Southern New Mexico Ozone Study
CAMx 2011 Model Performance Evaluation

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ACRONYMS AND ABBREVIATIONS

3SAQS	Three-State Air Quality Study
AIRS	Aerometric Information Retrieval System
AMET	Atmospheric Model Evaluation Tool
APCA	Anthropogenic Precursor Culpability Assessment
AQ	Air Quality
AQS	Air Quality System
BC	Boundary Condition
BLM	Bureau of Land Management
CAMx	Comprehensive Air-quality Model with extensions
CARB	California Air Resources Board
CASTNet	Clean Air Status and Trends Network
CB6r2	Carbon Bond mechanism version 6, revision 2
CMAQ	Community Multiscale Air Quality modeling system
CONUS	Continental United States
CPC	Center for Prediction of Climate
CSAPR	Cross State Air Pollution Rule
CSN	Chemical Speciation Network
EC	Elemental Carbon Fine Particulate Matter
ECMWF	European Center for Medium Range Weather Forecasting
EGU	Electrical Generating Units
EIS	Environmental Impact Statement
EPA	Environmental Protection Agency
FB	Fractional Bias
FE	Fractional Error
FRM	Federal Reference Method
GCM	Global Chemistry Model
GEOS-Chem	Goddard Earth Observing System (GEOS) global chemistry model
GIRAS	Geographic Information Retrieval and Analysis System
IMPROVE	Interagency Monitoring of PROtected Visual Environments
IWDW	Intermountain West Data Warehouse
LCP	Lambert Conformal Projection
LSM	Land Surface Model
MADIS	Meteorological Assimilation Data Ingest System
MATS	Modeled Attainment Test Software
MCIP	Meteorology-Chemistry Interface Processor
MEGAN	Model of Emissions of Gases and Aerosols in Nature
MNGE	Mean Normalized Gross Error
MNB	Mean Normalized Bias
MNE	Mean Normalized Error
MOVES	Motor Vehicle Emissions Simulator
MOZART	Model for OZone And Related chemical Tracers
MPE	Model Performance Evaluation

MSKF	Multi-Scale Kain-Fritsch Cumulus Parameterization
NAAQS	National Ambient Air Quality Standard
NAM	North American Mesoscale Forecast System
NCAR	National Center for Atmospheric Research
NCEP	National Center for Environmental Prediction
NCDC	National Climatic Data Center
NEI	National Emissions Inventory
NEPA	National Environmental Policy Act
NH_4	Ammonium Fine Particulate Matter
NMB	Normalized Mean Bias
NME	Normalized Mean Error
NO_2	Nitrogen Dioxide
NO_3	Nitrate Fine Particulate Matter
NOAA	National Oceanic and Atmospheric Administration
OA	Organic Aerosol Fine Particulate Matter
OC	Organic Carbon Fine Particulate Matter
OSAT	Ozone Source Apportionment Technology
PAVE	Package for Analysis and Visualization
PBL	Planetary Boundary Layer
PGM	Photochemical Grid Model
PM	Particulate Matter
PPM	Piecewise Parabolic Method
QA	Quality Assurance
QC	Quality Control
RMP	Resource Management Plan
RRF	Relative Response Factor
SCC	Source Classification Code
SIP	State Implementation Plan
SMOKE	Sparse Matrix Kernel Emissions modeling system
SNMOS	Southern New Mexico Ozone Study
SOA	Secondary Organic Aerosol
SO_2	Sulfur Dioxide
SO_4	Sulfate Fine Particulate Matter
TCEQ	Texas Commission on Environmental Quality
UNC-IE	University of North Carolina Institute for the Environment
USFS	United States Forest Service
VERDI	Visualization Environment for Rich Data Interpretation
VMT	Vehicle Miles Traveled
WBD	Wind Blown Dust model
WAQS	Western Air Quality Study
WESTAR	Western States Air Resources Council
WestJumpAQMS	West-Wide Jump-Start Air Quality Modeling Study
WESTUS	Western United States
WRAP	Western Regional Air Partnership

WGA	Western Governors' Association
WRF	Weather Research Forecast model

1.0 EXECUTIVE SUMMARY

The Southern New Mexico Ozone Study (SNMOS) performed photochemical grid modeling for the year 2011 using the Comprehensive Air Quality Model with Extensions (CAMx) version 6.20. The SNMOS Work Plan for the 2011 Modeling Year (Adelman et al., 2015a) details the CAMx configuration and justification for the model's selection for the SNMOS. This document presents the CAMx model performance evaluation (MPE) for the SNMOS 2011 ozone season modeling episode. We present the evaluation of CAMx model performance against concurrent measured ambient concentrations using graphical displays of model performance and statistical model performance measures. We compare these measures against established model performance goals and criteria following the procedures recommended in EPA's photochemical modeling guidance documents.

Model performance was evaluated in New Mexico and surrounding regions for two CAMx runs that used different meteorological inputs, but were otherwise identical. The University of North Carolina Institute for the Environment (UNC-IE) carried out a series of Weather Research and Forecasting Model (WRF; Skamarock et al., 2005) meteorological model simulations of the SNMOS modeling episode and compared model performance in each run against observed weather data (UNC-IE and Ramboll Environ, 2015). The WRF model runs differed in their cumulus parameterizations and the datasets used for initial conditions and analysis nudging. The two WRF runs that produced the best model performance over the SNMOS WRF 12/4 km modeling domains used the Multi-Scale Kain-Fritsch (MSKF) cumulus scheme (Alapaty et al., 2014; Herwehe et al., 2014). One of the MSKF WRF runs used the National Center for Environmental Prediction (NCEP) North American Mesoscale Forecast System (NAM) analysis for initial conditions and analysis nudging, while the other MSKF run used the European Center for Medium Range Weather Forecasting (ECMWF) ERA-Interim analysis. We refer to the two WRF simulations hereafter as the WRF ERA and WRF NAM runs and the two CAMx runs that used these WRF runs as the CAMx ERA and CAMx NAM runs.

For both CAMx runs, model performance was acceptable for daily maximum 8-hour average (MDA8) ozone based on comparison with EPA statistical performance benchmarks. Both CAMx runs had an overall high bias when all episode days were considered, but underestimated ozone on high ozone days, which are defined to be days with observed MDA8 ozone > 60 ppb. The CAMx run using ERA WRF meteorology performed slightly better than CAMx with NAM WRF meteorology on days when MDA8 > 60 ppb. The CAMx NAM run performed slightly better when all days were considered (i.e. on lower MDA8 ozone days).

We examined performance at the ground level ozone monitors within Doña Ana County in light of the form of the National Ambient Air Quality Standard (NAAQS) for ozone and the EPA's recommended method for performing modeled attainment demonstrations (EPA, 2014). The SNMOS will perform a modeled attainment demonstration for Doña Ana County using the 2011 base case model described in this document and a 2025 future year model that is currently under development. Future year emissions sensitivity modeling will then be used to evaluate the impacts of emissions reductions on future attainment of the ozone NAAQS. In carrying out the base case model performance, we considered how CAMx performance in the 2011 base year runs would affect the modeled attainment demonstration and selected the CAMx model run that will provide the most reliable future year ozone projection.

For both CAMx runs, many of the high ozone days that would be used to develop future year ozone projections for Doña Ana County monitors using EPA's recommended method have significant region-wide overestimates of ozone. Most of the highest modeled MDA8 ozone days did not have high observed MDA8 ozone in Doña Ana County. Future year projections based on these days would therefore not reflect conditions that cause high observed ozone in Doña Ana County so would not be useful in evaluating the impacts of local emissions control strategies.

We propose an alternate method of making future year projections in which the model projections are developed using a model performance criterion that selects only days when modeled ozone is high and model performance is within acceptable bias limits. When this alternate procedure for developing future year projections is used, the CAMx ERA run is clearly superior to the CAMx NAM run in performance on the high ozone days that would be used in future year ozone projections.

We therefore select the CAMx ERA run as the SNMOS 2011 base year run due to its better performance within the 4 km and 12 km domain on days where observed MDA8 ozone > 60 ppb as well as the fact that future year design value projections formed with the CAMx ERA run will be based on high modeled ozone days that correspond more closely to high observed MDA8 days than with the CAMx NAM run.

Having selected the CAMx ERA run, we then conducted a model performance evaluation for this run for ozone precursors and fine particulate matter ($PM_{2.5}$) and its component species with a focus on the modeling results for Dona Ana County. We evaluated the ozone precursors carbon monoxide (CO) and nitrogen dioxide (NO_2), but did not include volatile organic compound (VOC) species due to lack of observed data. Although the main focus of this study was ozone, the $PM_{2.5}$ evaluation included total $PM_{2.5}$ along with the component species sulfate (SO_4), nitrate (NO_3), ammonium (NH_4), elemental carbon (EC), and organic carbon (OC).

NO_2 and CO performance are typical of photochemical model simulations of the Western U.S. and are comparable to performance noted in the WAQS 2011b modeling (Adelman et al., 2016) and the Three State Air Quality Study (3SAQS; Adelman et al., 2015b). The SNMOS PM performance evaluation showed that $PM_{2.5}$ was underestimated across the New Mexico and the surrounding region and that the underestimate of total $PM_{2.5}$ was consistent with modeled underestimates of several of its component species including NH_4, NO_3, and SO_4. While there are shortcomings in model performance for the CAMx ERA simulation of $PM_{2.5}$ and its component species, performance is roughly comparable to that of other similar studies in the western U.S. such as the WAQS and 3SAQS. PM performance is not the main focus of the SNMOS, and so no effort was expended to try to diagnose and improve model performance for PM. We note the reasonable model performance and conclude that the CAMx 2011 SNMOS model is functioning as expected.

In summary, we conclude that model performance for ozone, ozone precursors NO_2 and CO and PM is adequate for the SNMOS in the CAMx ERA run.

2.0 INTRODUCTION

In this Section, we review recent ambient ozone measurements and the ozone attainment status of Doña Ana County, NM. We then give an overview of the modeling approach used in the study and provide an outline of this report.

2.1 Recent Ambient Ozone Levels in Dona Ana County

The U.S. EPA sets a National Ambient Air Quality Standard (NAAQS) for ozone in order to protect public health and the environment. The 8-hour ozone NAAQS prescribes a maximum level for the three-year running average of the annual fourth-highest daily maximum 8-hour average (MDA8) concentration; this quantity is known as the design value. EPA's most recent review of the ozone standard was finalized on October 1, 2015. On October 1, the EPA lowered the ozone NAAQS from the 75 parts per billion (ppb) level set in 2008 to a more stringent value of 70 ppb[1]. The 2015 NAAQS is violated by a design value of 71 ppb or greater.

Doña Ana County in Southern New Mexico experiences some of the highest observed ground-level ozone concentrations in the state. The Sunland Park Ozone Nonattainment Area (NAA), which lies within Doña Ana County, was designated as marginal nonattainment for the 1-hour ozone standard on June 12, 1995 (60 FR 30789). With the revocation of the 1-hour ozone standard in 2004, the Sunland Park NAA was designated a maintenance area for 8-hour ozone (NMED, 2007). The lowering of the 8-hour ozone standard by EPA in 2008 to 0.75 ppm (75 ppb) and again in 2015 to 0.70 ppm (70 ppb) will likely lead to the Sunland Park NAA receiving a nonattainment designation for 8-hour ozone. In addition, the New Mexico Air Quality Control Act (NMAQCA) requires the New Mexico Environment Department (NMED) to develop a plan for reducing ozone levels in areas that are within 95% of the ozone standard (NMSA 1978, § 74-2-5.3). Table 2-1 shows the 1st through 4th highest MDA8 concentrations measured from 2011 to 2014 at the EPA Air Quality System (AQS) monitors in Doña Ana County. This table shows that all but a handful of the measurements at these monitors exceeded either the 2015 NAAQS for ozone (orange) or the NMAQCA 95% threshold (yellow).

Table 2-1. Daily maximum 8-hour average ozone measurements from 2011-2014 at AQS sites in Doña Ana County, NM.

	1st Highest		2nd Highest		3rd Highest		4th Highest	
Station	Date	ppmV	Date	ppmV	Date	ppmV	Date	ppmV
La Union	5/24/2011	0.064	6/22/2011	0.064	7/28/2011	0.064	4/26/2011	0.063
SPCY	6/22/2011	0.078	6/4/2011	0.076	7/28/2011	0.068	6/27/2011	0.067
Chaparral	8/2/2011	0.074	5/24/2011	0.073	5/25/2011	0.071	6/22/2011	0.07
Desert V	6/4/2011	0.084	6/22/2011	0.081	8/27/2011	0.073	7/28/2011	0.072
Sta Teresa	6/22/2011	0.078	5/24/2011	0.074	4/26/2011	0.07	6/27/2011	0.07
Solano	5/24/2011	0.068	5/25/2011	0.068	8/6/2011	0.068	8/27/2011	0.067
La Union	8/31/2012	0.079	7/13/2012	0.078	6/28/2012	0.075	7/14/2012	0.074
SPCY	8/31/2012	0.078	7/13/2012	0.076	7/12/2012	0.075	6/28/2012	0.073
Chaparral	6/2/2012	0.075	6/1/2012	0.07	7/13/2012	0.069	6/3/2012	0.067

[1] https://www.epa.gov/ozonepollution/2015-national-ambient-air-quality-standards-naaqs-ozone

Station	1st Highest		2nd Highest		3rd Highest		4th Highest	
	Date	ppmV	Date	ppmV	Date	ppmV	Date	ppmV
Desert V	7/13/2012	0.077	8/31/2012	0.077	7/12/2012	0.076	6/28/2012	0.075
Sta Teresa	8/31/2012	0.083	7/13/2012	0.08	7/12/2012	0.078	9/1/2012	0.077
Solano	5/16/2012	0.069	6/3/2012	0.068	7/13/2012	0.067	6/2/2012	0.066
La Union	8/17/2013	0.066	8/16/2013	0.065	8/21/2013	0.065	8/4/2013	0.064
SPCY	7/3/2013	0.068	6/11/2013	0.063	6/9/2013	0.063	8/17/2013	0.062
Chaparral	5/24/2013	0.074	6/15/2013	0.074	7/3/2013	0.071	7/5/2013	0.07
Desert V	7/3/2013	0.076	8/16/2013	0.072	7/27/2013	0.072	6/9/2013	0.071
Sta Teresa	7/27/2013	0.089	7/3/2013	0.081	7/25/2013	0.081	7/7/2013	0.08
Solano	7/31/2013	0.066	7/27/2013	0.065	7/16/2013	0.065	5/20/2013	0.064
La Union	6/10/2014	0.07	5/29/2014	0.07	8/18/2014	0.068	5/28/2014	0.066
SPCY	6/10/2014	0.073	5/29/2014	0.068	8/30/2014	0.068	7/22/2014	0.068
Chaparral	8/6/2014	0.075	6/10/2014	0.071	7/18/2014	0.069	5/29/2014	0.068
Desert V	6/10/2014	0.077	5/29/2014	0.074	7/15/2014	0.073	5/28/2014	0.072
Sta Teresa	7/15/2014	0.071	8/18/2014	0.07	7/31/2014	0.069	6/10/2014	0.067
Solano	6/10/2014	0.072	6/7/2014	0.069	5/29/2014	0.068	6/9/2014	0.067

The aim of the SNMOS is to study the factors contributing to high ozone in Doña Ana County and investigate future emissions scenarios that will produce NAAQS attainment. The SNMOS is a collaborative project between NMED, the Western Regional Air Partnership (WRAP), the Western Air Resources Council (WESTAR), Ramboll Environ, Corporation (RE), and the University of North Carolina Institute for the Environment (UNC-IE). The SNMOS builds off of the Western Air Quality Study (WAQS), a cooperative project that is intended to facilitate air resource analyses for federal and state agencies in the intermountain western U.S. toward improved information for the public and stakeholders as a part of air quality planning. The WAQS grew out of the West-Wide Jump-Start Air Quality Modeling Study (WestJumpAQMS), which modeled the year 2008. The WAQS modeled a more recent year, 2011. The Intermountain West Data Warehouse (IWDW) at the Cooperative Institute for Research in the Atmosphere (CIRA) at Colorado State University is the source for the regional air quality modeling data and software resources from the WAQS. The SNMOS leveraged the WAQS 2011 version B (WAQS_2011b) modeling platform to conduct base and future year air quality modeling for Doña Ana County.

