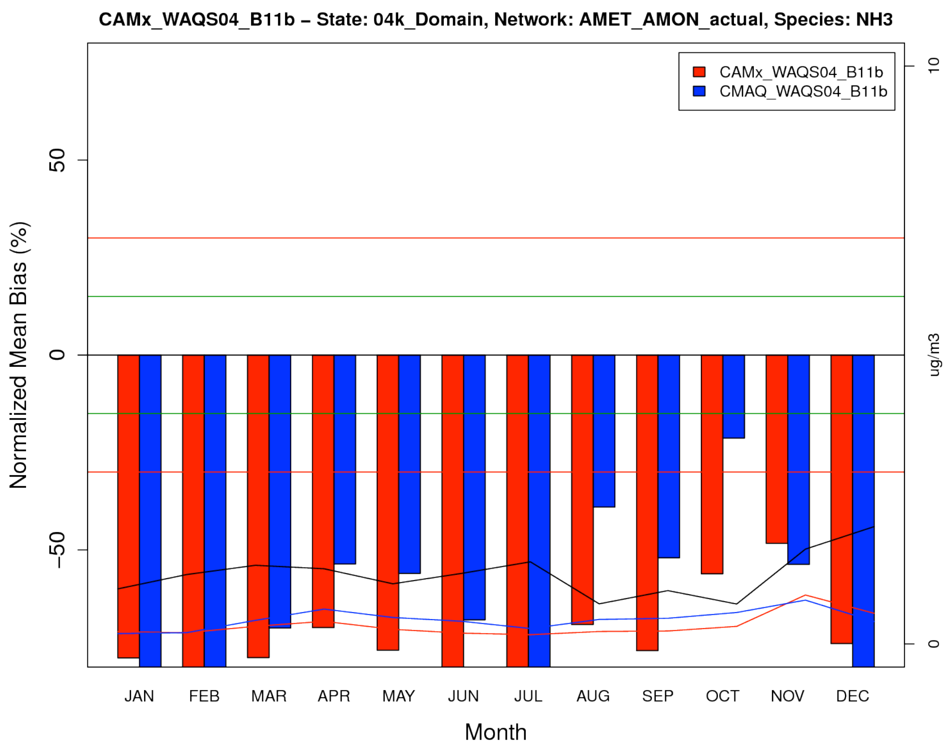


Figure 4-73. AMON NH_3 monthly bias-concentration plot.

4.4 WET DEPOSITION MODEL PERFORMANCE

We examined the model performance for wet deposition through comparison to the National Atmospheric Deposition Program (NADP) network measurements. The available measurements are for SO_4, NO_3 and NH_4. As in the Base11a evaluation (UNC and Environ, 2015), we followed the approaches of Appel et al (2011) and normalized the CAMx and CMAQ deposition species to match the observations. We also adjusted the model results to account for biases in the modeled precipitation. The normalized CAMx SO_4 deposition estimates include 150% of the estimated SO_2 deposition (based on the ratio of the molecular weights) because the SO_2 is fully oxidized to SO_4 in the NADP bucket by the time the measurements are collected. Similarly, the NH_4 deposition estimates include 106% of the CAMx NH_3 deposition and the NO_3 deposition estimates include 98.4% of the CAMx HNO_3 deposition. Table A.1 shows the expressions that we used to normalize the CAMx output deposition species with the NADP observations.

To account for the fact that some of the biases in the CAMx deposition estimates are due to biases in the simulated precipitation, we adjusted the CAMx annual and seasonal accumulated deposition results at each NADP monitor by the ratio of the observed to modeled accumulated precipitation over the same period. The effectiveness of the adjustment is highly dependent on the precipitation predictions in the model: sites impacted by particularly poor simulated meteorology estimates respond most favorably to the adjustment.

In general, the WAQS SO_4 deposition performance shows the most favorable response (lower bias and error) to the precipitation adjustment, while NO_3 and NH_4 do not respond as well. These trends are consistent with the results of Appel et al. (2011) and indicate that the biases in NO_3 and NH_4 performance are strongly influenced by errors in other model parameters. The NO_3 performance is likely impacted by poor predictions of lightning NO and NH_4 performance by surface NH_3 emissions. Additional details of the simulated deposition performance are provided in this section.

Table 4-14 summarize annual wet deposition species CAMx and CMAQ performance averaged across all sites in the 12-km WAQS modeling domain. The performance indicators in these tables include the impacts of the precipitation adjustments described above. On an annual basis, both models underestimate wet deposition for all species. Sulfate deposition shows the best performance across all sites in the 12-km domain (CAMx NMB: -22.3%; CMAQ NMB: -18.9%), followed by nitrate (CAMx NMB: -49.3%; CMAQ NMB: -38.8%) and ammonium (CAMx NMB: -50.4%; CMAQ NMB: -45.9%).

The scatter plots in Figure 4-74 through Figure 4-76 compare CAMx and CMAQ to NADP observations of accumulated annual wet deposition for all sites in the 12-km domain for SO_4, NO_3, and NH_4. Each point on these plots represents the accumulated deposition for an individual NADP monitor. The model results in these figures include the impacts of the precipitation adjustments described above. The CAMx model performance is plotted as red circles; the CMAQ model is plotted as blue circles. The important features of these plots include:

- All of these plots show relatively high r^2 values for the adjusted model, meaning that CAMx and CMAQ are generally good models for wet deposition and account for a high percentage of the variance in the observations
- Negative biases in the deposition estimates indicate that both models underestimate at least one key deposition parameter.
- Although the deposition estimates are still low relative to the observations, CMAQ estimates higher deposition than CAMx resulting in smaller negative biases for all species.

Figure 4-77 through Figure 4-80 compare observed and modeled (12-km domain CAMx and CMAQ) accumulated monthly wet deposition at all NADP sites in Colorado, New Mexico, Utah, and Wyoming. These plots confirm the annual deposition performance statistics that the models are systematically underestimating all deposition species in all states.

Figure 4-81 through Figure 4-84 are daily accumulated wet deposition time series plots for the following NADP sites:

- Rocky Mountain National Park, Colorado (CO19)
- Canyonlands National Park, Utah (UT09)
- Bandolier National Park, New Mexico (NM07)
- Pinedale, Wyoming (WY06)

These plots illustrate the daily variability in the wet deposition observations and model predictions. Additional site-specific wet deposition model performance plots are available on the IWDW.

Table 4-14. Accumulated annual wet deposition species performance indicators at all NADP sites in the 12-km modeling domain

Species		R^2	NMB	NME	FB	FE	Mean Obs	Mean Mod
Units			%	%	%	%	kg/ha	kg/ha
CAMx	NH4	0.73	-50.4	53.0	-74.4	80.5	1.39	0.69
CMAQ	NH4	0.75	-45.9	48.9	-56.1	63.3	1.46	0.79
CAMx	NO3	0.75	-49.3	49.4	-77.5	77.6	3.09	1.56
CMAQ	NO3	0.78	-38.8	40.5	-51.9	54.1	3.20	1.96
CAMx	SO4	0.86	-22.3	29.7	-43.1	50.4	2.33	1.81
CMAQ	SO4	0.88	-18.9	27.0	-30.5	38.1	2.41	1.96

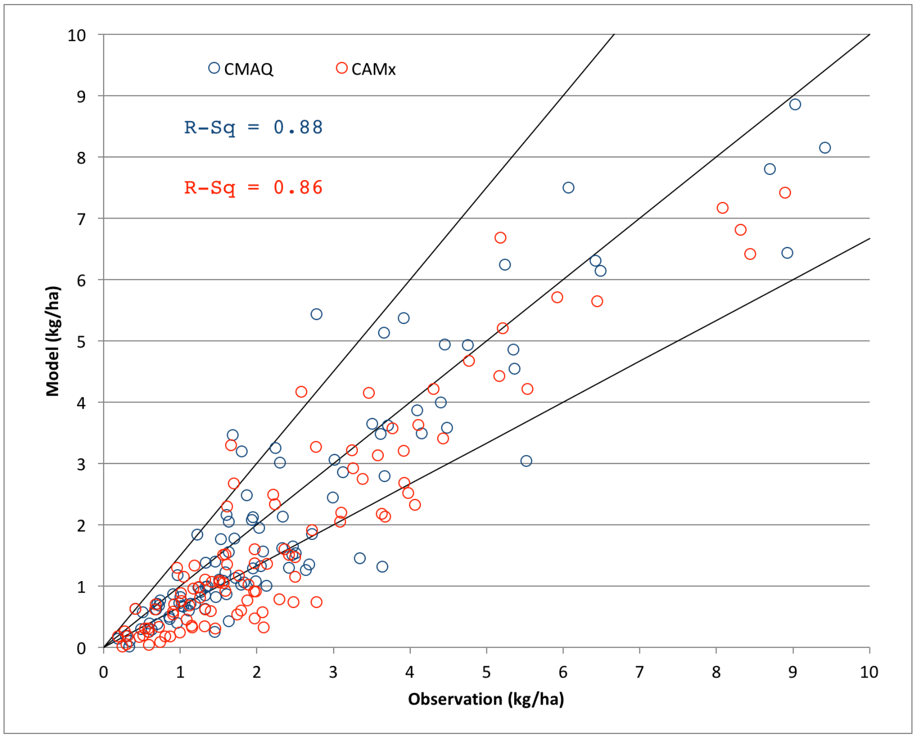


Figure 4-74. CAMx and CMAQ 2011b 12-km domain accumulated annual sulfate wet deposition model performance.