2.2 Overview of the SNMOS Modeling Approach

The SNMOS modeling platform was derived from the WAQS_2011b regional modeling platform. A regional modeling platform is the suite of data and software required for conducting a regional-scale air quality modeling study. The procedures for the SNMOS 2011 modeling followed those performed for the 2011 WAQS with adjustments to the meteorology and modeling domains to optimize the modeling platform for application to southern New Mexico. The SNMOS modeling platform included nested 36, 12 and 4 km resolution meteorology modeling domains. The regional air quality modeling was conducted at 12 and 4 km resolution. The SNMOS 12 and 4 km domains were designed to encompass the meteorology and emissions features that are most important to ground-level ozone formation in southern New Mexico. We simulated the 2011 ozone season and evaluated the meteorology and air quality model performance against surface and aloft monitors that operated in the modeling domains during the study period. After the first air quality model simulation of the 2011 season was completed, we performed a second simulation using different meteorological input data in an effort to improve the model's simulation of ozone in Southern New Mexico. We selected the better performing simulation based on the model performance evaluation results for both runs.

Now that the base year model performance evaluation is completed and a base year 2011 model run has been selected, we will use projected emissions data to simulate air quality in the year 2025. Along with future year attainment tests, the future year modeling will include ozone source apportionment modeling of source region and source category contributions to ozone concentrations and ozone design values at ozone monitoring in Doña Ana County (and elsewhere in the region). A summary of the SNMOS 2011 modeling approach is given below, with more details provided in the SNMOS Modeling Work Plan (Adelman et al., 2015a).

- The 2011 ozone season for New Mexico (May 1 – September 30) was selected for the modeling period.
- Year 2011 and 2025 inventories are being used to estimate base and future year emissions.
- The modeling domains include a 36 km continental U.S. (CONUS36) domain, a 12 km western U.S. (WESTUS12) domain, and a 4 km New Mexico (SNMOS04) domain. The WESTUS12 photochemical modeling domain encompasses regional metropolitan areas and large emissions sources likely to contribute to ozone in Doña Ana County, while the high resolution SNMOS4 domain focuses on Doña Ana County and its immediate vicinity.
- The Weather Research Forecasting (WRF) version 3.7.1 was used to simulate meteorology data for this study.
- Emissions processing was primarily conducted using the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system version 3.7 using emissions data from the EPA 2011-based modeling platform (2011v6) version 2 and the WAQS (2011b).
- Photochemical grid modeling (PGM) is being done with the Comprehensive Air-quality Model with extensions (CAMx) version 6.20. The Carbon Bond 6 revision 2 (CB6r2) photochemical mechanism is being used for the SNMOS 2011 and 2025 modeling.
- For the SNMOS 2011 modeling, hourly boundary conditions (BCs) for the lateral boundaries of the SNMOS WESTUS12 PGM domain that lies within the larger WAQS WESTUS12 domain were extracted from the WAQS 36 km CONUS CAMx modeling.
- Model evaluation was conducted for meteorology, ozone, and ozone precursor and product species.
- A diagnostic sensitivity test was conducted to determine sensitivity of the PGM model estimates to meteorological input data in order to improve the 2011 base year model performance.

- Future year modeling will be used to estimate air quality in 2025 and to conduct attainment tests for Doña Ana County.
- Future year emissions sensitivity modeling will be used to evaluate the impacts of emissions reductions on future attainment of the ozone NAAQS.
- Future year CAMx source apportionment modeling will be used to quantify the source region and source category contributions to ozone concentrations and ozone design values at ozone monitoring in Dona Ana County.

2.3 Overview of Report

The SNMOS performed photochemical grid modeling for the year 2011 using the Comprehensive Air Quality Model with Extensions (CAMx) version 6.10 (Ramboll Environ, 2015). The SNMOS 2011 Work Plan (Adelman et al., 2015) details the CAMx configuration and justification for why it was chosen for the SNMOS. Section 3 of this document summarizes the CAMx 2011 configuration, the model performance evaluation approach and the available ambient data for the SNMOS 2011 base year simulations on the 12 km and 4 km modeling grids. Statistics used for the MPE and the model performance goals are also presented in Section 3. Section 4 presents the model performance evaluation for ozone and its precursors on the 12/4 km grids, which encompass Southern New Mexico and surrounding regions. Note that the 3SAQS 2011 modeling study (Adelman et al., 2015b) presents an evaluation of the CAMx results for 36 km CONUS modeling that was used to provide boundary conditions for the SNMOS 12/4 km grid modeling. Section 5 of this document presents the MPE for particulate matter and Section 6 provides a summary of the 2011 modeling results and conclusions of the study.

3.0 CAMX MODELING AND EVALUATION APPROACH

3.1 Model Selection

The SNMOS used the Weather Research and Forecasting Model (WRF; Skamarock et al., 2004; 2005; 2006) meteorological model and the Comprehensive Air Quality Model with Extensions (CAMx; Ramboll Environ, 2015) to carry out the 2011 base year modeling. A detailed justification for the selection of these models is provided in Adelman et al. (2015a), and a brief summary of each model is provided below.

3.1.1 WRF Meteorological Model

The non-hydrostatic version of the Advanced Research version of the Weather Research Forecast (WRF-ARW) model is a three-dimensional, limited-area, primitive equation, prognostic model that has been used widely in regional air quality model applications. The basic model has been under continuous development, improvement, testing and open peer-review for more than 10 years and has been used world-wide by hundreds of scientists for a variety of mesoscale studies, including cyclogenesis, polar lows, cold-air damming, coastal fronts, severe thunderstorms, tropical storms, subtropical easterly jets, mesoscale convective complexes, desert mixed layers, urban-scale modeling, air quality studies, frontal weather, lake-effect snows, sea-breezes, orographically induced flows, and operational mesoscale forecasting. WRF is a next-generation mesoscale prognostic meteorological model routinely used for urban- and regional-scale photochemical, fine particulate and regional haze regulatory modeling studies. Developed jointly by the National Center for Atmospheric Research and the National Centers for Environmental Prediction, WRF is maintained and supported as a community model by researchers and practitioners around the globe. The code supports two modes: the Advanced Research WRF (ARW) version and the Non-hydrostatic Mesoscale Model (NMM) version. It is suitable for use in a broad spectrum of applications across scales ranging from hundreds of meters to thousands of kilometers.

WRF-ARW version 3.7.1 was used for the SNMOS.

3.1.2 CAMx Photochemical Grid Model

The CAMx modeling system is a state-of-science ‘One-Atmosphere’ photochemical grid model capable of addressing ozone, particulate matter (PM), visibility and acid deposition at regional scale for periods up to one year. CAMx is a publicly available open-source computer modeling system for the integrated assessment of gaseous and particulate air pollution. Built on today’s understanding that air quality issues are complex, interrelated, and reach beyond the urban scale, CAMx is designed to (a) simulate air quality over many geographic scales, (b) treat a wide variety of inert and chemically active pollutants including ozone, inorganic and organic $PM_{2.5}$ and PM_{10} and mercury and toxics, (c) provide source-receptor, sensitivity, and process analyses and (d) be computationally efficient and easy to use. The U.S. EPA has approved the use of CAMx for numerous Ozone and PM State Implementation Plans throughout the U.S. and EPA has used CAMx to evaluate regional mitigation strategies including those for recent regional rules (e.g., CSAPR, CATR, CAIR, NOx SIP Call, etc.) in the eastern U.S. Use of CAMx in the present study allows the SNMOS to leverage the WAQS CAMx 2011 modeling platform and to take advantage of the CAMx source apportionment functions.

CAMx Version 6.20 (released in March 2015) was used for the SNMOS modeling.

3.2 Modeling Episode Selection for the SNMOS

EPA's modeling guidance lists primary criteria for selecting episodes for ozone, $PM_{2.5}$ and visibility SIP modeling along with a set of secondary criteria that should also be considered.

3.2.1 EPA Primary Episode Selection Criteria

EPA's modeling guidance (EPA, 2007; EPA, 2014) identifies four specific primary criteria to consider when selecting episodes for use in demonstrating attainment of the 8-hour ozone NAAQS:

1. A variety of meteorological conditions should be covered, including the types of meteorological conditions that produce 8-hour ozone exceedances in the region of interest;
2. Choose episodes having days with monitored 8-hour daily maximum ozone concentrations close to the ozone Design Values;
3. To the extent possible, the modeling data base should include days for which extensive data bases (i.e. beyond routine aerometric and emissions monitoring) are available; and
4. Sufficient days should be available such that relative response factors (RRFs) for ozone projections can be based on several (i.e., > 10) days with at least 5 days being above or equal to the absolute minimum MDA8 ozone value of 60 ppb.

3.2.2 EPA Secondary Episode Selection Criteria

EPA also lists four "other considerations" to bear in mind when choosing potential 8-hour ozone episodes, including:

1. Choose periods which have already been modeled;
2. Choose periods that are drawn from the years upon which the current Design Values are based;
3. Include weekend days among those chosen; and
4. Choose modeling periods that meet as many episode selection criteria as possible in the maximum number of nonattainment areas possible.

EPA suggests that modeling an entire summer ozone season for ozone would be a good way to ensure that a variety of meteorological conditions are captured and that sufficient days are available to construct robust RRFs for the 8-hour ozone Design Value projections.

3.2.3 SNMOS Modeling Episode

May through September 2011 was selected for the SNMOS modeling because it builds off the WAQS modeling. The selection of this period also satisfies several of the episode selection criteria listed above:

1. Modeling the entire 2011 ozone season captures a variety of conditions that lead to elevated ozone in southern New Mexico
2. 2011 is also a National Emissions Inventory (NEI) update year and the NEI is an important database required for modeling.
3. The five-month ozone season simulation assures sufficient days are available to analyze ozone formation and impacts. Simulating the entire season also provides the opportunity to simulate the North American Monsoon season, which strongly influences ozone concentrations in the region.
4. In addition to the WAQS, 2011 is being used for other studies including several BLM Environmental Impact Statements (EISs) and Resource Management Plans (RMPs).
5. Many weekday-weekend cycles and synoptic weather cycles are included in the entire ozone season simulation.

The decision to model just the summer ozone season and not the entire year is based on the need to only address ozone and not $PM_{2.5}$, visibility and deposition issues.

3.3 CAMx Modeling Domains

The SNMOS modeling domains were selected to facilitate high resolution modeling for sources around Doña Ana County and to enable regional source apportionment modeling among all of the surrounding Western states. The SNMOS meteorology modeling will use 36, 12 and 4 km one-way nested domains. The WRF meteorological model requires use of an odd nesting ratio so the 36/12/4 km domains are using a 3:1 grid-nesting ratio. Consistent with the majority of regional modeling studies over the mid-latitudes, a Lambert Conformal Projection (LCP) centered on 40°N and 97°W was used for horizontal modeling domains using the parameters in Table 3-1.

Figure 3-1 illustrates the SNMOS WRF domains, which are considerably larger than the CAMx modeling domains. The WRF domains were chosen for the following reasons:

- The 36 km continental U.S. (d01; CONUS36) domain is the same as used by the RPOs (e.g., WRAP) and most other recent modeling studies (e.g., WAQS). It is defined to be large enough so that the outer boundaries are far away from the primary areas of interest (i.e., New Mexico and the surrounding region).
- The 12 km western U.S. (d02; WESTUS12) domain is the same size as the WAQS 12 km domain but shifted south to support the resolution of North American Monsoon features that influence weather throughout the southern portion of the modeling domain.
- The 4 km southern New Mexico (d03; SNMOS04) domain focuses on Doña Ana County.

CAMx modeling of 2011 for the SNMOS was performed on nested 12/4 km modeling grids focused on Doña Ana County. Figure 3-2 displays the 12 km WESTUS12 and 4 km SNMOS04 CAMx and emissions processing domains. Table 3-2 details the CAMx domain parameters. The CAMx and emissions domains for modeling of 2011 were chosen for the following reasons:

- New continental-scale coarse grid modeling was not needed for the SNMOS because we were able to extract BCs for the 12 km domain from the WAQS 2011 CAMx modeling results. The WAQS modeling used the 36 km RPO grid and a 12 km modeling domain that encompassed much of the western U.S. As we used the same emissions data and CAMx configuration for the SNMOS as were used for the WAQS, there is consistency between these simulations, enabling the use of the WAQS modeling as BCs for the SNMOS domains.
- The SNMOS WESTUS12 CAMx domain encompasses all of New Mexico, extends west to include the metropolitan area of Phoenix, east to include East Texas, and south to include the Carbon II power plant in Coahuila, Mexico. This facility is a large source of NOx emissions and lies in a region that was sometimes upwind of Doña County on high ozone days during 2011. The SNMOS WESTUS12 domain was designed as a trade-off between computational efficiency and the need to model transport from sources likely to influence Doña Ana County at 12 km resolution.
- The SNMOS04 4 km Doña Ana County domain focuses on Southern New Mexico and the major source regions in the immediate vicinity, including Ciudad Juarez, Mexico and El Paso, TX.

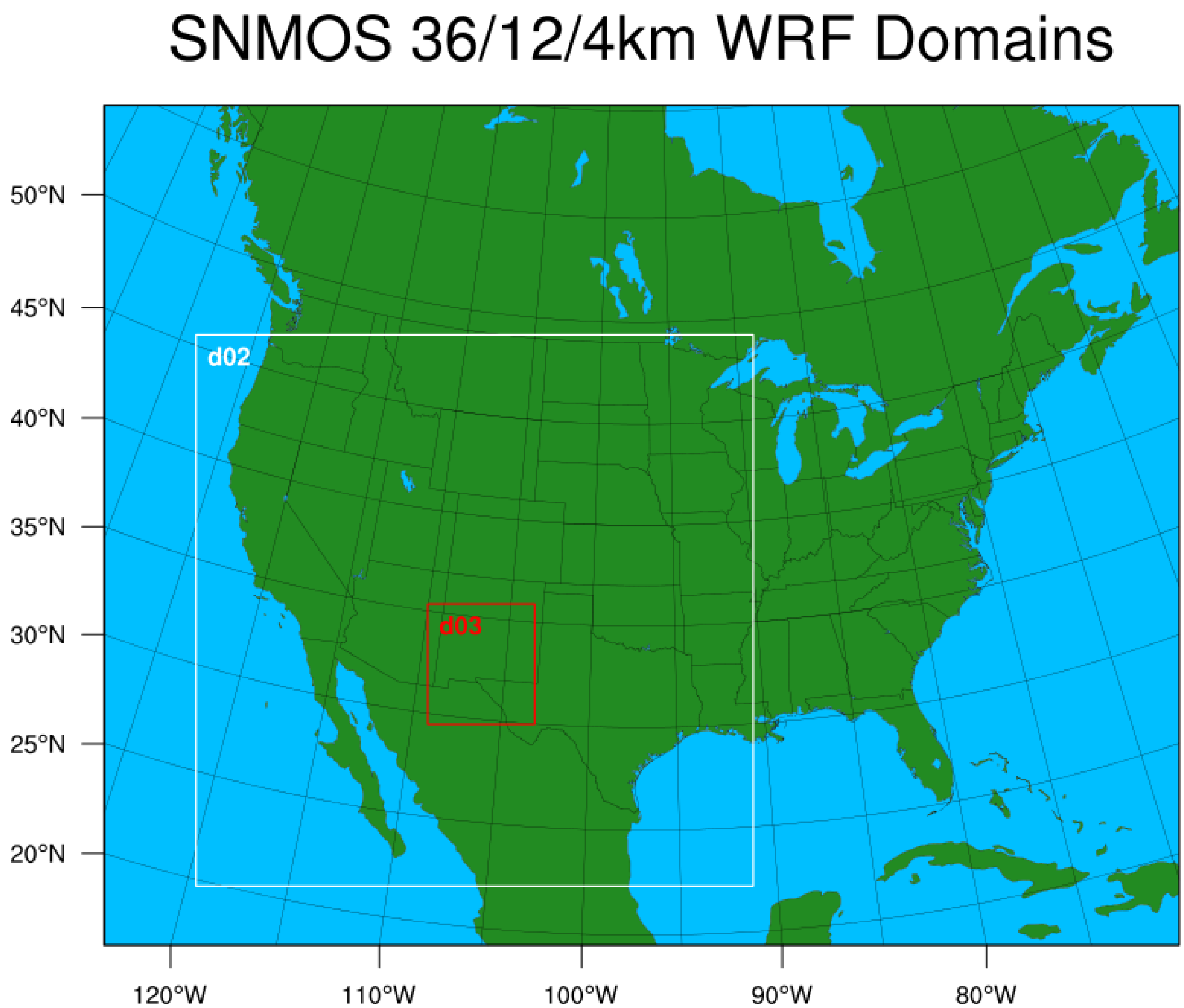


Figure 3-1. SNMOS WRF modeling domains.

Table 3-1. SNMOS WRF domain projection and grid parameters.

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 = -2196, d03 = -912
Y-orig (km)	d01 = -2088, d02 = -1728, d03 = -828
# cols	d01 = 165, d02 = 256, d03 = 148
# rows	d01 = 129, d02 = 253, d03 = 166

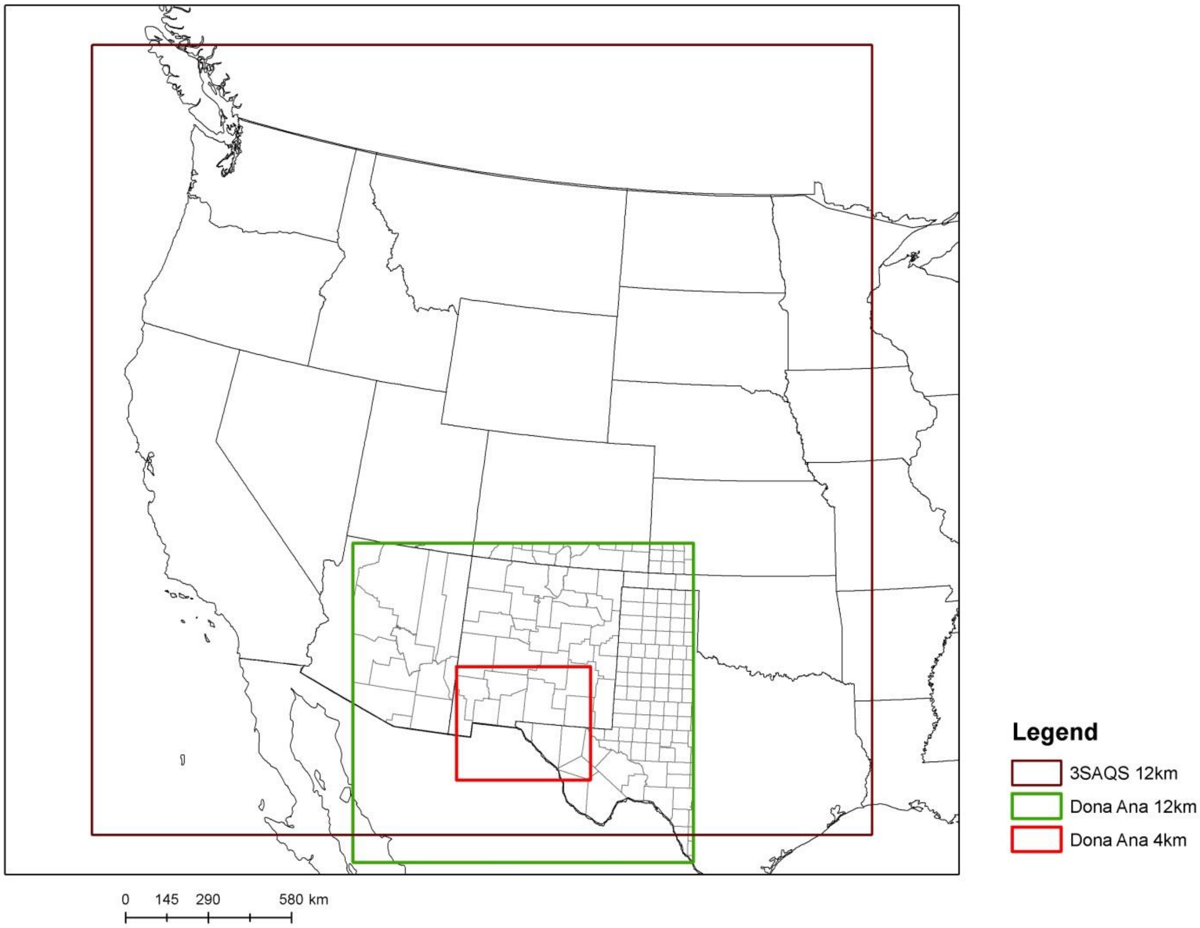


Figure 3-2. SNMOS 2011 CAMx 12/4 km modeling domains and the WAQS 2011b 12 km grid.

Table 3-2. SNMOS CAMx domain projection and grid parameters.

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 = -1476, d03 = -1116
Y-orig (km)	d01 = -2088, d02 = -1332, d03 = -1044
# cols	d01 = 148, d02 = 99, d03 = 117
# rows	d01 = 112, d02 = 93, d03 = 99

The SNMOS WRF and CAMx modeling used the vertical domain structure shown in Table 3-3. WRF was run with 33 vertical layer interfaces (32 vertical layers using the CAMx definition of layer thicknesses). The WRF model employs a terrain-following coordinate system defined by pressure, using multiple layers that extend from the surface to 50 mb (approximately 19 km above mean sea level). No layer averaging (collapsing) scheme was used for the CAMx simulations; CAMx used the same vertical layers as WRF. The 32 layer structure presented here is unique to the SNMOS and was designed to resolve the impacts of local, regional, and long-range sources of air pollution on receptor sites in the 4 km SNMOS modeling domain. The shallow layers (< 42 m) near the surface are configured to resolve the boundary layer dynamics that are crucial to simulating ground-level emissions and air pollution. Maintaining relatively shallow layers (< 2 km) aloft without layer collapsing is designed to improve the simulation of stratosphere-troposphere ozone exchange. Having more layers aloft also improves the simulation of the impacts of long-range air pollutant transport on regional background air quality.

Table 3-3. 33 vertical layer interface definition for WRF and CAMx simulations.

WRF and CAMx Levels				
WRF Level	**Sigma**	**Pressure (mb)**	**Height (m)**	**Thickness (m)**
33	0.0000	50.00	19260	2055
32	0.0270	75.65	17205	1850
31	0.0600	107.00	15355	1725
30	0.1000	145.00	13630	1701
29	0.1500	192.50	11930	1389
28	0.2000	240.00	10541	1181
27	0.2500	287.50	9360	1032
26	0.3000	335.00	8328	920
25	0.3500	382.50	7408	832
24	0.4000	430.00	6576	760
23	0.4500	477.50	5816	701
22	0.5000	525.00	5115	652
21	0.5500	572.50	4463	609
20	0.6000	620.00	3854	461
19	0.6400	658.00	3393	440
18	0.6800	696.00	2954	421
17	0.7200	734.00	2533	403
16	0.7600	772.00	2130	388
15	0.8000	810.00	1742	373
14	0.8400	848.00	1369	271
13	0.8700	876.50	1098	177
12	0.8900	895.50	921	174
11	0.9100	914.50	747	171
10	0.9300	933.50	577	84
9	0.9400	943.00	492	84
8	0.9500	952.50	409	83
7	0.9600	962.00	326	83
6	0.9700	971.50	243	81
5	0.9800	981.00	162	65

WRF and CAMx Levels				
WRF Level	Sigma	Pressure (mb)	Height (m)	Thickness (m)
4	0.9880	988.60	97	41
3	0.9930	993.35	56	32
2	0.9970	997.15	24	24
1	1.0000	1000	0	

3.4 CAMx Model Configuration

The SNMOS project conducted photochemical modeling of the 2011 New Mexico ozone season (May 1 – September 30) on the 36/12/4 km modeling domains shown in Figure 3-2 using the CAMx photochemical grid model. The CAMx configuration used for the 2011 base year modeling was directly derived from the WAQS 2011b modeling platform, although the most recent version of the CAMx model (6.20) available at the time of the SNMOS was used. At the time of the WAQS 2011b modeling, the most recently available version of CAMx was version 6.10, which was used in the WAQS 2011b platform. Table 3-4 summarizes the CAMx version 6.20 (March 2015 release) science configuration and options used for the 2011 ozone season simulation. CAMx was configured to predict ozone and PM species as well as nitrogen and sulfur deposition.

We used the PPM advection solver for horizontal transport (Colella and Woodward, 1984) along with the spatially varying (Smagorinsky) horizontal diffusion approach. CAMx used K-theory for vertical diffusion using the CMAQ-like vertical diffusivities from the WRFCAMx v4.4 meteorological preprocessor (Ramboll Environ, 2015; www.camx.com). WRFCAMx v4.4 was the most recent version of WRFCAMx available at the time of the SNMOS modeling and contains several updates relative to the WRFCAMx version used in the WAQS 2011b modeling. The CB6r2 gas-phase chemical mechanism (Yarwood et al., 2012) was selected for CAMx because it includes the latest chemical kinetic rates and represents improvements over the other alternative CB05 and SAPRC chemical mechanisms in its treatment of the cycling of nitrogen as well as active methane chemistry. Additional CAMx inputs included:

Meteorological Inputs: Two sets of meteorological inputs were used in the SNMOS 2011 CAMx modeling. UNC-IE carried out a series of WRF model simulations of the SNMOS modeling episode and compared model performance in each run against observed weather data (UNC-IE and Ramboll Environ, 2015). The WRF model runs differed in their cumulus parameterizations and the datasets used for initial conditions and analysis nudging. The two WRF runs that produced the best model performance over the SNMOS WRF 12/4 km modeling domains used the Multi-Scale Kain-Fritsch (MSKF) cumulus scheme (Alapaty et al., 2014; Herwehe et al., 2014). One of the MSKF WRF runs used the National Center for Environmental Prediction (NCEP) North American Mesoscale Forecast System (NAM) analysis for initial conditions and analysis nudging, while the other MSKF run used the European Center for Medium Range Weather Forecasting (ECMWF) ERA-Interim analysis. We refer to the two WRF simulations hereafter as the WRF ERA and WRF NAM runs and the two CAMx runs that used these WRF runs as the CAMx ERA and CAMx NAM runs.

The meteorological model performance evaluation showed that the two WRF runs were roughly comparable in their performance. The WRF ERA run was generally wetter than the WRF NAM run, with better water vapor mixing ratio performance but positively biased overall. The NAM run produced a better simulation of temperature at surface weather stations in the 12/4 km grids, but the WRF ERA runs simulated the surface winds more accurately. Simulations of precipitation were comparable between the two runs, with one run performing better than the other on some days and vice versa. Therefore, the modeling team elected to perform two CAMx runs using the WRF NAM and WRF ERA to develop meteorological inputs. Then, the CAMx run that performed best in simulating air quality observations in the 12/4 km grids would be selected as the final base case 2011 CAMx model run.

The WRF-derived meteorological fields for the WRF ERA and NAM simulations were processed in the same way to generate CAMx meteorological inputs using the WRFCAMx preprocessor. The CAMx model was run twice for the May 1 - September 30 modeling episode. One CAMx run used the WRF NAM run and the other CAMx run used the WRF ERA run. The two CAMx runs were identical except for the different meteorological inputs.

<u>Initial/Boundary Conditions</u>: The boundary conditions (BCs) for the WAQS 36 km CONUS domain simulation used in the SNMOS were extracted from a MOZART global chemistry model (GCM) simulation of 2011. MOZART output species were interpolated from the MOZART horizontal and vertical coordinate system to the CAMx LCP coordinate system and vertical layer structure and the MOZART chemical species were mapped to the chemical mechanism used by CAMx. The MOZART dust and sea salt species were zeroed out based on findings from the WAQS 2011 modeling (Adelman et al., 2015b). The WAQS 2011 36 km CONUS CAMx simulation was then driven with the MOZART-derived BCs. The SNMOS 2011 12 km modeling was in turn driven with the WAQS CONUS 36 km CAMx outputs as BCs.

<u>Photolysis Rates:</u> The modeling team prepared the photolysis rate inputs as well as albedo/haze/ozone/snow inputs for CAMx. Day-specific ozone column data were based on the Total Ozone Mapping Spectrometer (TOMS) data measured using the satellite-based Ozone Monitoring Instrument (OMI). Albedo was based on land use data. In CAMx, there is an ancillary snow cover input that was used to override the land use based albedo input. Average values for typical snow cover were utilized. Although we are simulating a late spring/summer episode, there are mountains exceeding 3,000 m above ground level within the 12 km domain where snow may have been present during the modeling period. For CAMx, the TUV photolysis rate processor was used. CAMx was configured to use the in-line TUV to adjust for cloud cover and account for the effects aerosol loadings have on photolysis rates; this latter effect on photolysis is especially important in adjusting the photolysis rates due to the occurrence of PM concentrations associated with emissions from fires.

<u>Landuse:</u> We generated landuse fields based on USGS Geographic Information Retrieval and Analysis System (GIRAS) data.

Spin-Up Initialization: A ten day period of model spin up was performed on the 2011 CAMx 12/4 km grid before the first day of the modeling episode.

Table 3-4. SNMOS CAMx version 6.20 configuration

Science Options	Configuration	Details
Model Codes	CAMx V6.20 – March 2015 Release	
Horizontal Grid Mesh	36/12/4 km	
36 km grid	148 x 112 cells	36 km CONUS domain
12 km grid	99 x 93 cells	12 km SNMOS WESTUS12 regional domain
4 km grid	117 x 99 cells	4 km Dona Ana domain
Vertical Grid Mesh	34 vertical layers defined by WRF; no layer collapsing	Layer 1 thickness ~12 m. Model top at ~19-km above MSL
Grid Interaction	12/4 km two-way nesting for CAMx (2011) 36/12/4 km two way nesting for CAMx (2025)	
Initial Conditions	10 day spin-up on 12/4 km grid before first day with MDA8 ozone>70 ppb at any Dona Ana County monitor (2011) 14 day spin-up on 36/12/4 km grid (2025)	Clean initial conditions
Boundary Conditions	12 km SNMOS grid from 36/12 km WAQS modeling (2011) 36 km grid from global chemistry model (2025)	MOZART GCM data for 2011; zeroed out dust and sea salt.
Emissions		
Baseline Emissions Processing	SMOKE, MOVES and MEGAN	
Sub-grid-scale Plumes		
Chemistry		
Gas Phase Chemistry	CB6r2	Active methane chemistry and ECH4 tracer species
Meteorological Processor	WRFCAMx v4.4	Compatible with CAMx V6.20
Horizontal Diffusion	Spatially varying	K-theory with Kh grid size dependence
Vertical Diffusion	CMAQ-like in WRF2CAMx	
Diffusivity Lower Limit	Kz_min = 0.1 to 1.0 m^2/s or 2.0 m^2/s	Land use dependent
Deposition Schemes		
Dry Deposition	Zhang dry deposition scheme (CAMx)	Zhang 2003
Wet Deposition	CAMx-specific formulation	rain/snow/graupel/virga
Numerics		
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) -- Fast Solver	
Vertical Advection Scheme	Implicit scheme w/ vertical velocity update (CAMx)	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	Collela and Woodward (1984)

Science Options	Configuration	Details
Integration Time Step	Wind speed dependent	~0.1-1 min (4 km), 1-5 min (1 -km), 5-15 min (36 km)

3.5 CAMx Model Performance Evaluation Approach

Using the inputs and model configurations described above in Sections 3.3 and 3.4, two CAMx 2011 base case simulations were conducted on the nested 12 and 4 km modeling domains for the 2011 ozone season; one CAMx run was performed with the WRF ERA meteorology inputs and one CAMx run was performed using the WRF NAM meteorology inputs. The SNMOS CAMx simulation results for ozone, carbon monoxide (CO), nitrogen dioxide (NO_2), total $PM_{2.5}$ mass and speciated $PM_{2.5}$ concentrations were evaluated against concurrent measured ambient concentrations using graphical displays of model performance and statistical model performance measures that were compared against established model performance goals and criteria. The CAMx performance evaluation followed the procedures recommended in EPA's photochemical modeling guidance documents (EPA, 2014) and described in detail in the SNMOS Modeling Work Plan (Adelman et al., 2015a). While the focus of the SNMOS is on ozone, a cursory evaluation of the PM performance was conducted to assess the overall validity of the model for the application period and domains.