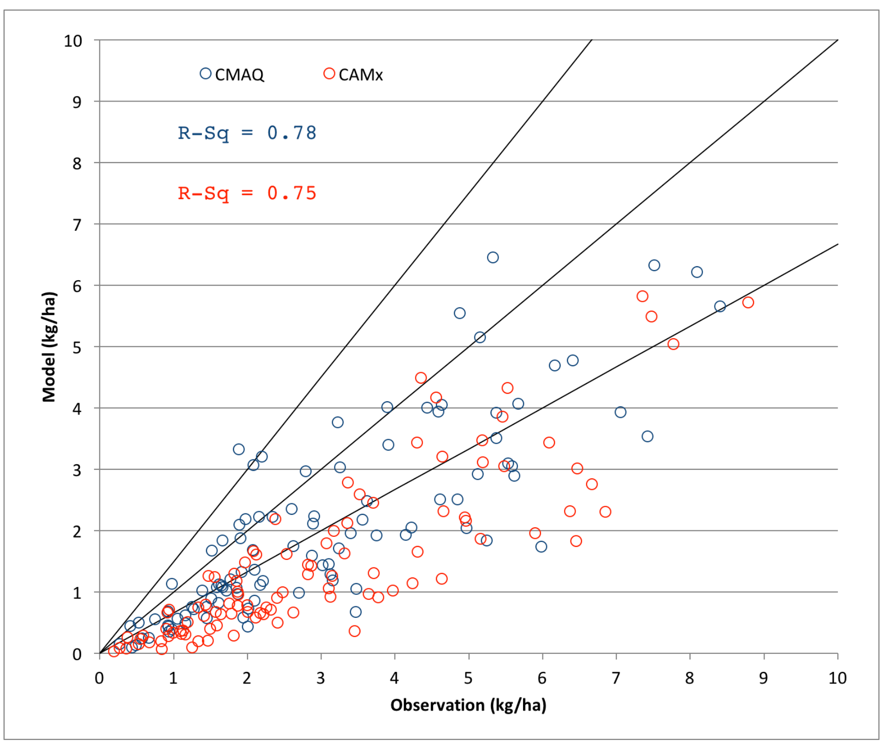


Figure 4-75. CAMx and CMAQ 2011b 12-km domain accumulated annual nitrate wet deposition model performance.

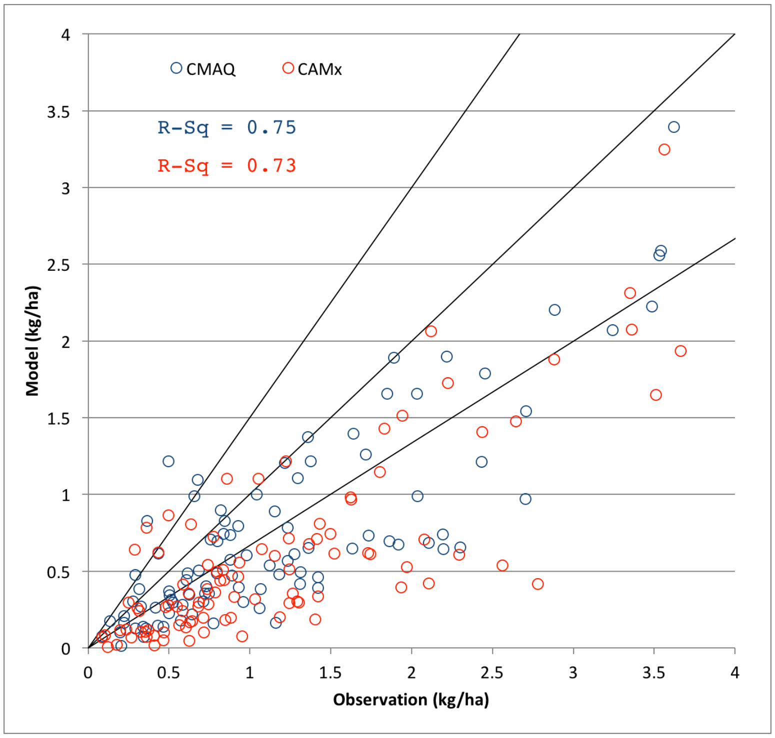


Figure 4-76. CAMx and CMAQ 2011b 12-km domain accumulated annual ammonium wet deposition model performance.

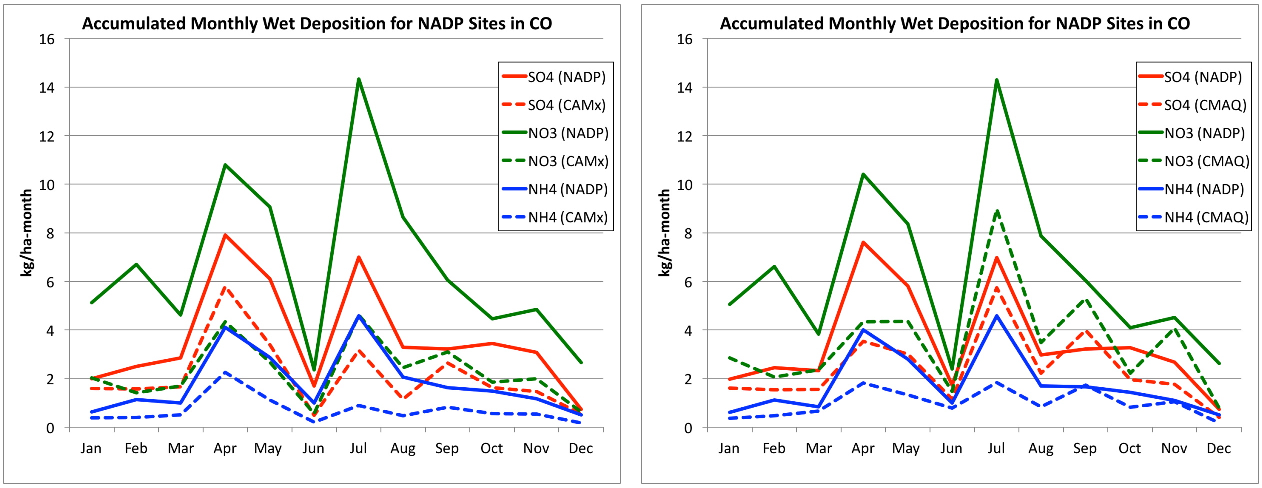


Figure 4-77. Accumulated monthly wet deposition performance at NADP sites in Colorado

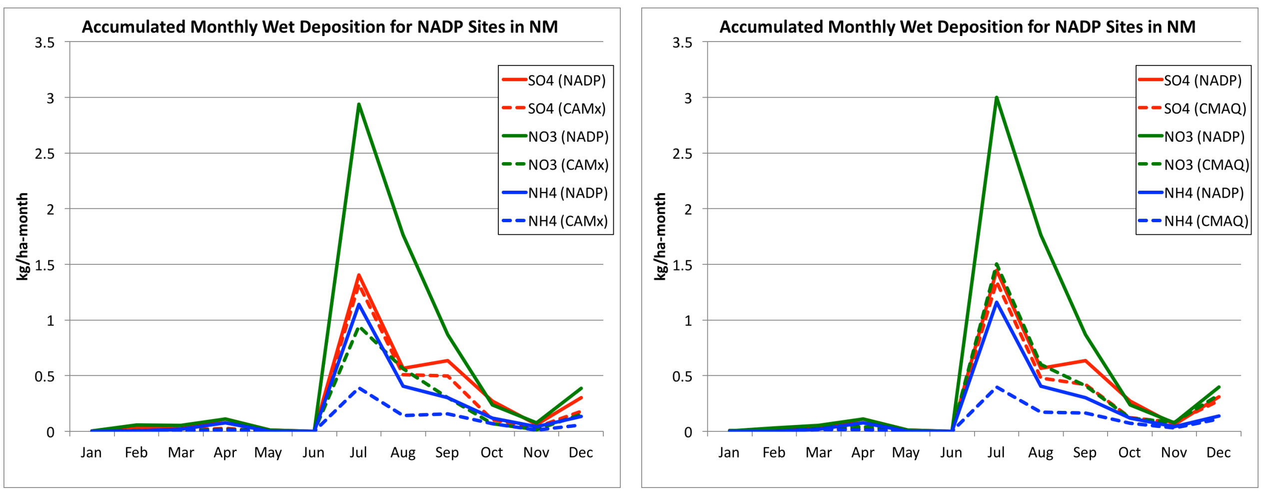


Figure 4-78. Accumulated monthly wet deposition performance at NADP sites in New Mexico