Detailed evaluation of ozone and its precursor species focused on the model performance at monitors in the 4 km modeling domain. Figure 3-3 is a map of the SNMOS modeling region showing the locations of air quality monitors that were used for the CAMx evaluation. This map shows a cluster of ozone monitors in the Doña Ana County region extending from Las Cruces southeast to El Paso and Ciudad Juarez. The data from these monitors were key inputs to the evaluation of the surface ozone and PM concentrations predicted by CAMx.

3.5.1 Available Aerometric Data for Model Performance Evaluation

The following routine air quality measurement data networks operating in 2011 were used in the SNMOS model performance evaluation:

<u>EPA AQS Surface Air Quality Data</u>: Data files containing hourly-averaged concentration measurements at a wide variety of state and EPA monitoring networks are available in the Air Quality System (AQS) database throughout the U.S. The AQS consists of many sites that tend to be mainly located in and near major cities. The standard hourly AQS AIRS monitoring stations typically measure hourly ozone, NO_2, NOx and CO concentrations and there are thousands of sites across the U.S. There are several AQS sites in Doña Ana County and another group of AQS sites in nearby El Paso, TX. There is a monitoring site in Ciudad Juarez that is part of the AQS network, but this site was not used in calculating episode average, domain-wide MPE statistical metrics due to concerns about the reliability of the data (personal communication from Michael Baca, NMED, 2016). However, we do present model performance statistics for this monitor in several plots in which monitor performance is broken out separately (e.g. Figure 4-4). This allows the reader to view the data for the Ciudad Juarez monitor without introducing possible bias from this monitor into the overall statistical evaluation of the two CAMx runs.

<u>Chemical Speciation Network (CSN)</u>: This network measures speciated $PM_{2.5}$ concentrations including SO_4, NO_3, NH_4, EC, OC and elements at 24-hour averaging time period using a 1:3 or 1:6 day sampling frequency.

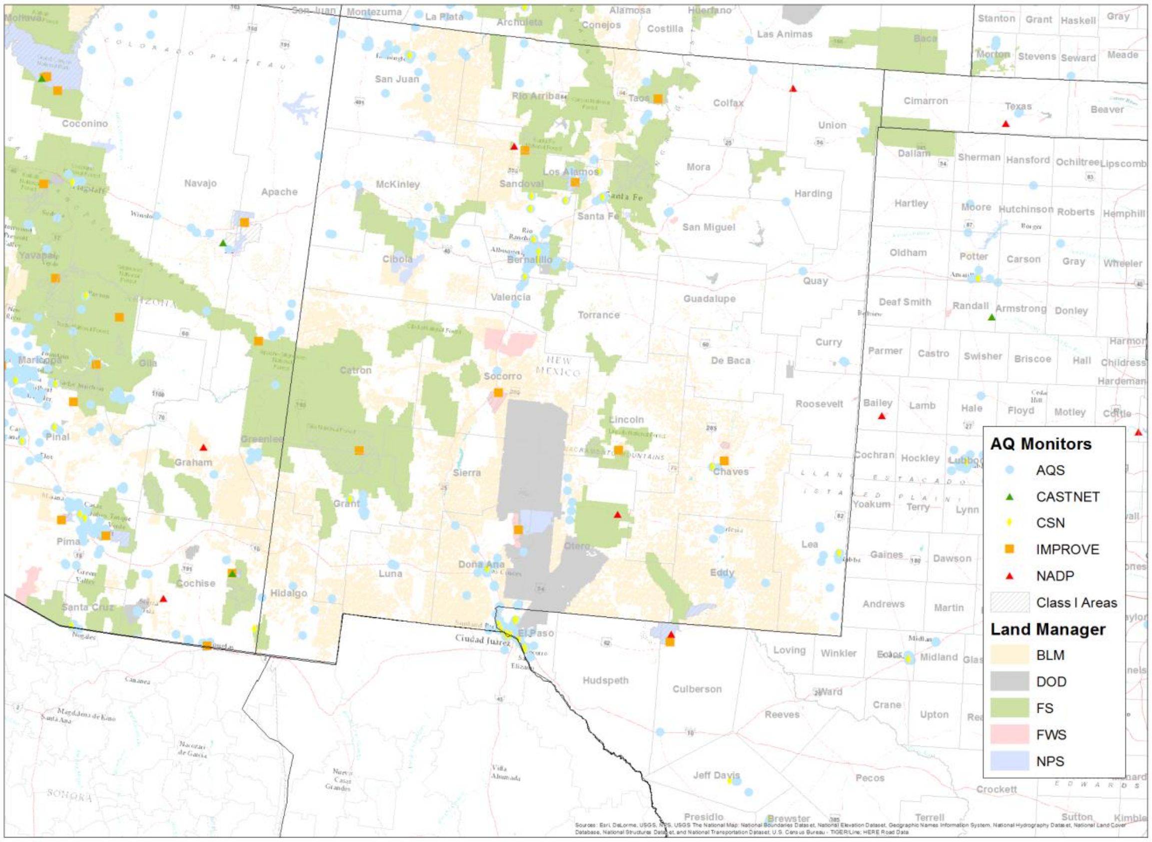


Figure 3-3. Air quality monitors in New Mexico and the surrounding area.

<u>IMPROVE Monitoring Network</u>: The Interagency Monitoring of PROtected Visual Environments (IMPROVE) network collects 24-hour average $PM_{2.5}$ and PM_{10} mass and speciated $PM_{2.5}$ concentrations (with the exception of ammonium) using a 1:3 day sampling frequency. IMPROVE monitoring sites are mainly located at more rural Class I area sites that correspond to specific National Parks, Wilderness Areas and Fish and Wildlife Refuges across the U.S. with a large number of sites located in the western U.S., although there are also some IMPROVE protocol sites that are more urban-oriented.

<u>CASTNet Monitoring Network</u>: The Clean Air Status and Trends Network (CASTNet) operates approximately 80 monitoring sites in mainly rural areas across the U.S. CASTNet sites typically collected hourly ozone, temperature, wind speed and direction, sigma theta, solar radiation, relative humidity, precipitation and surface wetness. CASTNet also collects weekly (Tuesday to Tuesday) samples of speciated $PM_{2.5}$ sulfate, nitrate, ammonium and other relevant ions and weekly gaseous SO_2 and nitric acid (HNO_3).

3.5.2 Model Performance Statistics and Evaluation Approach

For over two decades, ozone model performance has been compared against EPA's 1991 ozone modeling guidance performance goals (EPA, 1991). For PM species, a separate set of model performance statistics and performance goals and criteria have been developed as part of the regional haze modeling performed by several Regional Planning Organizations (RPOs). EPA's modeling guidance notes that PM models might not be able to achieve the same level of model performance as ozone models. Indeed, $PM_{2.5}$ species definitions are defined by the measurement technology used to measure them and different measurement technologies can produce very different $PM_{2.5}$ concentrations. Given this, several researchers have developed PM model performance goals and criteria that are less stringent than the ozone goals as shown in Table 3-5 (Boylan, 2004; Boylan and Russell, 2006; Morris et al., 2009a,b).

Table 3-5. Ozone and PM model performance goals and criteria

Fractional Bias (FB)	Fractional Error (FE)	Comment
≤±15%	≤35%	Ozone model performance goal that would be considered very good model performance for PM species
≤±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.

EPA compiled and interpreted the model performance from 69 PGM modeling studies in the peer-reviewed literature between 2006 and March 2012 and developed recommendations on what should be reported in a model performance evaluation (Simon et al., 2012). Although these recommendations are not official EPA guidance, they are useful and were considered in developing the plan for the SNMOS model performance evaluation. Model performance statistics described below are defined in Table 3-6.

- PGM MPE studies should at a minimum report the Mean Bias (MB) and Error (ME or RMSE), and Normalized Mean Bias (NMB) and Error (NME) and/or Fractional Bias (FB) and Error (FE). Both the MNB and FB are symmetric around zero with the FB bounded by -200% to +200%.
- Use of the Mean Normalized Bias (MNB) and Gross Error (MNGE) is not encouraged because they are skewed toward low observed concentrations and can be misinterpreted due to the lack of symmetry around zero.
- Given this recommendation, the bias and error metrics were calculated for ozone using an appropriate observed ozone cut-off concentration (SNMOS used a 60 ppb cut-off).
- The model evaluation statistics should be calculated for the highest resolution temporal resolution available and for important regulatory averaging times (e.g., daily maximum 8-hour ozone).
- It is important to report processing steps in the model evaluation and how the predicted and observed data were paired and whether data are spatially/temporally averaged before the statistics are calculated.
- Predicted values should be taken from the grid cell that contains the monitoring site, although bilinear interpolation to the monitoring site point can be used for higher resolution modeling (< 12 km).

Table 3-6. Model performance evaluation statistical measures used to evaluate CTMs.

Statistical Measure	Mathematical Expression	Notes
Accuracy of paired peak (Ap)	$\frac{P - O_{peak}}{O_{peak}}$	Comparison of the peak observed value (O_{peak}) with the predicted value at same time and location
Coefficient of determination (r2)	$\frac{\left[\sum_{i=1}^{N}(P_i - \overline{P})(O_i - \overline{O})\right]^2}{\sum_{i=1}^{N}(P_i - \overline{P})^2 \sum_{i=1}^{N}(O_i - \overline{O})^2}$	Pi = prediction at time and location i; Oi = observation at time and location i; $\overline{P}$ = arithmetic average of Pi, i=1,2,…, N; $\overline{O}$ = arithmetic average of Oi, i=1,2,…,N
Normalized Mean Error (NME)	$\frac{\sum_{i=1}^{N}\left\|P_i - O_i\right\|}{\sum_{i=1}^{N}O_i}$	Reported as %
Root Mean Square Error (RMSE)	$\left[\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2\right]^{1/2}$	Reported as concentration (e.g., $\mu g/m^3$)
Fractional Gross Error (FE)	$\frac{2}{N}\sum_{i=1}^{N}\left\|\frac{P_i - O_i}{P_i + O_i}\right\|$	Reported as % and bounded by 0% to 200%
Mean Error (ME)	$\frac{1}{N}\sum_{i=1}^{N}\left\|P_i - O_i\right\|$	Reported as concentration (e.g., $\mu g/m^3$)
Mean Normalized Gross Error (MNGE)	$\frac{1}{N}\sum_{i=1}^{N}\frac{\left\|P_i - O_i\right\|}{O_i}$	Reported as %
Mean Bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$	Reported as concentration (e.g., $\mu g/m^3$)
Mean Normalized Bias (MNB)	$\frac{1}{N}\sum_{i=1}^{N}\frac{(P_i - O_i)}{O_i}$	Reported as %
Mean Fractionalized Bias (Fractional Bias, FB)	$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$	Reported as %, bounded by -200% to +200%
Normalized Mean Bias (NMB)	$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N}O_i}$	Reported as %
Bias Factor (BF)	$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{P_i}{O_i}\right)$	Reported as BF:1 or 1: BF or in fractional notation (BF/1 or 1/BF).

- $PM_{2.5}$ should also be evaluated separately for each major component species (e.g., SO_4, NO_3, NH_4, EC, OA and $OPM_{2.5}$).
- Evaluation should be performed for subsets of the data including, high observed concentrations (e.g., ozone > 60 ppb), by sub-regions and by season or month.
- Evaluation should include more than just ozone and $PM_{2.5}$, such as SO_2, and CO.
- Spatial displays should be used in the model evaluation to evaluate model predictions away from the monitoring sites. Time series of predicted and observed concentrations at a monitoring site should also be used.
- It is necessary to understand measurement artifacts in order to make meaningful interpretation of the model performance evaluation.

We incorporated the recommendations of Simon, Baker and Philips (2012) into the SNMOS model performance evaluation within the constraints of the available data. The SNMOS evaluation products included qualitative and quantitative evaluation for the following model output species:

- 1-hour average ozone and maximum daily 8-hour average (MDA8) ozone, with and without a 60 ppb threshold
- Carbon monoxide, nitrogen dioxide; VOC measurements were not readily available
- Total $PM_{2.5}$, elemental carbon, organic carbon, sulfate, nitrate, and ammonium

3.6 CAMx Post-Processing and Model Performance Evaluation Tools

3.6.1 Atmospheric Model Evaluation Tool (AMET)

The Atmospheric Model Evaluation Tool (AMET) (Appel et al., 2013) is a suite of software designed to facilitate the analysis and evaluation of meteorological and air quality models. AMET matches the model output for particular locations to the corresponding observed values from one or more networks of monitors (Appendix A). These pairings of values (model and observation) are then used to statistically and graphically analyze the model's performance. AMET version 2.1 (AMETv1.2) was the primary tool used to generate the performance statistics and plots used to conduct the model performance evaluation.

3.7 CAMx Post-processing and Model-Observations Pairing

This section details how we processed and compared the CAMx output data to ambient air quality observations. The general procedure involved the following steps:

1. Convert the CAMx average (avrg) hourly output files from UAM to I/O API-netCDF format with the utility camx2ioapi. This utility is available from http://www.camx.com.
2. Run the program Combine to post-process the model output species. One function of Combine is to simply convert the units of the gas-phase model species from ppmV to ppbV. Combine also calculates lumped species, such as total volatile organic compounds and NOx. Finally Combine is used to calculate the model PM species for comparison to

observations. Combine is distributed with the CMAQ air quality model package available from http://www.cmaq-model.org.

3. Run the programs sitecmp, cmp_airs, and cmp_castnet to pair in space and time the model output data from Combine with the surface monitoring networks described above. The programs cmp_airs and cmp_castnet also compute MDA8 values for comparison to the reported MDA8 concentrations in the observational databases. These programs are distributed with AMET available from http://www.cmascenter.org.
4. Load the paired model-observations tables output from sitecmp, cmp_airs, and cmp_castnet into the AMET database using the scripts provided with AMET
5. Run the AMET analysis scripts to calculate the model performance statistics and create plots of the performance results

4.0 CAMX MODEL PERFORMANCE EVALUATION FOR OZONE AND ITS PRECURSORS

We begin the ozone model performance evaluation with a domain-wide overview of the ozone simulation. In Section 4.1, we present regional ozone performance across the entire 12 km and 4 km modeling domains and compare with performance benchmarks shown in Table 3-5. Evaluation focused on specific time periods and monitors is presented in Section 4.2

4.1 Episode Average Performance Metrics

Episode average statistical performance metrics for the 4 km domain are shown in Table 4-1 and episode average metrics for the 12 km domain are shown in Table 4-2. Table 4-1 and Table 4-2 include bias, error and correlation metrics for modeled ozone averaged over all AQS monitoring sites across the 4 km and 12 km modeling domains, respectively. Values shown in red indicate performance metrics for which CAMx does not achieve the model performance goals shown in Table 3-5. For both CAMx runs, the SNMOS 12 km domain-wide performance meets all bias and error goals for hourly and MDA8 ozone with and without the 60 ppb threshold. The 4 km domain-wide ozone model performance meets the bias and error performance goals for MDA8 ozone at the AQS monitoring locations with and without application of the 60 ppb threshold. Several key points of CAMx ozone model performance across the 12/4 km domains include:

- Fractional bias (FB=24.6% for ERA, FB=20.5% for NAM) for AQS hourly ozone is the only ozone performance metric for which CAMx misses the performance goal on the 4 km grid. Both CAMx runs miss the goal.
- On an episode- and domain-wide average basis, both CAMx runs have a positive bias for hourly ozone and for MDA8 ozone when no ozone threshold is applied. This is true on both the 4 km and 12 km domains.
- When a 60 ppb observed ozone concentration threshold is applied, the model biases for hourly ozone and for MDA8 ozone switch from positive to negative for both CAMx runs. The model performance is better at the AQS sites at ozone values > 60 ppb, in that the absolute value of the bias is smaller when ozone exceeds 60 ppb. Model performance improves for higher values of observed ozone.
- The CAMx run with ERA WRF meteorology has lower bias and error than the CAMx run with NAM WRF meteorology when hourly or MDA8 ozone > 60 ppb. The reverse is true when ozone < 60 ppb. The CAMx ERA run performs better than the CAMx NAM run when ozone is high and vice versa.
- Values of R^2 are higher for hourly ozone than for MDA8 ozone and are comparable in both CAMx runs.

Figure 4-1 and Figure 4-2 show scatter plots (CAMx modeled ozone vs. observed ozone) for all AQS sites in the 4 km domain for the CAMx runs with WRF ERA and WRF NAM meteorology, respectively. The figures include both hourly ozone (upper panels) and MDA8 ozone (lower panels) and results are shown with and without a 60 ppb ozone concentration threshold applied to the observations. CAMx has a positive bias in predicting the observed hourly and MDA8 ozone values in both runs, with higher bias in the ERA run compared to the NAM when no threshold is applied.

Table 4-1. 4 km domain ozone performance indicators. Red type indicates a metric that exceeds the ozone performance goal in Table 3-5.

Species		Network	FB	FE	MB	ME	NMB	NME	R^2	RMSE
		Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)		(ppb)
O3	CAMx with ERA WRF	AQS Hourly	24.6	32.4	9.35	12.7	23	31.2	0.34	15.8
	CAMx with NAM WRF	AQS Hourly	20.5	31.1	7.42	11.8	18.3	29.2	0.31	15
O3 > 60 ppb	CAMx with ERA WRF	AQS Hourly	-5.6	12.5	-3.23	7.97	-4.9	12	0.01	10.4
	CAMx with NAM WRF	AQS Hourly	-9.1	13.9	-5.39	8.64	-8.1	13	0.01	11.3
O3	CAMx with ERA WRF	AQS MDA8	13.8	17.7	7.56	9.83	14.2	18.4	0.17	12.1
	CAMx with NAM WRF	AQS MDA8	11.0	16.9	5.9	9.25	11.1	17.4	0.09	11.7
O3 > 60 ppb	CAMx with ERA WRF	AQS MDA8	-0.50	9.46	-0.14	6.20	-0.22	9.5	0.00	7.79
	CAMx with NAM WRF	AQS MDA8	-4.4	10.5	-2.54	6.69	-3.89	10.2	0.00	8.64

Table 4-2. 12 km domain ozone performance indicators. Red type indicates a metric that exceeds the ozone performance goal in Table 3-5.

Species		Network	FB	FE	MB	ME	NMB	NME	R^2	RMSE
		Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)		(ppb)
O3	CAMx with ERA WRF	AQS Hourly	11	31.8	4.48	11.7	10.6	27.5	0.36	14.9
	CAMx with NAM WRF	AQS Hourly	10.1	30.7	3.72	11.2	8.77	26.5	0.36	14.5
O3 > 60 ppb	CAMx with ERA WRF	AQS Hourly	-8.16	15	-4.4	9.18	-6.56	13.7	0.04	12.3
	CAMx with NAM WRF	AQS Hourly	-10.1	15.8	-5.65	9.63	-8.42	14.3	0.04	12.7
O3	CAMx with ERA WRF	AQS MDA8	6.92	13.9	3.95	7.96	7.04	14.2	0.28	10.1
	CAMx with NAM WRF	AQS MDA8	4.65	13.6	2.65	7.73	4.73	13.8	0.26	9.98
O3 > 60 ppb	CAMx with ERA WRF	AQS MDA8	-1.7	10.4	-0.83	6.81	-1.26	10.3	0.03	8.54
	CAMx with NAM WRF	AQS MDA8	-3.95	11.2	-2.24	7.24	-3.38	10.9	0.03	9.11

On the days with elevated ozone measurements (> 60 ppb), CAMx has a negative bias (i.e. underestimates ozone) in both runs, and the CAMx run with ERA WRF had a smaller absolute value of the bias (i.e. better performance) than the CAMx NAM run. The domain-wide and episode-wide evaluation shows that the CAMx run with ERA WRF performed better when observed ozone values were high, and the CAMx run with NAM WRF performed better on days with low ozone.

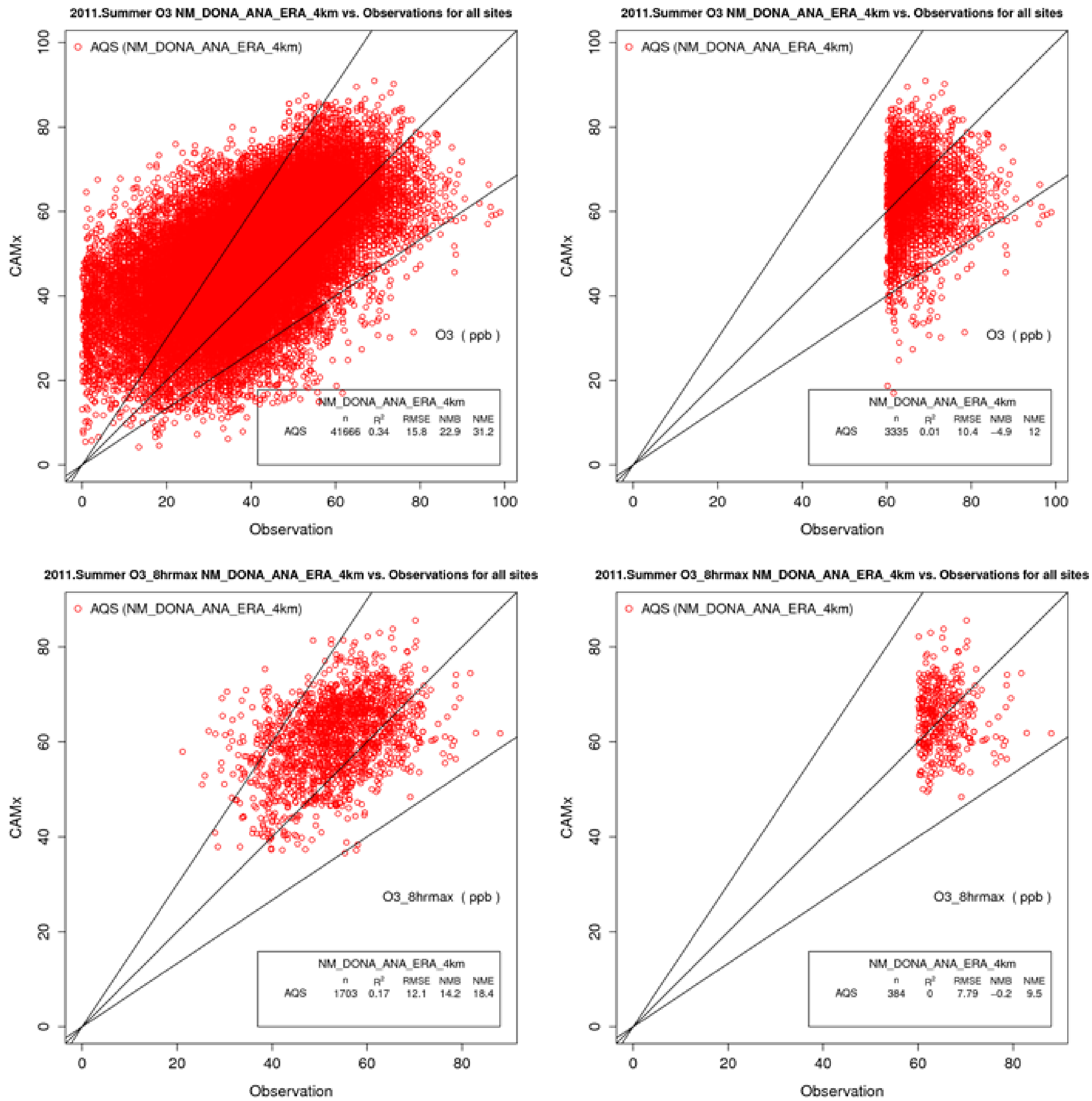


Figure 4-1. Scatter plots showing modeled versus observed ozone. SNMOS 2011 base case model performance for the CAMx run using ERA WRF meteorology for hourly (top) and MDA8 (bottom) ozone concentrations for all AQS sites in the 4 km domain with (right) and without (left) using a 60 ppb observed ozone cut-off threshold.

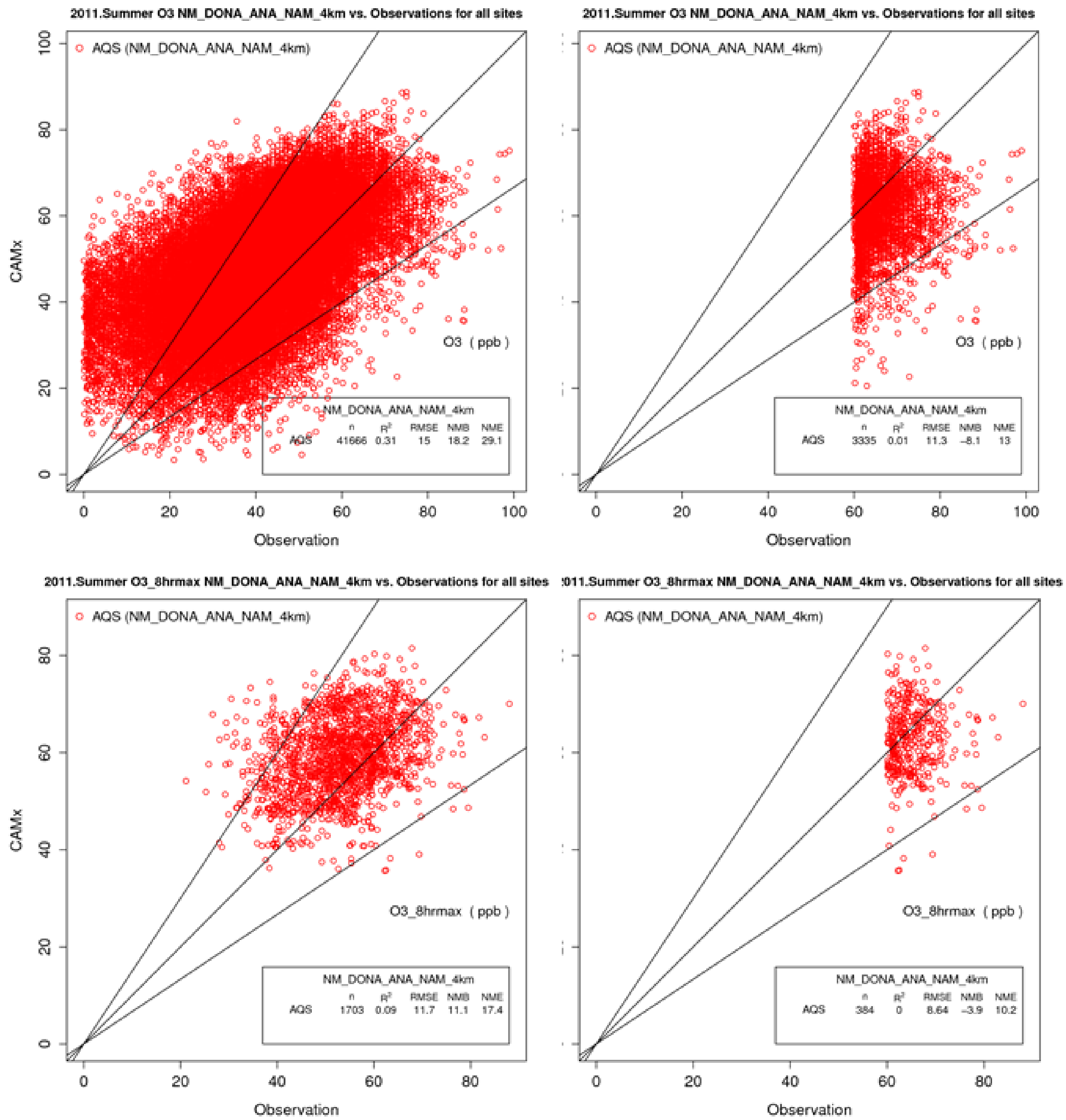


Figure 4-2. Scatter plots showing modeled versus observed ozone. SNMOS 2011 base case model performance for the CAMx run using NAM WRF meteorology for hourly (top) and MDA8 (bottom) ozone concentrations for all AQS sites in the 4 km domain with (right) and without (left) using a 60 ppb observed ozone cut-off threshold.

4.2 Model Performance at Doña Ana County Monitors

Next, we focus on the performance of the two CAMx simulations in reproducing observed ozone in Doña Ana County within the 4 km grid. Figure 4-3 shows ozone monitors within the 4 km domain that had ozone data for more than 75% of the hours in the SNMOS modeling episode. The greatest concentration of sites is in southern Doña Ana County and nearby El Paso, TX. Data for the Ciudad Juarez Advance monitor is shown in this section with the caveat that the observations are likely to be unreliable.

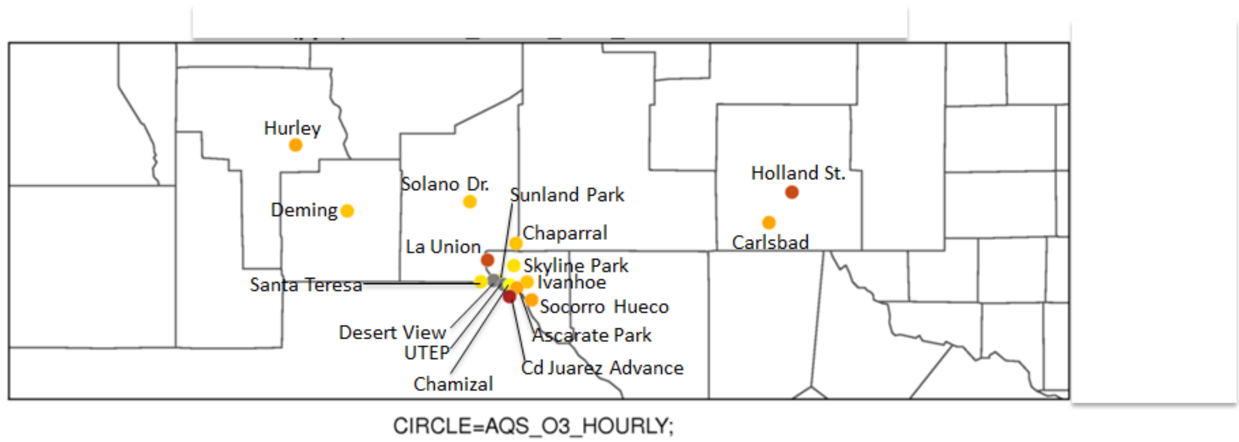


Figure 4-3. Monitor site map for 4 km grid AQS sites used in AMET analysis.

Figure 4-4 shows a spatial summary of model performance for episode average correlation between observed and modeled MDA8 ozone within the 4 km domain. Results are shown for both CAMx model runs with and without application of a 60 ppb threshold for the observed MDA8 ozone. In both CAMx runs, the modeled MDA8 ozone is less well-correlated with the observations for values of observed MDA8 > 60 ppb. For MDA8 ozone > 60 ppb, correlation performance in the two runs is comparable. For MDA8 ozone < 60 ppb, the CAMx ERA run is better correlated with observations for monitors in southern Doña Ana County and the El Paso area than the CAMx NAM run.

For NMB (Figure 4-5), all monitors except the Hurley monitor are within the ±15% EPA bias goal when the 60 ppb MDA8 ozone threshold is applied; this is true for both CAMx runs. When observed ozone MDA8 < 60 ppb, both runs show similar performance. Without the 60 ppb threshold, a number of sites in the 4 km domain show a high bias that exceeds the 15% performance goal. The higher values of bias occur outside of Doña Ana County (with the exception of the La Union monitor) and are more prevalent in El Paso than in Doña Ana. The Ciudad Juarez NMB value is higher than that of any other monitor within the modeling domain.

For NME (Figure 4-6), both model runs show better performance when observed MDA8 ozone exceeded 60 ppb. When the 60 ppb threshold was applied, all sites in both runs have NME less than 35% except the Hurley monitor. When the 60 ppb threshold is used, the CAMx ERA run has lower NME than the CAMx NAM run. In both CAMx runs, the NME is larger when the 60 ppb threshold is not used, consistent with the larger positive bias seen in Figure 4-5.