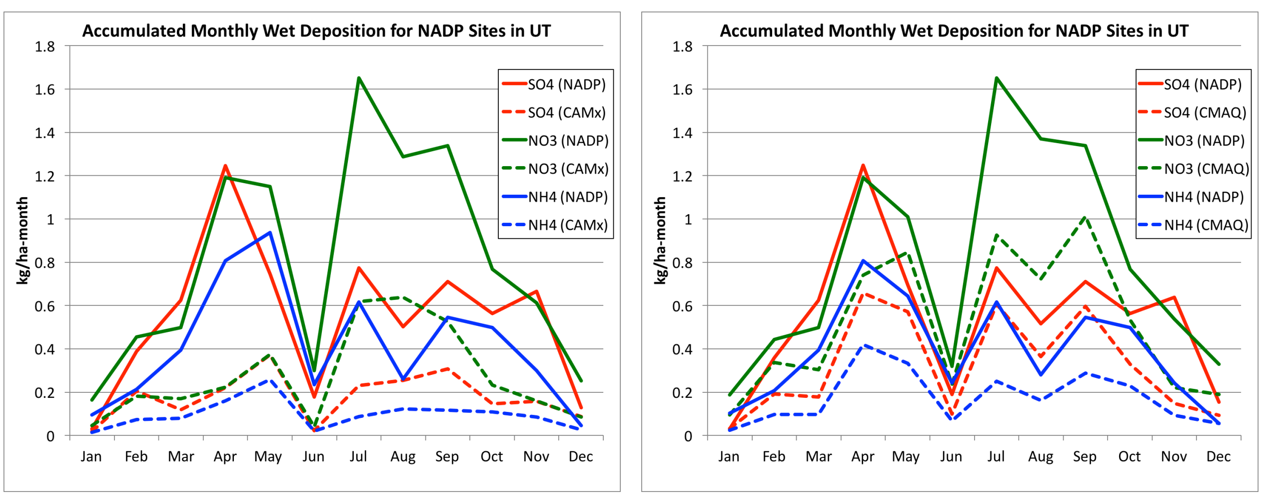


Figure 4-79. Accumulated monthly wet deposition performance at NADP sites in Utah

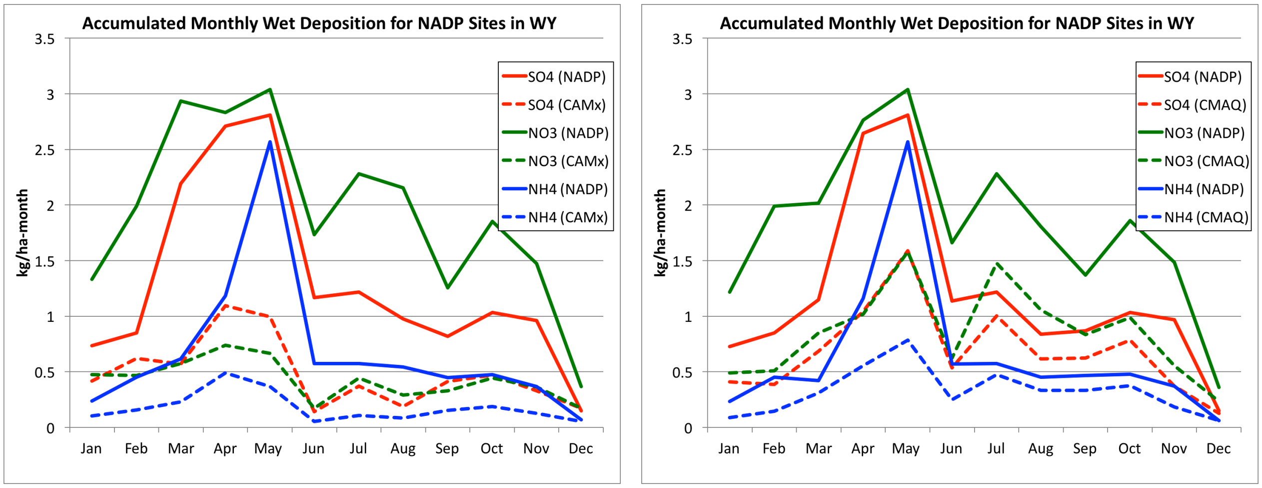


Figure 4-80. Accumulated monthly wet deposition performance at NADP sites in Wyoming

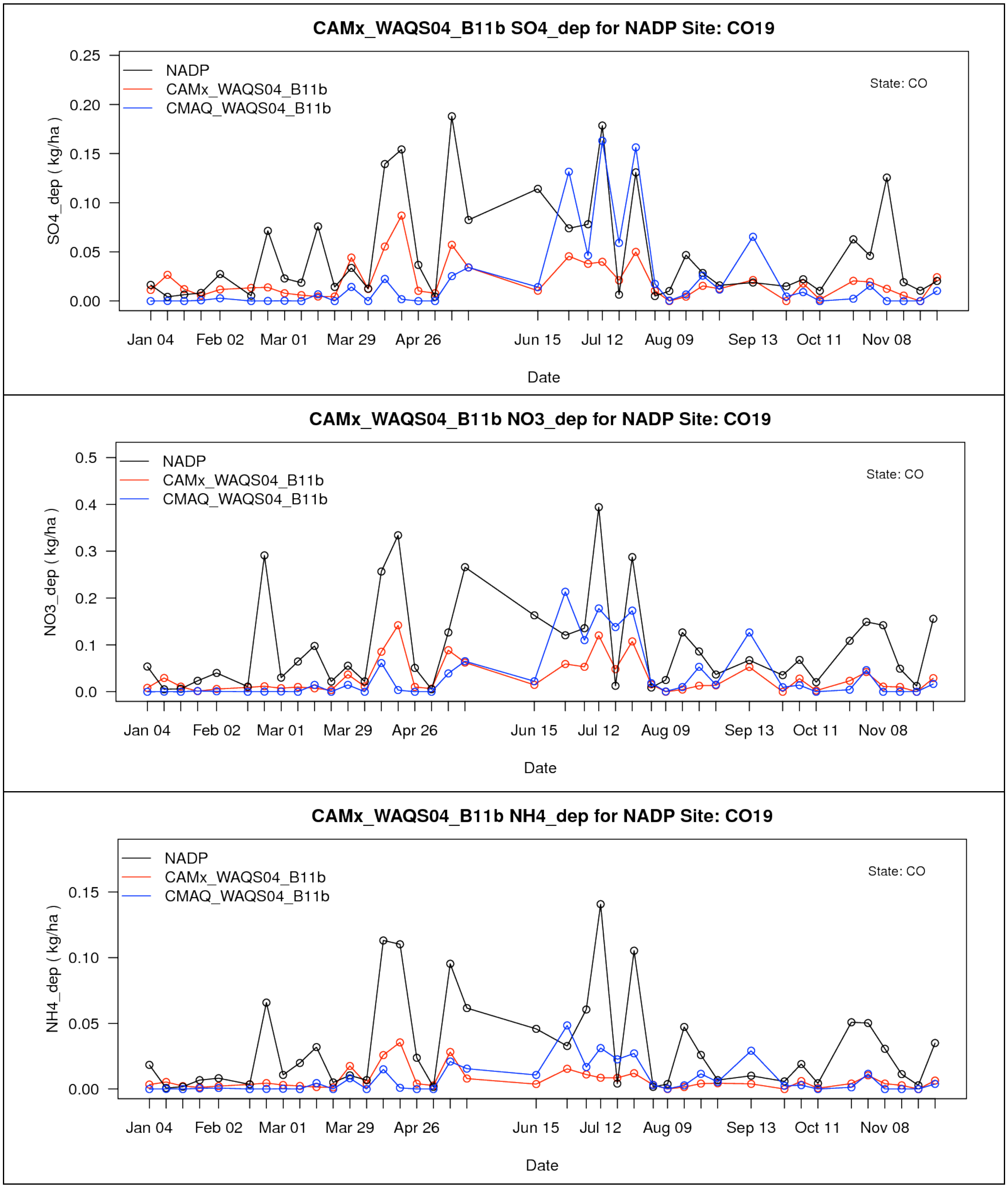


Figure 4-81. Rocky Mountain National Park, Colorado Wet Deposition Performance (unadjusted).