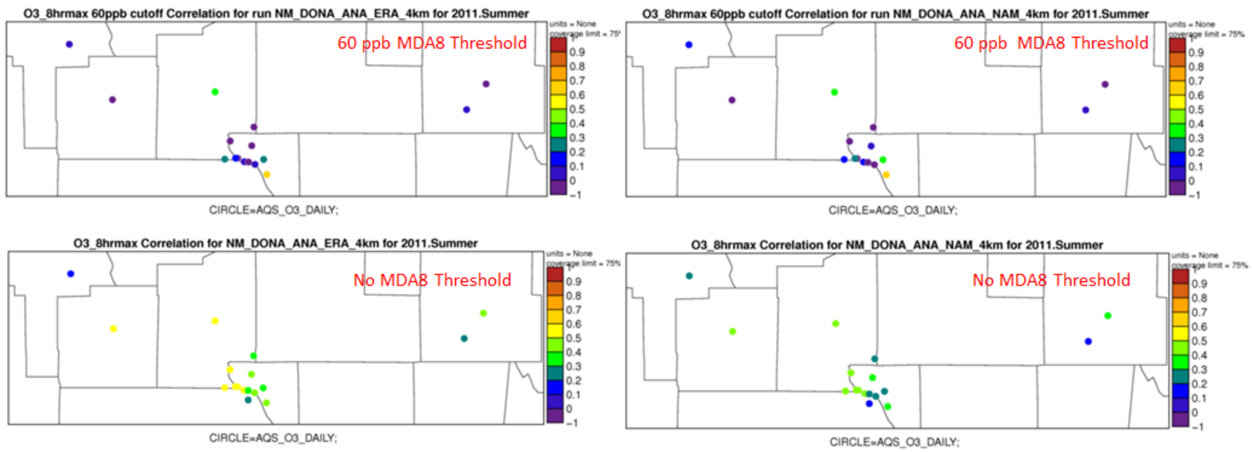


Figure 4-4. Comparison of correlation for the CAMx ERA (left) and CAMx NAM (right) model runs. Upper figures have 60 ppb MDA8 threshold and no threshold was used for the lower figures.

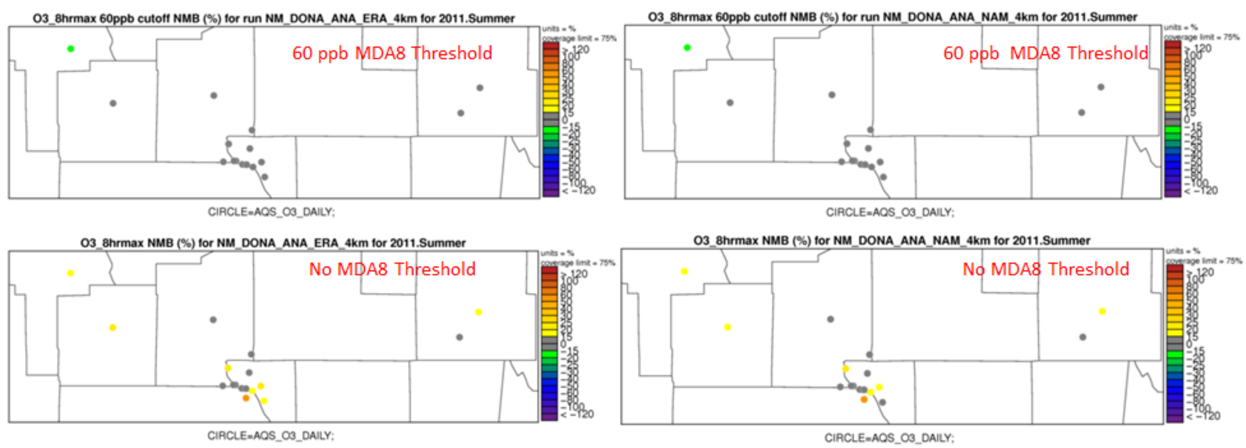


Figure 4-5. Comparison of NMB for the CAMx ERA (left) and CAMx NAM (right) model runs. Upper figures have 60 ppb MDA8 threshold and no threshold was used for the lower figures.

The MDA8 ozone MB for both CAMx runs is shown in Figure 4-7. When no threshold is used, both model runs show an overall high bias. Performance is better in the CAMx NAM run, which has smaller values of the MB for sites in the vicinity of the Mexico-U.S. border. However, when the 60 ppb threshold is applied to the observed MDA8 ozone, the CAMx ERA run has a smaller MB than the CAMx NAM run (Figure 4-7). The underprediction of MDA8 ozone is more pronounced in CAMx NAM run on days when the observed MDA8 ozone is high, and the CAMx ERA run does a better job of simulating the higher observed ozone values.

The episode average statistical metrics indicate that both CAMx model runs have an overall high bias for hourly ozone and MDA8 in the 4 km domain when all days are included in the average. Overall performance is better in the CAMx NAM run when all days and hours are

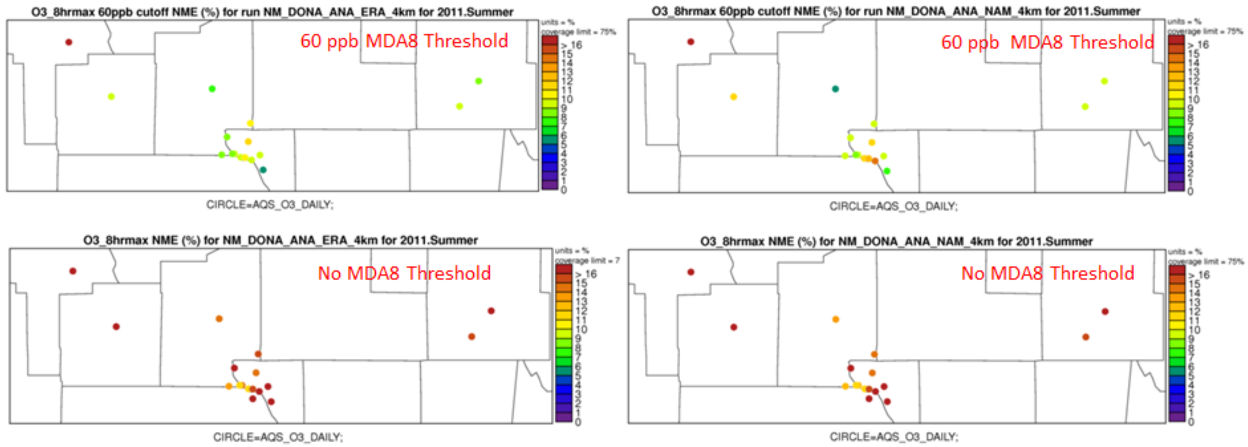


Figure 4-6. Comparison of NME for the CAMx ERA (left) and CAMx NAM (right) model runs. Upper figures have 60 ppb MDA8 threshold and no threshold was used for the lower figures.

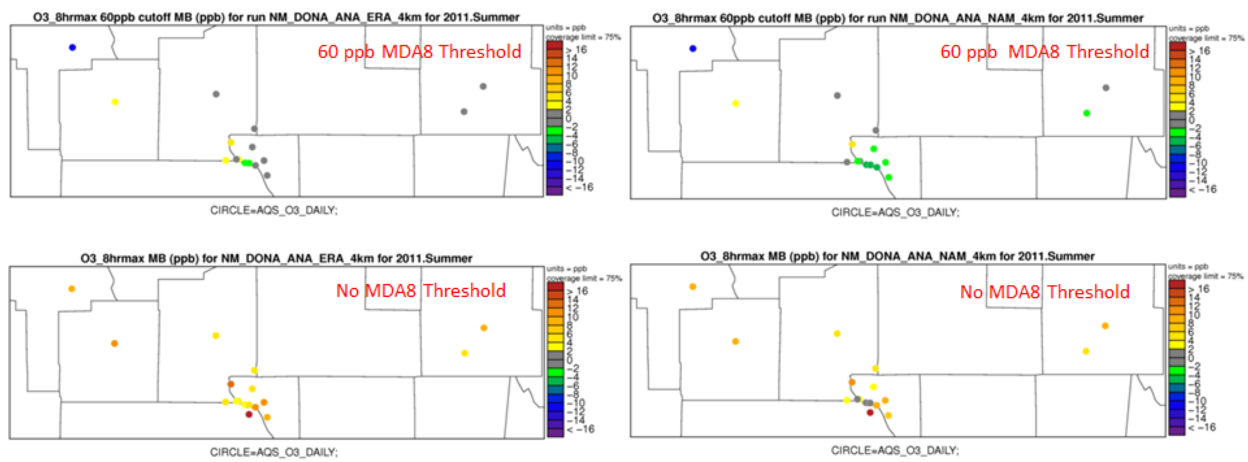


Figure 4-7. Comparison of MB for the CAMx ERA (left) and CAMx NAM (right) model runs. Upper figures have 60 ppb MDA8 threshold and no threshold was used for the lower figures.

considered. When only the observed days with MDA8 > 60 ppb are considered, CAMx tends to underestimate the MDA8, and the CAMx ERA run shows better performance than the CAMx NAM run.

Next, we examine performance at the ozone monitors within Doña Ana County in light of the form of the NAAQS for ozone and the EPA's recommended method for performing modeled attainment demonstrations. The SNMOS will perform a modeled attainment demonstration for Doña Ana County using the 2011 base case described in this document and a 2025 future year model that is currently under development (Adelman et al., 2015a). Future year emissions sensitivity modeling will then be used to evaluate the impacts of emissions reductions on future attainment of the ozone NAAQS at Doña Ana County monitors. In carrying out the base case model performance, we therefore consider how CAMx performance in the 2011 base year run will affect the modeled attainment demonstration and aim to choose the CAMx model run that will provide the most reliable results.

The ozone NAAQS are formulated in terms of a Design Value, which is calculated as the 3-year average of the fourth highest monitored MDA8 concentration at each monitoring site. To attain the 2015 ozone standard, the Design Value for a given monitor must not exceed 70 ppb. EPA's latest modeling guidance (EPA, 2014) for projecting future year 8-hour ozone Design Values recommends the use of modeling results in a relative sense to scale the observed base year 8-hour ozone Design Value (DVB) to obtain a future year 8-hour ozone Design Value (DVF). The model-derived scaling factors are referred to as Relative Response Factors (RRF) and are defined as The RRF is the ratio of the average future MDA8 values to the average base MDA8 values.

$$DVF_{monitor\ i} = DVB_{monitor\ i} \times RRF_{monitor\ i}$$

$$RRF_{monitor\ i} = \frac{\sum_{days}(MDA8\ ozone)_{future\ year}}{\sum_{days}(MDA8\ ozone)_{base\ year}}$$

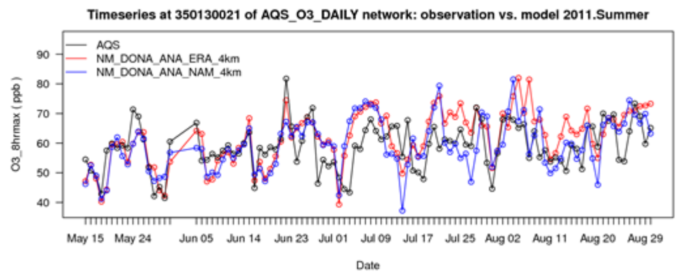
This technique is used to minimize the effect of model uncertainty on future year ozone projections. For example, if the model has a bias toward underestimating ozone at a given monitor, using the raw future year ozone predictions may result in an underestimate of future year ozone at that monitor. However, if the ratio of the future year to base year modeled ozone values at that monitor is multiplied by the observed base year Design Value to produce a predicted future year value, that future year value will better reflect the change in ozone due to changes in emissions between base and future year cases, and the effect of the model's bias toward lower ozone values will have been reduced.

EPA Modeling Guidance (EPA, 2014) recommends calculating the modeled RRF used in the attainment demonstration based on the days with the 10 highest modeled MDA8 ozone values in the simulated period at each monitoring site, as long as the MDA8 ozone for each day is ≥ 60 ppb. The default for EPA's Modeled Attainment test Software (MATS) is to use top 10 modeled MDA8 ozone days to construct RRFs. In the SNMOS MPE, we focused on model performance for MDA8 ozone on the 10 days at each monitor that would be used in calculating the RRF for each Doña Ana County monitor as part of the planned modeled attainment demonstration.

Figure 4-8 shows ranked lists of the 10 days with the highest modeled values of modeled MDA8 ozone at the Desert View, NM monitor for the CAMx ERA and CAMx NAM runs. The highest modeled MDA8 ozone days do not correspond well to high observed MDA8 ozone in either CAMx run. In general, the highest modeled days are days on which the model greatly overestimates the observed MDA8 ozone. For example, on the highest modeled MDA8 ozone day in the CAMx ERA run, the modeled MDA8 ozone was 82 ppb, while the observed MDA8 ozone was 65 ppb, corresponding to a model bias of 17 ppb in the MDA8. There was only one day out of the 10 highest modeled days in the CAMx ERA run that corresponded to a day when the observed MDA8 ozone exceeded 70 ppb: June 22. The CAMx ERA bias on June 22 was -7 ppb, consistent with the MPE statistical analysis that showed that CAMx ERA tended to underestimate observed ozone on high observed ozone days.

NM_DONA_ANA_ERA_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	8/5/2011	65.13	81.97	16.84
2	8/7/2011	55.00	81.43	26.43
3	7/21/2011	58.13	75.84	17.71
4	8/4/2011	67.88	75.79	7.91
5	6/22/2011	81.75	74.45	-7.30
6	7/9/2011	64.13	73.71	9.58
7	7/20/2011	65.50	73.57	8.07
8	7/25/2011	64.63	73.44	8.82
9	7/8/2011	68.00	73.34	5.34
10	8/30/2011	65.13	73.31	8.18

NM_DONA_ANA_NAM_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	8/4/2011	67.88	81.49	13.62
2	7/21/2011	58.13	79.34	21.22
3	8/26/2011	64.00	74.45	10.45
4	7/7/2011	64.38	74.05	9.67
5	7/8/2011	68.00	72.93	4.93
6	7/20/2011	65.50	72.03	6.53
7	7/9/2011	64.13	71.94	7.81
8	7/6/2011	58.00	71.82	13.82
9	7/5/2011	59.13	71.76	12.64
10	8/9/2011	55.25	71.40	16.15



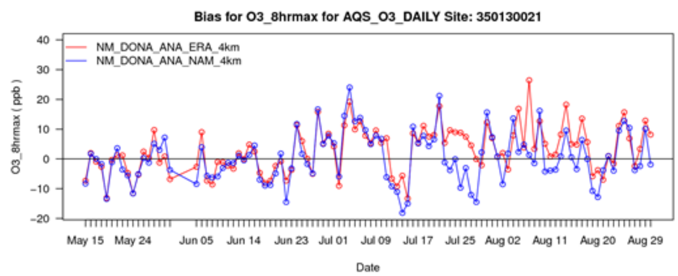
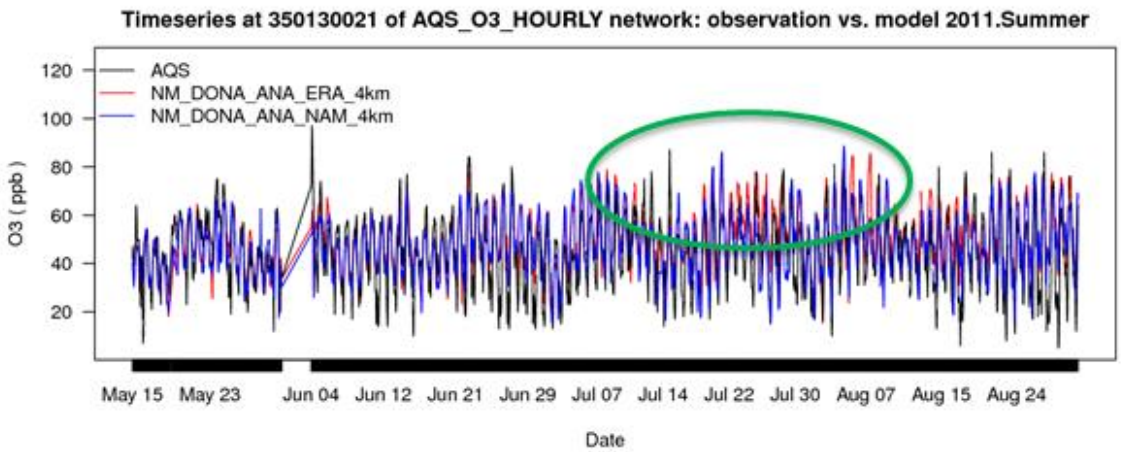


Figure 4-8. Upper (lower) left panel: Ranked list of the 10 days with the highest modeled values of modeled MDA8 ozone (ppb) at the Desert View, NM monitor for the CAMx ERA (NAM) run. Also shown are date, observed MDA8 (ppb) and the model bias (ppb). Upper right panel: time series of observed (black) and modeled MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the Desert View monitor. Lower right panel: Model bias in MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the Desert View monitor.

In the CAMx NAM run, none of the 10 highest modeled days corresponded to a day with observed MDA8 exceeding 70 ppb. The CAMx NAM run bias was positive on all 10 of the highest modeled days. For both the CAMx ERA and CAMx NAM runs, the 10 highest modeled days occurred mainly during July and August, which are periods when both runs saw persistent overestimates of MDA8 ozone at the Desert View monitor (right panel of Figure 4-8). Figure 4-9 shows the observed and modeled hourly ozone time series for the modeling episode as well as modeled bias. The green circled portions of the time series indicate periods of July and August when many of the 10 highest days shown in Figure 4-8 occurred. Both CAMx ERA and CAMx NAM runs have a persistent bias in hourly ozone during this period, and during the last week of July, the ozone overestimate is higher in the CAMx ERA run.

Figure 4-10 shows observed ozone (filled diamonds) and CAMx modeled surface layer ozone for August 7, 2011 for the CAMx ERA and CAMx NAM runs on the 4 km and 12 km domains. August 7 was the day with the 2nd highest modeled MDA8 ozone for the CAMx ERA run (Figure 4-8). Both model runs show a region of relatively low ozone in the western portion of the 12 km modeling domain and a region of higher ozone in the eastern portion of the domain. The observations indicate that both CAMx runs overestimate ozone across broad regions of New



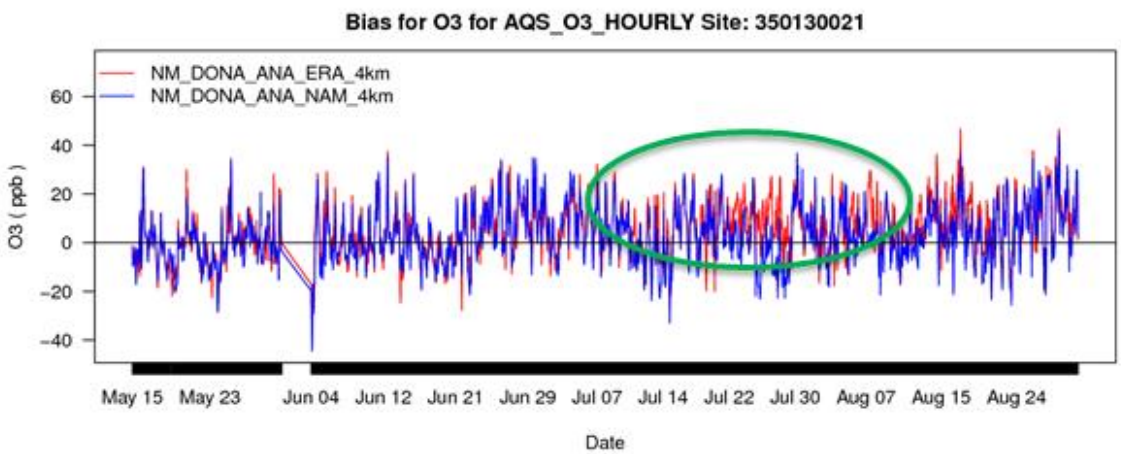


Figure 4-9. Upper panel: observed 1-hour ozone time series and modeled 1-hour time series for the CAMx NAM and CAMx ERA runs at the Desert View monitor in Doña Ana County. Lower panel: Model bias for hourly ozone in the CAMx NAM and CAMx ERA runs at the Desert View monitor.

Mexico and Texas, with the CAMx ERA run showing a more pronounced high bias. The 4 km domain results (upper panels) show that ozone is overestimated across Doña Ana County as well as in the El Paso area, with the CAMx ERA run making a larger overestimate than the CAMx NAM run.

Overall, neither CAMx run shows good skill in simulating MDA8 ozone on the highest modeled days at Desert View, and the only observed day with MDA8 ozone > 70 ppb that appears among the top 10 modeled days is June 22. This day appears only in the 10 highest days for the CAMx ERA run. The high modeled values that appear in the list of 10 highest modeled MDA8 ozone days occur during July and August periods when modeled ozone is overestimated across broad areas of New Mexico and Texas.

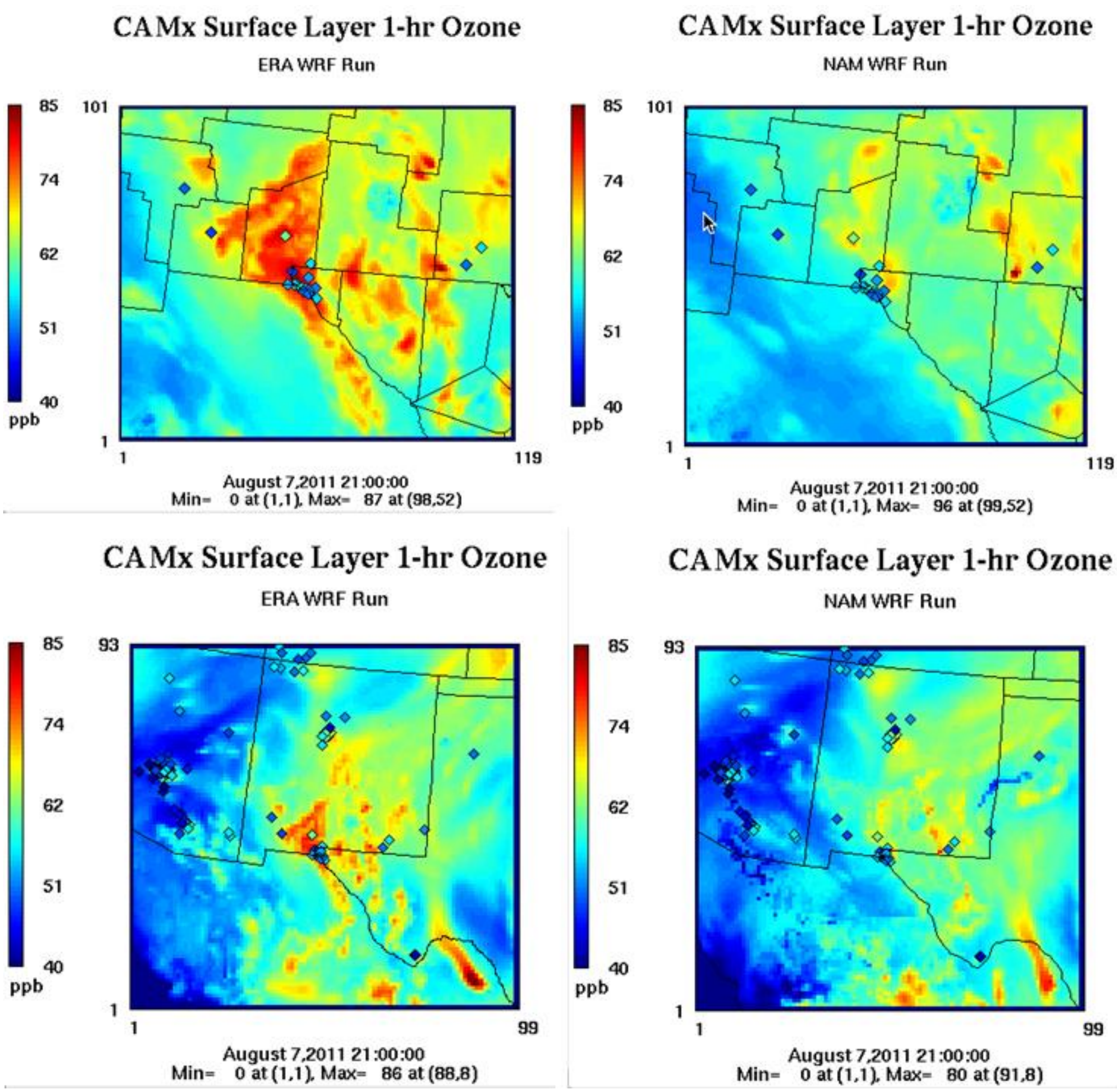


Figure 4-10. CAMx modeled surface layer ozone for August 7, 2011 at 21Z. Upper left panel: CAMx ERA run, 4 km domain. Lower left panel: CAMx ERA run: 12 km domain. Upper right panel: CAMx NAM run, 4 km domain. Lower right panel: CAMx NAM run: 12 km domain. Filled diamonds indicate surface AQS monitoring sites and their color scale is identical to that of the rest of the plot.

The 10 highest modeled MDA8 ozone days for the Sunland Park, NM monitor are shown in Figure 4-11. Results for Sunland Park are similar to those for Desert View in that the days with high modeled MDA8 ozone do not correspond to days with high observed MDA8 ozone except for June 22 in the CAMx ERA run only. Figure 4-12 illustrates the reason for the difference in CAMx ERA and CAMx NAM performance on June 22. The surface layer ozone plots correspond

NM_DONA_ANA_ERA_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	8/5/2011	62.63	82.99	20.37
2	8/7/2011	52.50	81.55	29.05
3	7/21/2011	56.50	76.74	20.24
4	8/30/2011	61.25	74.14	12.89
5	7/25/2011	63.13	74.08	10.96
6	8/4/2011	62.63	73.62	10.99
7	8/29/2011	55.00	72.78	17.78
8	7/9/2011	59.63	72.33	12.70
9	8/28/2011	61.25	72.06	10.81
10	6/22/2011	78.63	71.95	-6.68

NM_DONA_ANA_NAM_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	8/4/2011	62.63	79.85	17.22
2	7/21/2011	56.50	77.24	20.74
3	7/7/2011	64.63	72.94	8.31
4	8/26/2011	58.50	72.54	14.04
5	7/8/2011	64.25	72.30	8.05
6	7/9/2011	59.63	71.30	11.68
7	8/29/2011	55.00	71.04	16.04
8	8/9/2011	54.25	70.77	16.52
9	7/6/2011	53.50	70.76	17.26
10	7/5/2011	55.00	70.74	15.74

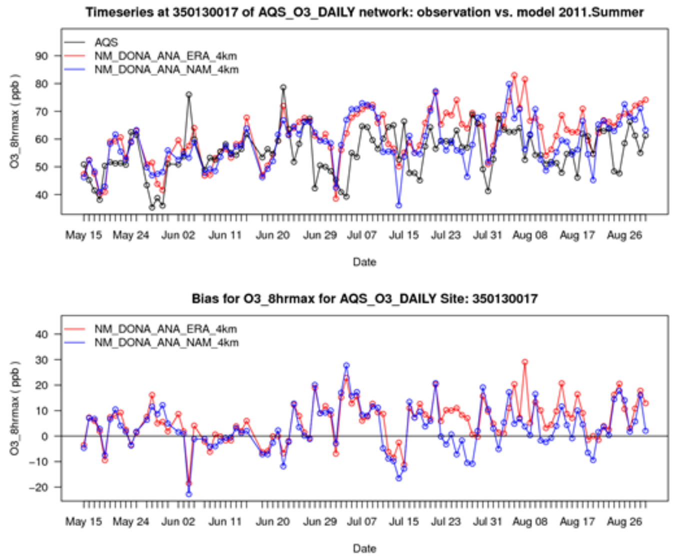


Figure 4-11. Upper (lower) left panel: Ranked list of the 10 days with the highest modeled values of modeled MDA8 ozone (ppb) at the Sunland Park, NM monitor for the CAMx ERA (NAM) run. Also shown are date, observed MDA8 (ppb) and the model bias (ppb). Upper right panel: time series of observed (black) and modeled MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the Sunland Park monitor. Lower right panel: Model bias in MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the Sunland Park monitor.

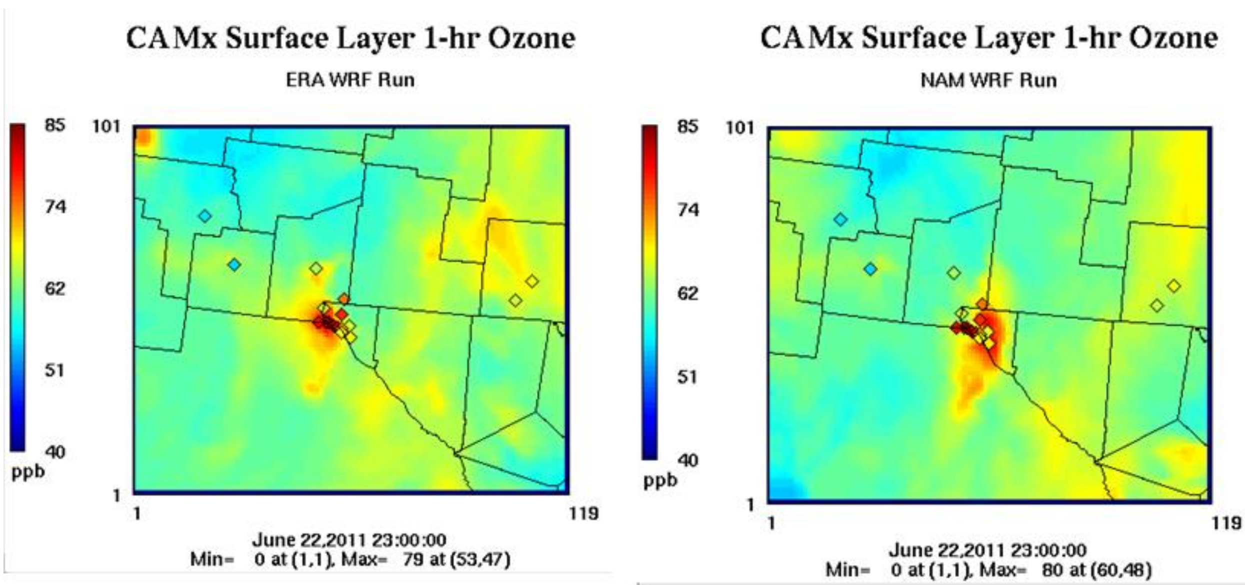


Figure 4-12. CAMx modeled surface layer ozone for June 22, 2011 at 23Z. Left panel: CAMx ERA run, 4 km domain. Right panel: CAMx NAM run, 4 km domain. Filled diamonds indicate surface AQS monitoring sites and their color scale is identical to that of the rest of the plot.

to the time of peak hourly ozone in the observations (Figure 4-13). Both CAMx runs do a reasonably good job of simulating the regional background ozone on June 22, as ozone values at most of the monitors outside the urbanized areas of southeastern Doña Ana and El Paso are well-simulated. The main difference between the simulations is that the CAMx NAM run places the plume of high ozone too far to the east of the cluster of monitors, while the CAMx ERA run captures the region of high observed ozone with greater skill, although still with some low bias. Time series of hourly observed and modeled ozone for the Sunland Park monitor are shown in Figure 4-13. Both CAMx model runs underestimate timing and intensity of peak observed hourly ozone, but do see enhanced ozone on this day.