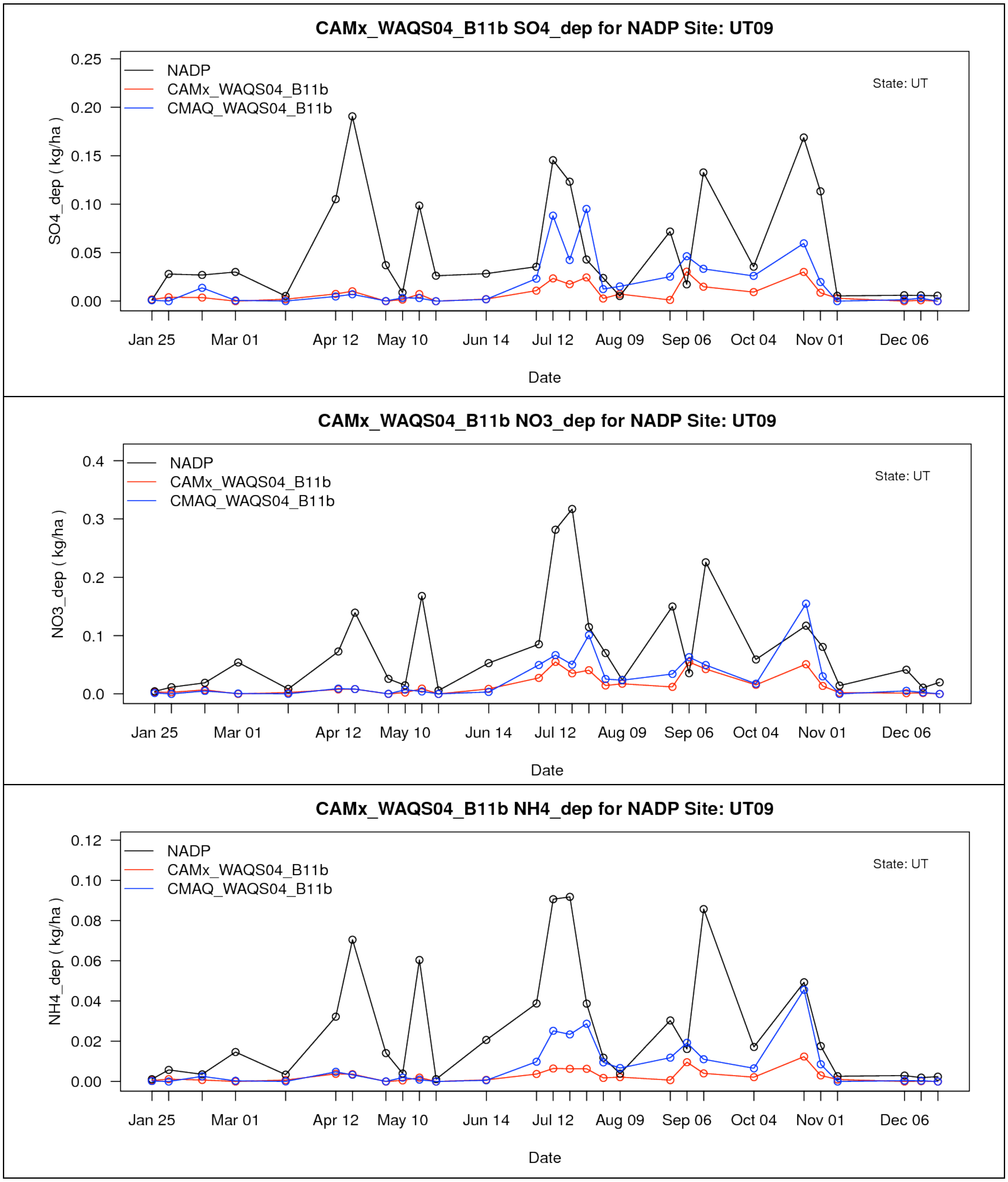


Figure 4-82. Canyonlands National Park, Utah Wet Deposition Performance (unadjusted).

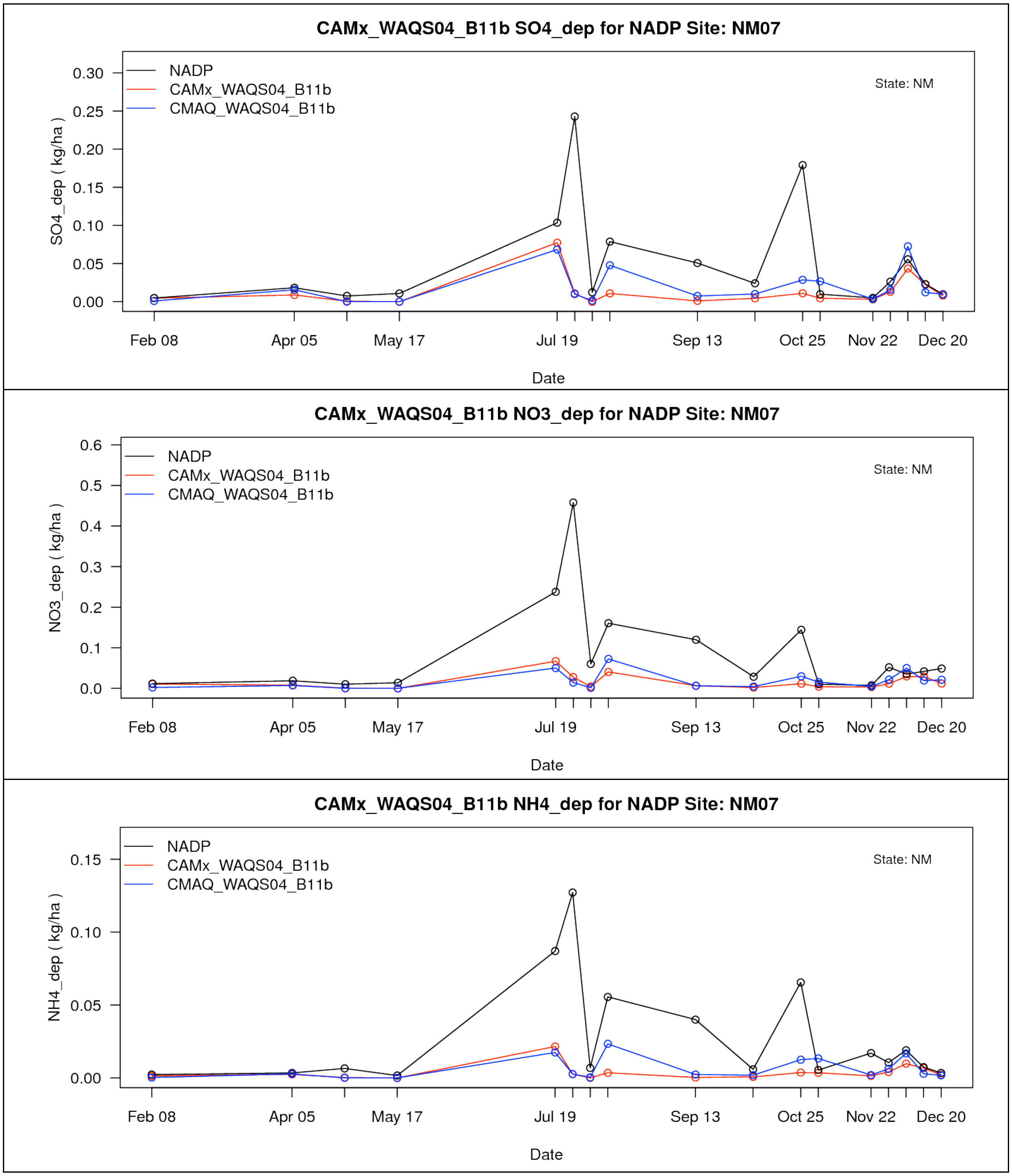


Figure 4-83. Bandolier National Park, New Mexico Wet Deposition Performance (unadjusted).

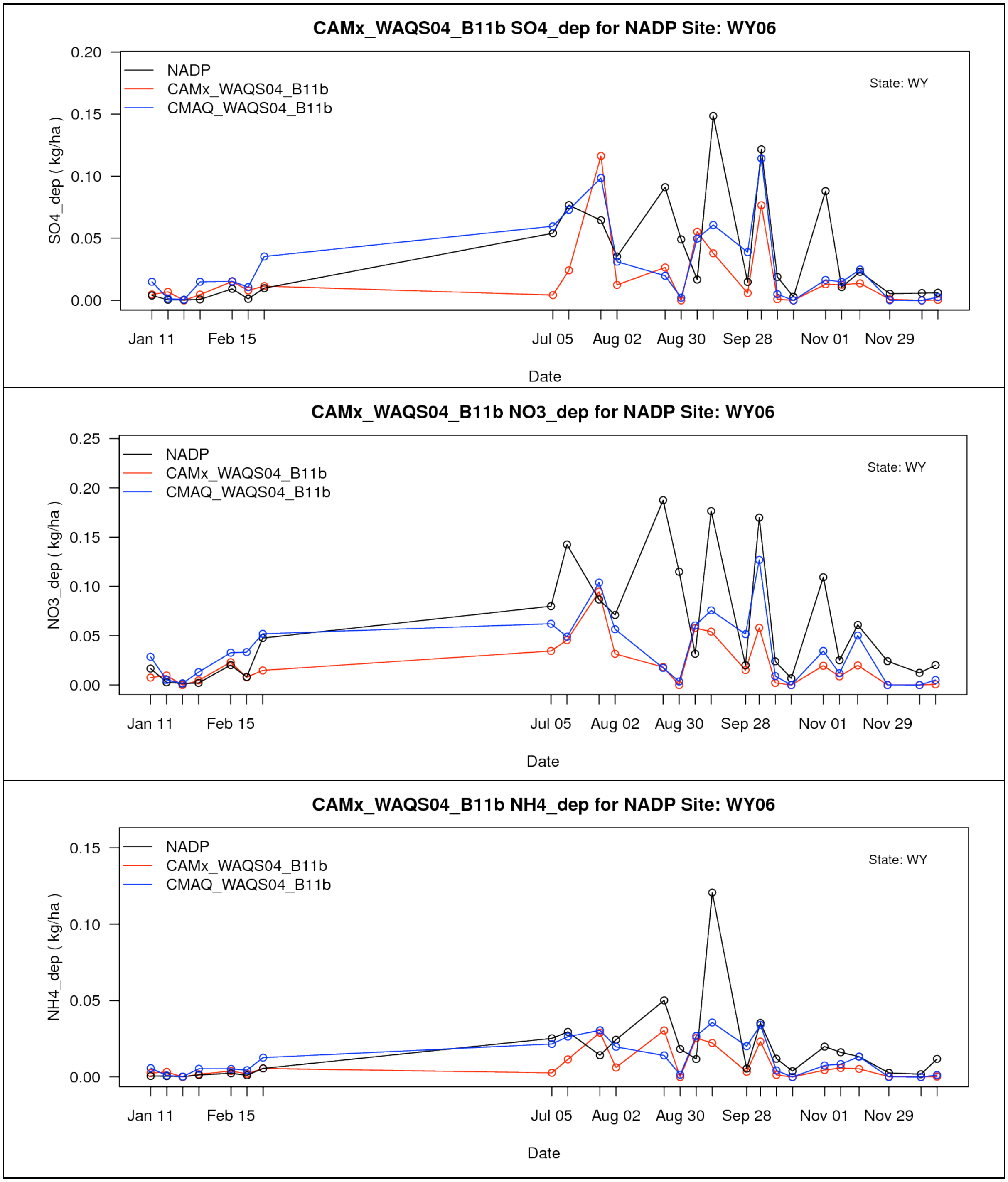


Figure 4-84. Pinedale, Wyoming Wet Deposition Performance (unadjusted).

4.5 REGIONAL HAZE MODEL PERFORMANCE

This section presents regional haze model performance metrics. Modeled and observed light extinctions are shown for both CAMx and CMAQ. We calculated species and total extinctions using the revised IMPROVE visibility equation (Pitchford et al., 2007).

Table 4-15 shows model bias and errors for the estimates of annual average light extinctions at all IMPROVE sites in the 4-km WAQS modeling domain and in the states of Colorado, New Mexico, Utah, and Wyoming. Total extinction and species extinction performance statistics are shown for both CAMx and CMAQ. This table shows that the model performance for total light extinction is comparable between the two models in all areas of the domain. Significant performance differences exist in the species light extinctions.

In general, both models underestimate light extinction, although some differences exist between species and in different parts of the modeling domain. CMAQ Base11b estimates higher SO_4, NO_3, and EC extinction than CAMx, resulting in lower biases than CAMx relative to the estimated IMPROVE observed light extinctions for these species. CAMx estimates higher OC and coarse mass light extinction than CMAQ. Even with the removal of sea salt from the boundary conditions, both models overestimate the contributions of sea salt to light extinction. CAMx underestimates the contribution of soil to light extinction, a trend that is likely related to the overcorrection of the boundary condition dust in simulation Base11b. CMAQ soil extinction estimates are not available for simulation Base11b because CMAQ does not track soil PM explicitly.

Figure 4-85 compares CAMx and CMAQ annual average modeled to observed light extinctions at each IMPROVE monitor in the 4-km domain. These plots supplement the domain average performance statistics in
Table 4-15 by showing the annual average light extinction estimates at each monitor. The CAMx underestimates of light extinction from SO_4 are offset by sea salt overestimates at many of the IMPROVE sites. The CMAQ performance is primarily impacted by underestimates of light extinction from course mass and soil.

Figure 4-86 through Figure 4-89 are stacked bar charts comparing the modeled light extinctions to IMPROVE observations for the 20% most impaired visibility days in each season. Spring season biases in both models are driven by underestimates in SO_4, soil and coarse mass. Summer and fall season biases result from modeled underestimates of OC, EC, dust, and coarse mass. Winter season biases are driven by underestimates of SO_4, NO_3, and coarse mass.

The CMAQ extinction estimates presented for simulation Base11b need to be reevaluated due to questions about the model species mapping for soil and coarse mass. As CMAQ does not explicitly track dust in the model output, we could not derive soil extinctions for the model. The definition of coarse mass in the CMAQ model outputs as it is applied to the IMPROVE visibility equation also warrants further investigation as there appears to be a mismatch between how we defined coarse mass from CMAQ and what is being reported by IMPROVE.

Table 4-15. Visibility model performance indicators.

Model	Species	4-km Domain		Colorado		New Mexico		Utah		Wyoming	
	Species	NMB	NME	NMB	NME	NMB	NME	NMB	NME	NMB	NME
	Units	%	%	%	%	%	%	%	%	%	%
CAMx	Total	-15.4	26.7	-15.5	22.2	-17.4	28.8	-14.4	21.1	-8.6	20.4
CMAQ	Total	-17.0	29.5	-19.8	25.5	-9.1	38.0	-20.3	24.6	-9.0	24.3
CAMx	SO4	-69.2	69.8	-68.3	68.6	-71.0	71.0	-71.6	71.7	-62.2	64.3
CMAQ	SO4	-14.7	42.2	-14.5	39.2	-13.5	40.9	-15.0	40.8	-10.2	45.4
CAMx	NO3	-30.6	97.6	-47.0	65.7	-8.8	84.8	-56.9	90.3	-49.2	83.0
CMAQ	NO3	-21.1	83.9	2.9	84.6	-8.7	83.5	-54.3	77.7	8.6	84.2
CAMx	OC	-23.1	74.3	0.8	67.9	-46.4	83.9	16.6	76.5	-25.9	80.6
CMAQ	OC	-28.8	73.0	-38.1	58.6	-21.0	97.9	-36.0	58.6	-27.6	75.8
CAMx	EC	-50.2	92.7	-47.9	85.8	-72.1	87.2	-35.4	91.7	-19.3	109.0
CMAQ	EC	10.9	73.9	-11.2	57.2	19.2	98.9	-16.3	47.1	1.5	61.7
CAMx	CM	-47.4	72.1	-58.8	68.9	-29.8	68.1	-48.3	63.2	-2.9	68.9
CMAQ	CM	-69.2	87.8	-84.0	87.4	-7.5	102.0	-69.9	76.9	-52.5	77.4
CAMx	SS	1520	1550	1950	1960	2230	2230	806	892	887	947
CMAQ	SS	43.3	167.0	53.4	176.0	25.2	161.0	-15.0	124.0	22.8	155.0
CAMx	Soil	-46.6	81.7	-58.9	74.8	-38.5	79.8	-42.6	74.6	-7.4	92.8
CMAQ	Soil										

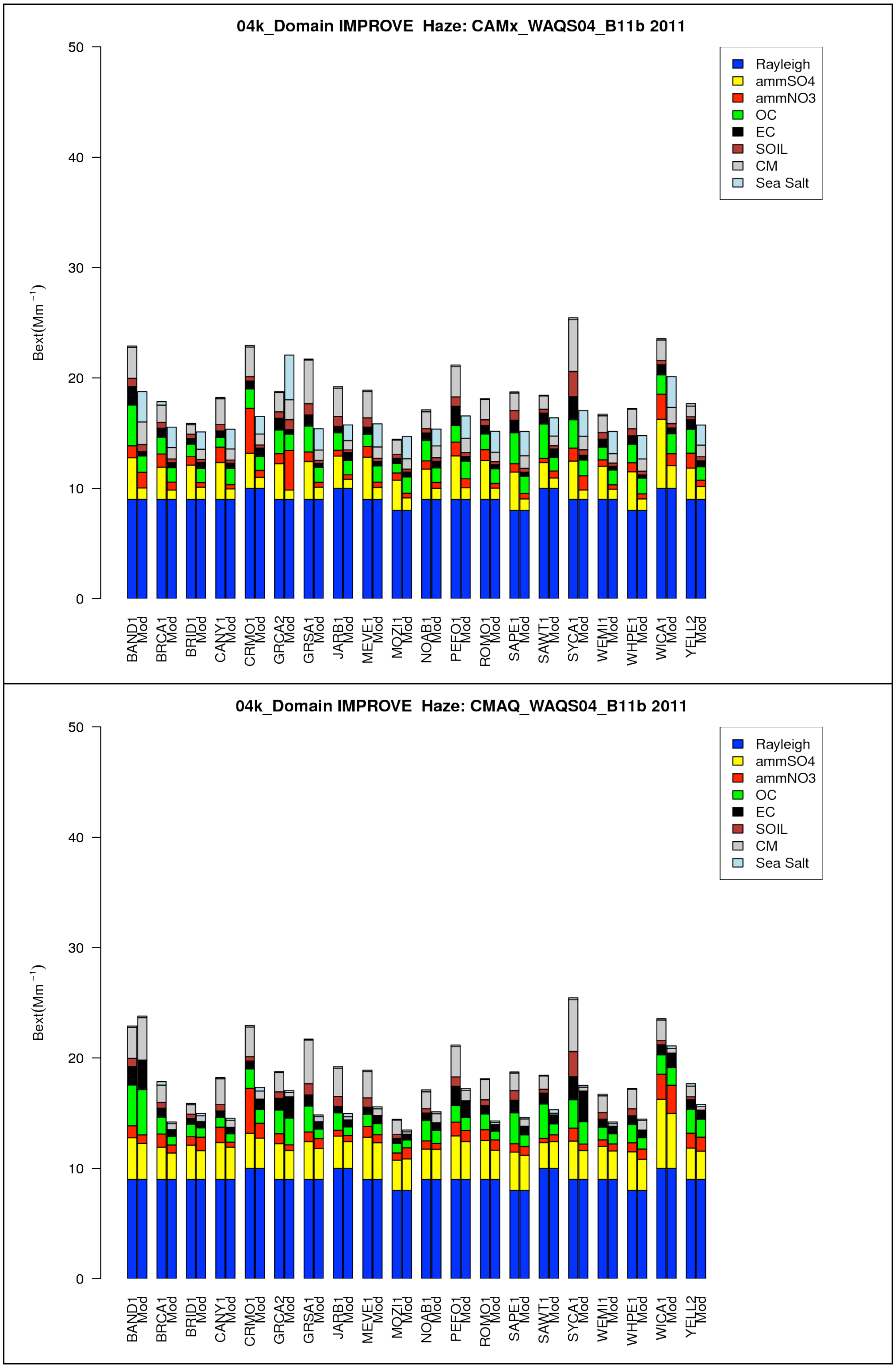


Figure 4-85. CAMx and CMAQ Base11b vs. IMPROVE annual average species extinctions.

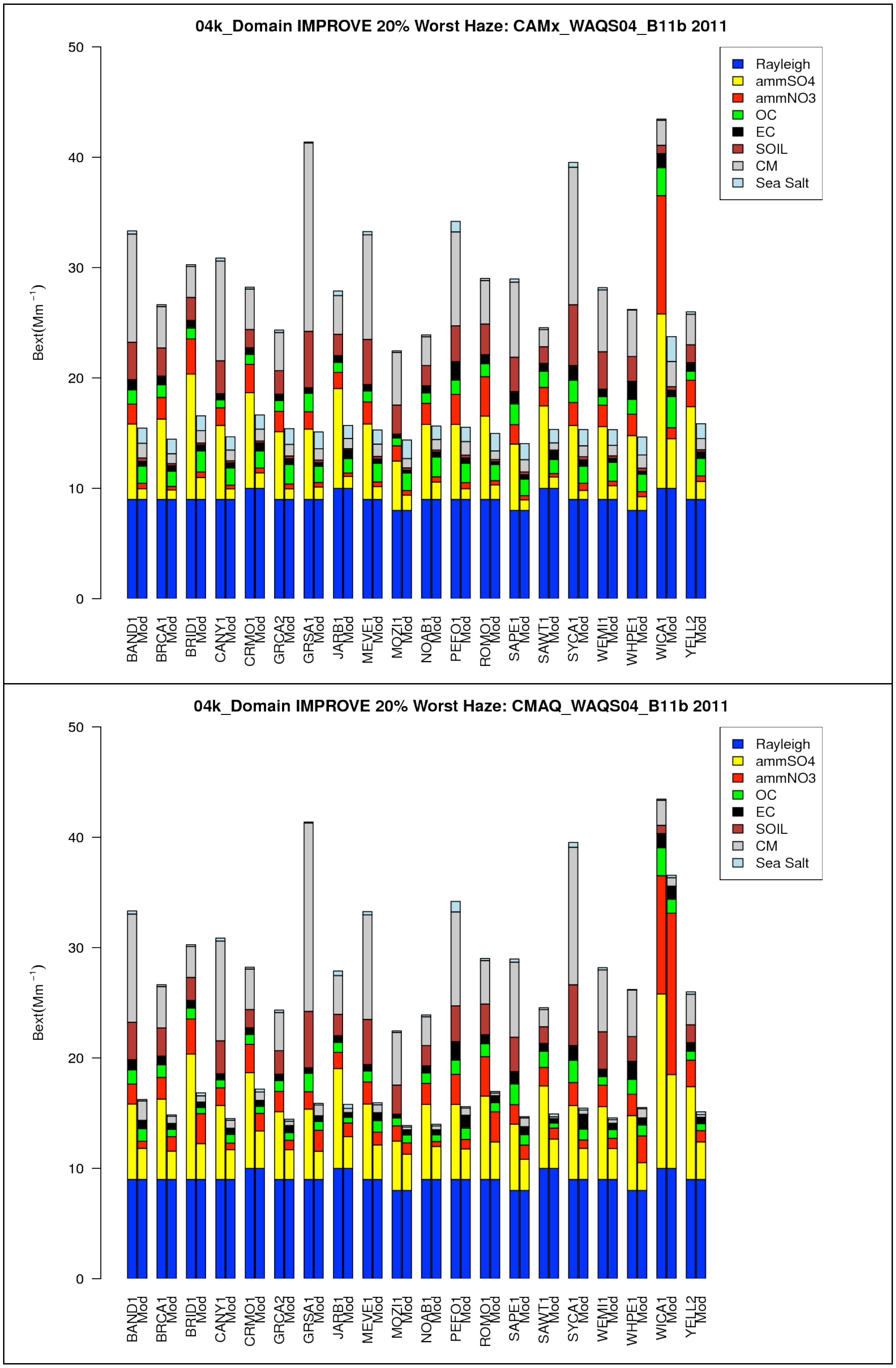


Figure 4-86. CAMx and CMAQ Base11b vs. IMPROVE species extinctions for spring season 20% most impaired visibility days.

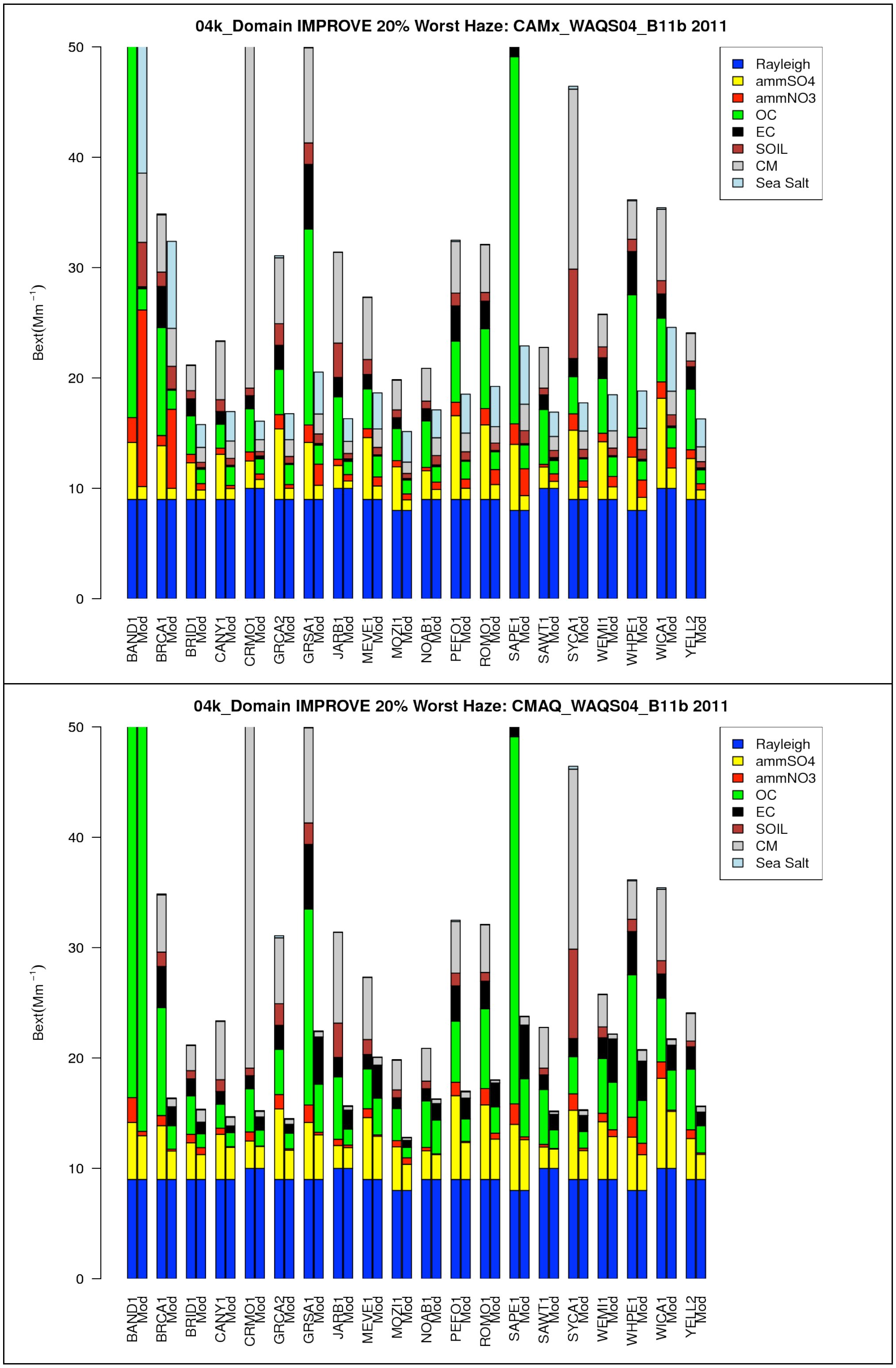
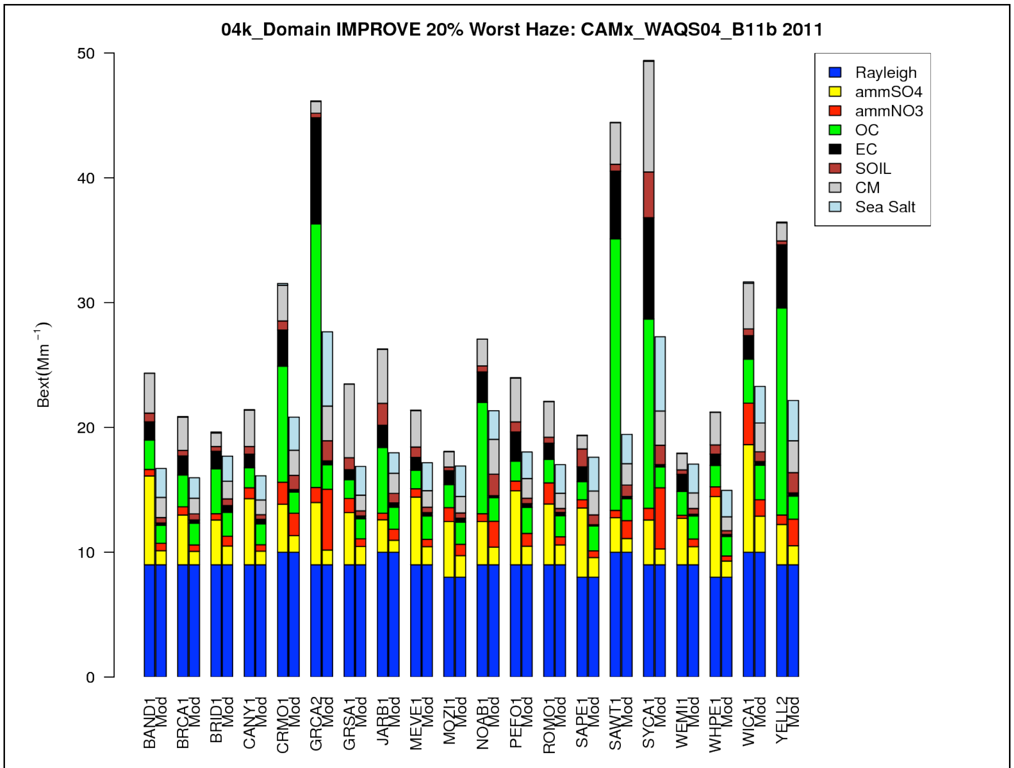


Figure 4-87. CAMx and CMAQ Base11b vs. IMPROVE species extinctions for summer season 20% most impaired visibility days.



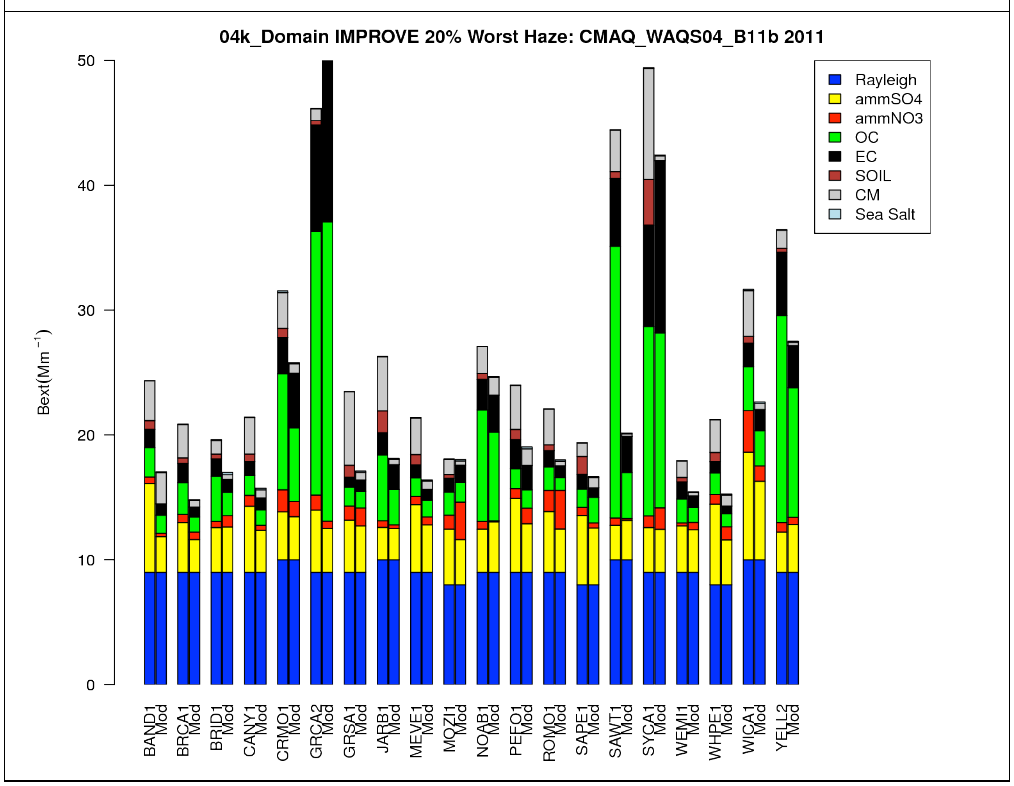


Figure 4-88. CAMx and CMAQ Base11b vs. IMPROVE species extinctions for fall season 20% most impaired visibility days.

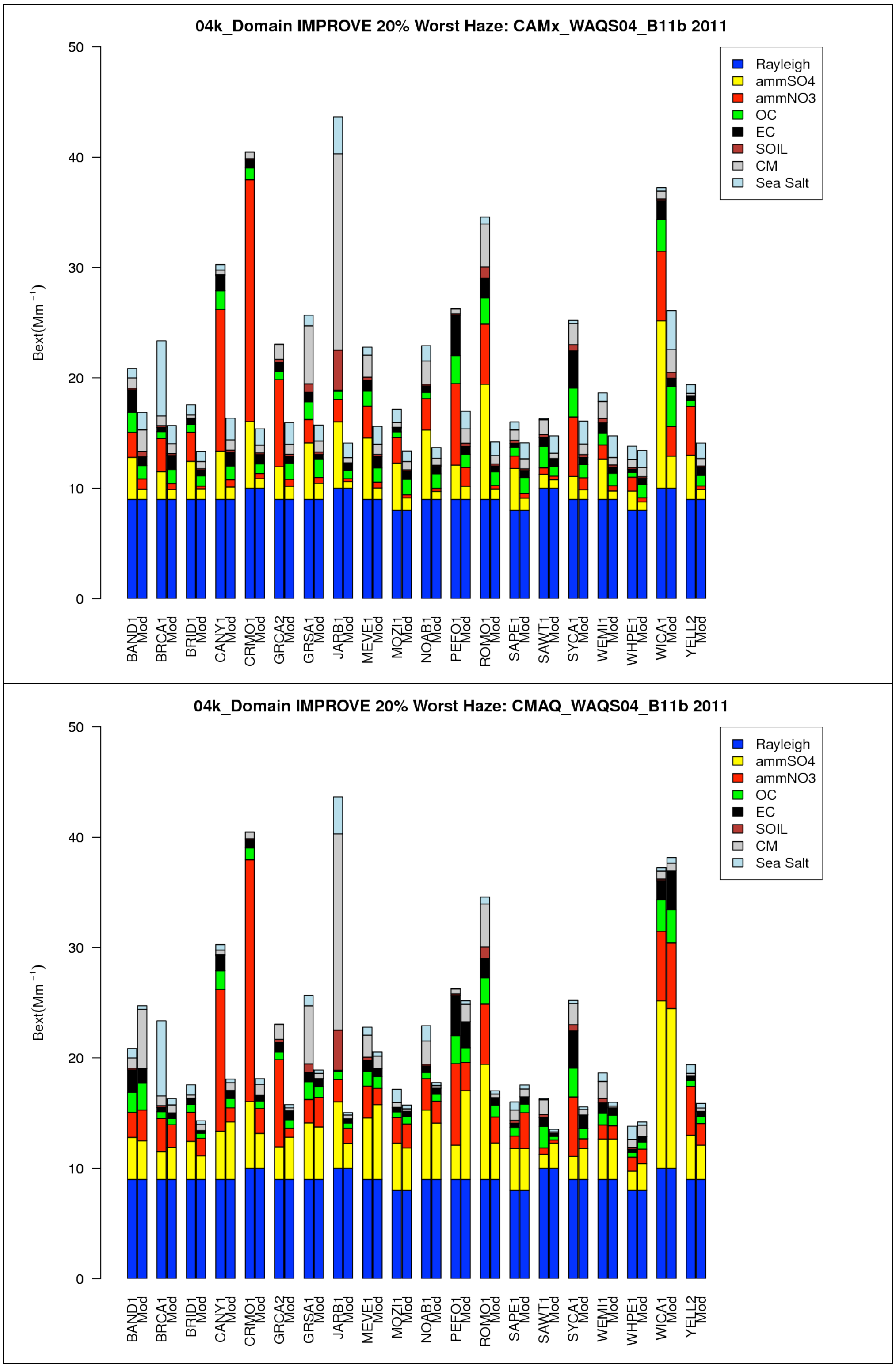


Figure 4-89. CAMx and CMAQ Base11b vs. IMPROVE species extinctions for winter season 20% most impaired visibility days.

5 RECOMMENDATIONS FOR FUTURE WORK

This section summarizes the recommendations for additional analysis and/or future work listed in the body of this report.

1) Additional investigation into the wind directions and speeds on the poor O_3 and NO_2 performance days is recommended.
2) Examine causes of NO_2 overestimates by the models.
3) Future work on improving ammonia model performance in the West should expand on the work of previous nitrogen modeling studies in the region. A bi-directional flux model should definitely be evaluated for the impacts on ammonia model performance. Further investigation of nitrogen deposition, ammonia and NOx emissions, regional flow regimes (i.e. up-slope and down-slope flows), and improvements to the temporal/spatial/magnitudes of emissions sources are needed to understand the deficiencies in the ammonia model and to identify areas for improvement.
4) Replace the boundary condition dust estimates with a model that simulates the global dust cycle.
5) Leverage work from studies on winter ozone and cold pool modeling to improve the model of winter ozone formation in oil and gas basins.
6) Continue to improve the organic PM species performance through investigation of combustion source speciation profiles and residential wood combustion emissions activities.
7) Investigate the PM species mappings for the CAMx and CMAQ output to the IMPROVE visibility equation species, particularly for coarse mass, dust, and seasalt.

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APPENDIX A

A.1 CAMx Species Post-processing Expressions

Output Species	Units	Formula (with CAMx species)
CO	ppbV	1000.0*CO
HNO3	ppbV	1000.0*HNO3
HNO3_UGM3	ug/m3	1000.0*(HNO3*2.1756*DENS)
NO	ppbV	1000.0*NO
NO2	ppbV	1000.0*NO2
ANO3_PPB	ppbV	(PNO3)/(DENS*(62.0/28.97))
O3	ppbV	1000.0*O3
SO2	ppbV	1000.0*SO2
SO2_UGM3	ug/m3	1000.0*(SO2*2.2118*DENS)
ALD2	ppbV	1000.0*ALD2
ALDX	ppbV	1000.0*ALDX
ETH	ppbV	1000.0*ETH
ETHA	ppbV	1000.0*ETHA
FORM	ppbV	1000.0*FORM
H2O2	ppbV	1000.0*H2O2
HONO	ppbV	1000.0*HONO
IOLE	ppbV	1000.0*IOLE
ISOP	ppbV	1000.0*ISOP
N2O5	ppbV	1000.0*N2O5
NH3	ppbV	1000.0*NH3
NH3_UGM3	ug/m3	1000.0*(NH3*0.5880*DENS)
NHX	ug/m3	1000.0*(NH3*0.5880*DENS)+PNH4
NOX	ppbV	1000.0*(NO+NO2+PAN)
NOY	ppbV	1000.0*(NO+NO2+NO3+2*N2O5+HONO+HNO3+PAN+PANX+PNA+NTR)+ANO3_PPB
NTR	ppbV	1000.0*NTR
OLE	ppbV	1000.0*OLE
PAR	ppbV	1000.0*PAR
PAN	ppbV	1000.0*PAN
PANX	ppbV	1000.0*PANX
SULF	ppbV	1000.0*SULF
TERP	ppbV	1000.0*TERP
TOL	ppbV	1000.0*TOL
VOC	ppbC	1000.0*(PAR+2.0*ETH+2.0*ETOH+2.0*OLE+7.0*TOL+8.0*XYL+FORM+2.0*ALD2+5.0*ISOP+2.0*ETHA+4.0*IOLE+2.0*AL

		DX+10.0*TERP)
XYL	ppbV	1000.0*XYL
CL	ug/m3	PCL
EC	ug/m3	PEC
NA	ug/m3	NA
NO3	ug/m3	PNO3
NH3	ug/m3	PNH4
POA	ug/m3	POA
SO4	ug/m3	PSO4
OA	ug/m3	POA+SOA1+SOA2+SOA3+SOA4+SOA5+SOA6+SOA7+SOPA+SOPB
PM25_OTHER	ug/m3	FPRM+FCRS
PM25_TOT	ug/m3	PM25_SO4+PM25_NO3+PM25_NH4+PM25_OA+PM25_EC+PM25_NA +PM25_CL+PM25_OTHER
PMC_TOT	ug/m3	CPRM+CCRS
TNO3	ug/m3	2175.6*(HNO3*DENS)+PNO3
WDEP_NHX	kg/ha	0.001*PNH4_WD + 0.017*1.059*NH3_WD
WDEP_TNO3	kg/ha	0.001*PNO3_WD + 0.063*0.984*HNO3_WD
WDEP_TSO4	kg/ha	0.001*PSO4_WD + 0.064*1.5*SO2_WD

A.2 CMAQ Species Post-processing Expressions

Output Species	Units	Formula (with CMAQ species)
CO	ppbV	1000.0*CO
HNO3	ppbV	1000.0*HNO3
HNO3_UGM3	ug/m3	1000.0*(HNO3*2.1756*DENS)
NO	ppbV	1000.0*NO
NO2	ppbV	1000.0*NO2
ANO3_PPB	ppbV	(PNO3)/(DENS*(62.0/28.97))
O3	ppbV	1000.0*O3
SO2	ppbV	1000.0*SO2
SO2_UGM3	ug/m3	1000.0*(SO2*2.2118*DENS)
ALD2	ppbV	1000.0*ALD2
ALDX	ppbV	1000.0*ALDX
ETH	ppbV	1000.0*ETH
ETHA	ppbV	1000.0*ETHA
FORM	ppbV	1000.0*FORM
H2O2	ppbV	1000.0*H2O2
HONO	ppbV	1000.0*HONO
IOLE	ppbV	1000.0*IOLE
ISOP	ppbV	1000.0*ISOP
N2O5	ppbV	1000.0*N2O5
NH3	ppbV	1000.0*NH3
NH3_UGM3	ug/m3	1000.0*(NH3*0.5880*DENS)
NHX	ug/m3	1000.0*(NH3*0.5880*DENS)+PNH4
NOX	ppbV	1000.0*(NO+NO2+PAN)
NOY	ppbV	1000.0*(NO+NO2+NO3+2*N2O5+HONO+HNO3+PAN+PANX+PNA+NTR)+ANO3_PPB
NTR	ppbV	1000.0*NTR
OLE	ppbV	1000.0*OLE
PAR	ppbV	1000.0*PAR
PAN	ppbV	1000.0*PAN
PANX	ppbV	1000.0*PANX
SULF	ppbV	1000.0*SULF
TERP	ppbV	1000.0*TERP
TOL	ppbV	1000.0*TOL
VOC	ppbC	1000.0*(PAR+2.0*ETH+2.0*ETOH+2.0*OLE+7.0*TOL+8.0*XYL+FORM+2.0*ALD2+5.0*ISOP+2.0*ETHA+4.0*IOLE+2.0*ALDX+10.0*TERP)

XYL	ppbV	1000.0*XYL
PM25_EC	ug/m3	AECI*PM25AT+AECJ*PM25AC
PM25_NO3	ug/m3	ANO3I*PM25AT+ANO3J*PM25AC+ANO3K*PM25CO
PM25_NH4	ug/m3	ANH4I*PM25AT+ANH4J*PM25AC+ANH4K*PM25CO
PM25_OC	ug/m3	AORGPAI*PM25AT+(AOCIJ-AORGPAI)*PM25AC
PM25_SO4	ug/m3	ASO4I*PM25AT+ASO4J*PM25AC+ASO4K*PM25CO
PM25_SOIL	ug/m3	(ASOIL+ACORS)*PM25CO
PM25_TOT	ug/m3	PM25_EC+PM25_NO3+PM25_NH4+PM25+PM25_OC+PM25_SO4+PM25_SOIL+PM25_NA+PM25_CL
PMC_TOT	ug/m3	PMC_SO4+PMC_NO3+PMC_NH4+PMC_NA+PMC_CL+PMC_OTHR
TNO3	ug/m3	2175.6*(HNO3*DENS)+ANO3I+ANO3J+ANO3K
WDEP_NHX	kg/ha	ANH4I+ANH4J+ANH4K+1.059*NH3
WDEP_TNO3	kg/ha	ANO3I+ANO3J+ANO3K+0.984*HNO3
WDEP_TSO4	kg/ha	ASO4I+ASO4J+ASO4K+1.5*SO2

A.3 AMET Model to Observations Pairing Expressions

IMPROVE				
Observation Species	**Input Unit**	**CAMx/Combine Species**	**Output Unit**	**Output Species**
SO4f_val	ug/m3	SO4	ug/m3	SO4
NO3f_val	ug/m3	NO3	ug/m3	NO3
0.2903*NO3f_val+0.375*SO4f_val	ug/m3	NH4	ug/m3	NH4
MF_val	ug/m3	PM25_TOT	ug/m3	PM25_TOT
OCf_val	ug/m3	OA	ug/m3	OC
ECf_val	ug/m3	EC	ug/m3	EC
OCf_val+ECf_val	ug/m3	OA+EC	ug/m3	TC
CSN				
Observation Species	**Input Unit**	**CAMx/Combine Species**	**Output Unit**	**Output Species**
m_so4	ug/m3	SO4	ug/m3	SO4
m_no3	ug/m3	NO3	ug/m3	NO3
m_nh4	ug/m3	NH4	ug/m3	NH4
oc_adj	ug/m3	OA	ug/m3	OC
ec_niosh	ug/m3	EC	ug/m3	EC
oc_adj+ec_niosh	ug/m3	OA+EC	ug/m3	TC
FRM PM2.5 Mass	ug/m3	PM25_TOT	ug/m3	PM25_TOT
CASTNET				
Observation Species	**Input**	**CAMx/Combine Species**	**Output**	**Output**

	Unit		Unit	Species
tso4	ug/m3	SO4	ug/m3	SO4
tno3	ug/m3	NO3	ug/m3	NO3
tnh4	ug/m3	NH4	ug/m3	NH4
tno3+nhno3	ug/m3	NO3+HNO3_UGM3	ug/m3	TNO3
ozone	ppb	O3	ppb	O3
NADP				
Observation Species	**Input Unit**	**CAMx/Combine Species**	**Output Unit**	**Output Species**
NH4	kg/ha	WDEP_NHX	kg/ha	NH4_dep
NO3	kg/ha	WDEP_TNO3	kg/ha	NO3_dep
SO4	kg/ha	WDEP_TSO4	kg/ha	SO4_dep
AQS				
Observation Species	**Input Unit**	**CAMx/Combine Species**	**Output Unit**	**Output Species**
O3	ppb	O3	ppb	O3
NOY	ppb	NOY	ppb	NOY
NO	ppb	NO	ppb	NO
NO2	ppb	NO2+PAN+PANX+HNO3	ppb	NO2
NOX	ppb	NO+NO2+PAN+PANX+HNO3	ppb	NOX
CO	ppb	CO	ppb	CO
SO2	ppb	SO2	ppb	SO2
PM25	ug/m3	PM25_TOT	ug/m3	PM25_TOT