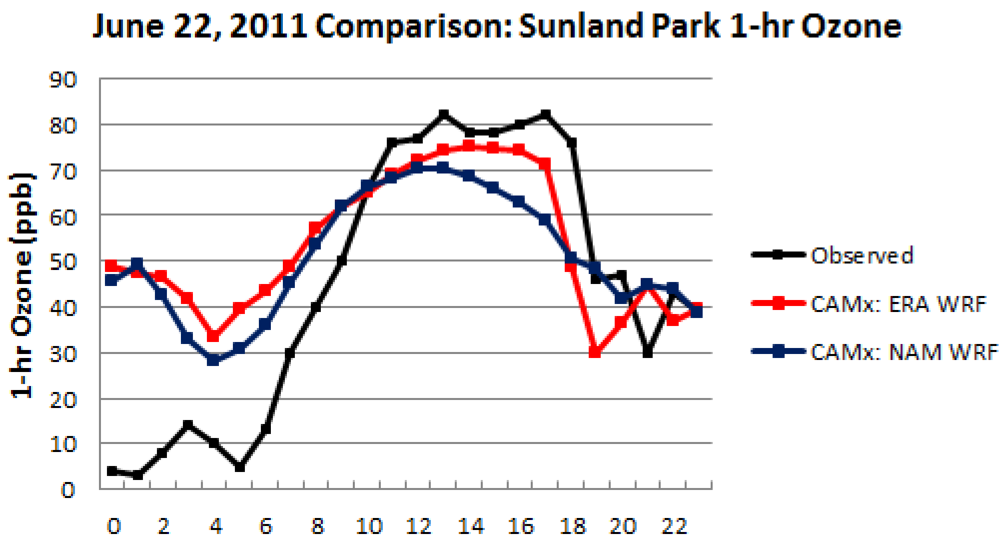


Figure 4-13. June 22 observed 1-hour ozone time series and modeled 1-hour time series for the CAMx NAM and CAMx ERA runs at the Sunland Park monitor in Doña Ana County.

For the CAMx NAM run, 5 of 10 highest modeled MDA8 ozone days occurred during July 5-9. This period was marked by pronounced, regional overestimates in modeled ozone. Figure 4-14 shows an example of a midday period when the model runs overestimated observed ozone. In both CAMx runs, modeled ozone is low across the western portion of the 12 km domain and higher to the east. There is an area of enhanced ozone along the Mexico-Texas border, and the ozone plume from the Carbon II power plant in Coahuila, Mexico is clearly visible. Both model runs overestimate ozone across New Mexico as well as in eastern Arizona and in West Texas. The hourly ozone and bias plots shown in Figure 4-15 confirm that the July and August periods during which most of the 10 highest modeled MDA8 ozone days occurred are periods of high bias for both runs. The high bias is frequently more pronounced in the CAMx ERA run, but on the only high observed MDA8 ozone day that appears in Figure 4-11 (June 22), the CAMx ERA run performs better than the CAMx NAM run, albeit with a low bias.

Figure 4-16 through Figure 4-19 summarize the 10 highest modeled days for the other Doña Ana County monitors. For all of the monitors, the results are similar to those for Desert View and Sunland Park. The 10 highest modeled MDA8 days are nearly always days in July and August that had observed MDA8 ozone well below 70 ppb and were characterized by modeled overestimates of ozone across broad regions of the 4 km and 12 km modeling domains.

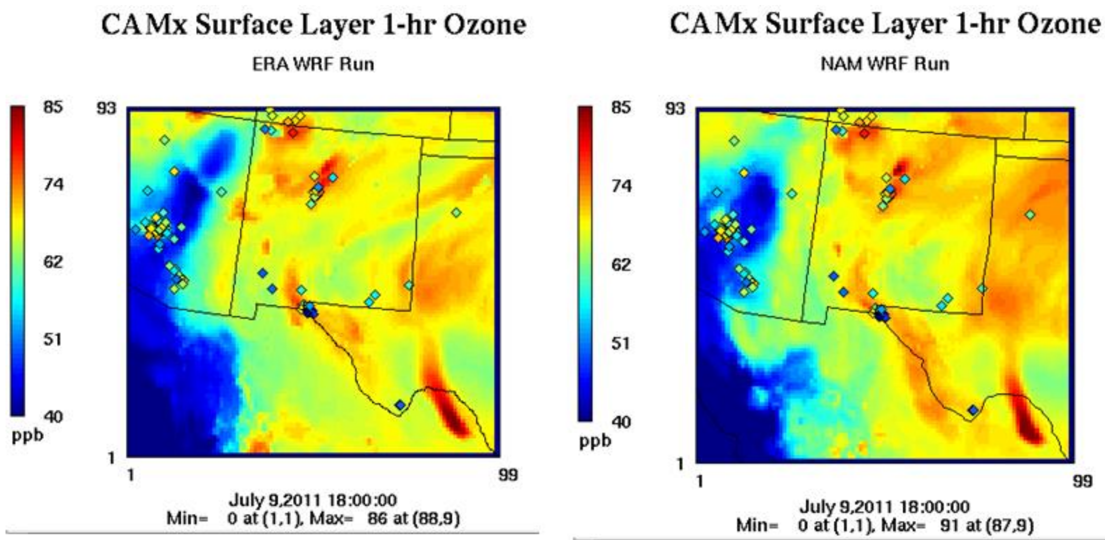


Figure 4-14. CAMx modeled surface layer ozone for July 9, 2011 at 18Z. Left panel: CAMx ERA run, 12 km domain. Right panel: CAMx NAM run, 12 km domain. Filled diamonds indicate surface AQS monitoring sites and their color scale is identical to that of the rest of the plot.

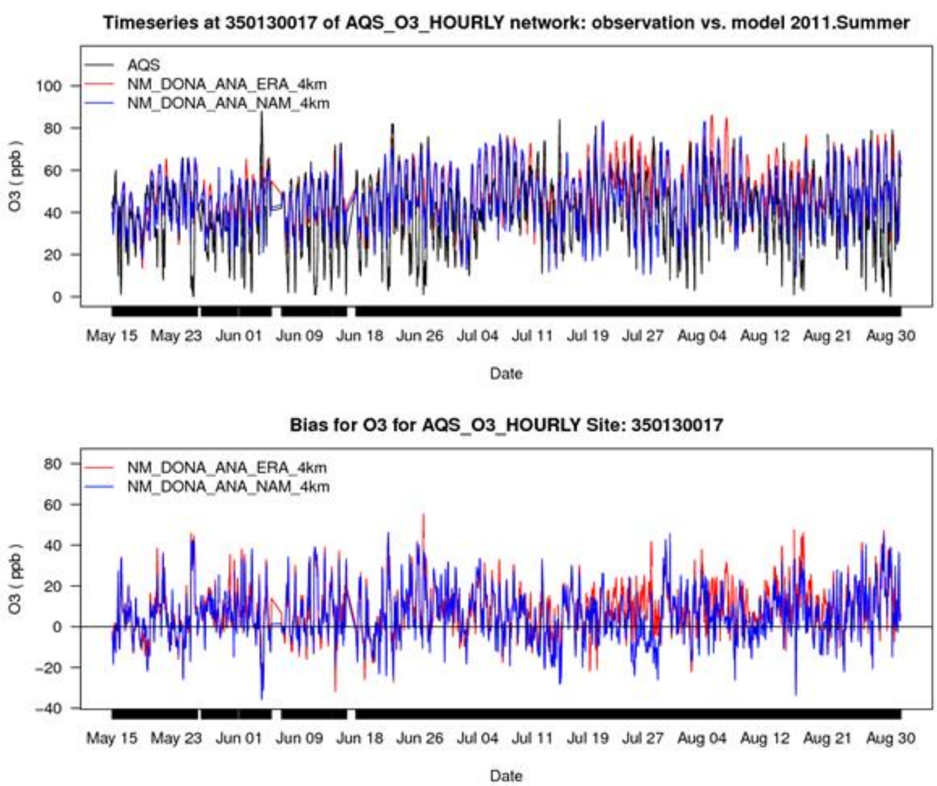


Figure 4-15. Upper panel: observed 1-hour ozone time series and modeled 1-hour time series for the CAMx NAM and CAMx ERA runs at the Sunland Park monitor in Doña Ana County. Lower panel: Model bias for hourly ozone in the CAMx NAM and CAMx ERA runs at the Sunland Park monitor.

NM_DONA_ANA_ERA_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	8/4/2011	68.50	78.86	10.36
2	8/7/2011	53.50	78.37	24.87
3	8/5/2011	59.88	76.03	16.15
4	7/7/2011	67.38	74.74	7.37
5	7/8/2011	64.38	74.17	9.80
6	6/22/2011	78.75	74.15	-4.60
7	7/9/2011	62.38	73.86	11.49
8	7/28/2011	63.75	73.67	9.92
9	7/25/2011	59.00	73.51	14.51
10	8/26/2011	60.88	73.51	12.64

NM_DONA_ANA_NAM_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	7/21/2011	55.75	78.44	22.69
2	8/4/2011	68.50	77.84	9.34
3	8/26/2011	60.88	76.08	15.20
4	7/7/2011	67.38	74.53	7.16
5	7/5/2011	56.50	72.64	16.14
6	7/6/2011	56.50	72.49	15.99
7	7/8/2011	64.38	72.12	7.74
8	7/9/2011	62.38	71.89	9.52
9	8/27/2011	67.25	71.61	4.36
10	7/20/2011	55.83	71.34	15.51

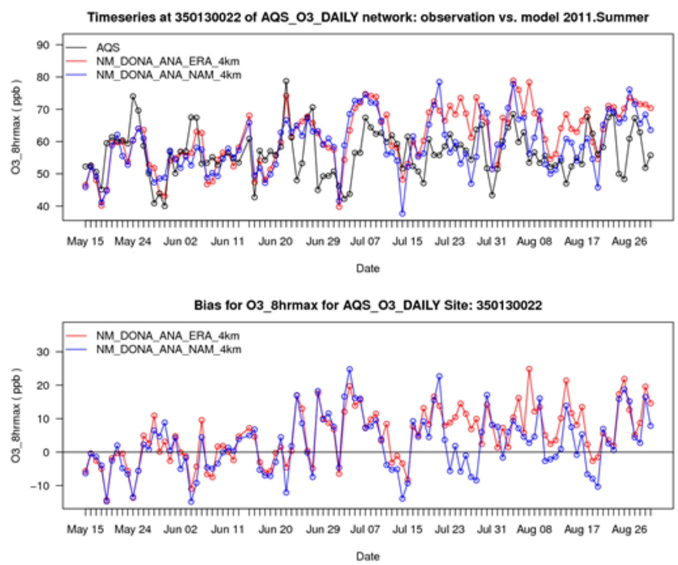


Figure 4-16. Upper (lower) left panel: Ranked list of the 10 days with the highest modeled values of modeled MDA8 ozone (ppb) at the Santa Teresa, NM monitor for the CAMx ERA (NAM) run. Also shown are date, observed MDA8 (ppb) and the model bias (ppb). Upper right panel: time series of observed (black) and modeled MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the Santa Teresa monitor. Lower right panel: Model bias in MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the Santa Teresa monitor.

NM_DONA_ANA_ERA_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	8/5/2011	65.38	83.78	18.41
2	8/29/2011	60.13	82.18	22.05
3	7/26/2011	58.63	78.53	19.90
4	7/27/2011	59.63	76.42	16.80
5	7/22/2011	60.00	73.24	13.24
6	8/4/2011	55.50	73.23	17.73
7	7/25/2011	62.13	72.71	10.59
8	7/21/2011	60.00	72.69	12.69
9	8/7/2011	56.50	71.64	15.14
10	8/16/2011	58.13	70.60	12.48

NM_DONA_ANA_NAM_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	8/29/2011	60.13	80.31	20.18
2	8/5/2011	65.38	79.22	13.85
3	8/4/2011	55.50	73.79	18.29
4	8/28/2011	53.00	73.73	20.73
5	8/26/2011	49.25	71.89	22.64
6	7/29/2011	58.13	69.64	11.51
7	7/23/2011	61.13	69.59	8.46
8	7/5/2011	54.88	69.43	14.56
9	7/20/2011	52.25	69.25	17.00
10	6/24/2011	52.00	68.99	16.99

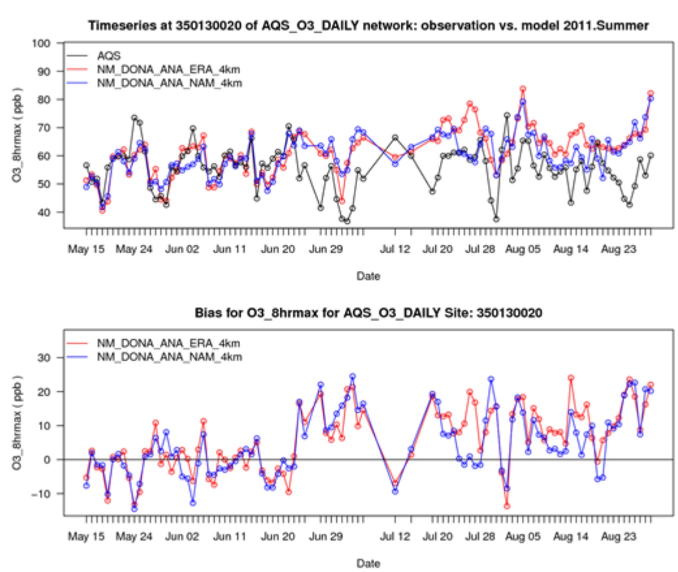
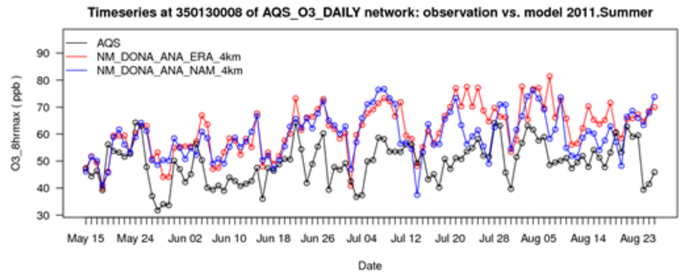


Figure 4-17. Upper (lower) left panel: Ranked list of the 10 days with the highest modeled values of modeled MDA8 ozone (ppb) at the Chaparral, NM monitor for the CAMx ERA (NAM) run. Also shown are date, observed MDA8 (ppb) and the model bias (ppb). Upper right panel: time series of observed (black) and modeled MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the Chaparral monitor. Lower right panel: Model bias in MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the Chaparral monitor.

NM_DONA_ANA_ERA_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	8/7/2011	48.63	81.38	32.75
2	8/2/2011	56.63	77.58	20.96
3	7/23/2011	53.63	77.48	23.85
4	7/25/2011	58.13	77.13	19.01
5	8/5/2011	57.63	77.07	19.45
6	7/21/2011	51.13	77.01	25.88
7	8/4/2011	61.63	76.63	15.01
8	7/8/2011	58.13	73.26	15.14
9	6/22/2011	64.25	73.20	8.95
10	6/27/2011	60.25	72.93	12.68

NM_DONA_ANA_NAM_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	7/8/2011	58.13	76.66	18.54
2	7/7/2011	58.63	76.41	17.79
3	8/4/2011	61.63	76.19	14.56
4	8/3/2011	63.00	73.96	10.96
5	8/26/2011	45.88	73.81	27.93
6	8/9/2011	50.13	73.57	23.44
7	7/21/2011	51.13	73.31	22.18
8	7/9/2011	53.50	73.27	19.77
9	8/5/2011	57.63	73.15	15.53
10	6/27/2011	60.25	72.13	11.88



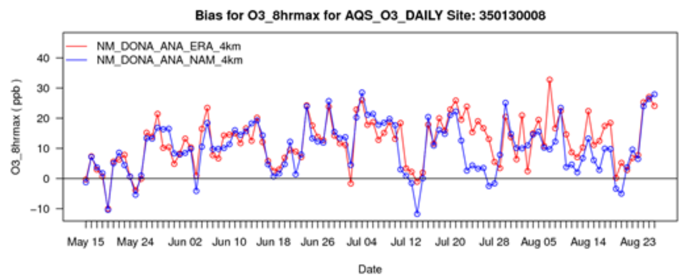
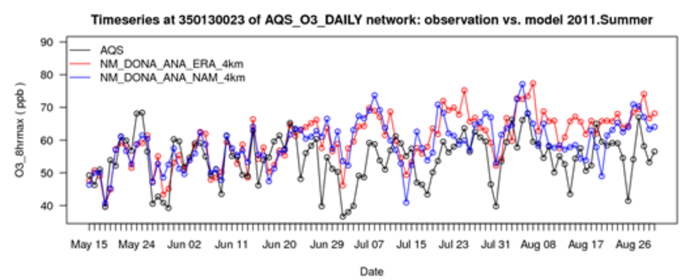


Figure 4-18. Upper (lower) left panel: Ranked list of the 10 days with the highest modeled values of modeled MDA8 ozone (ppb) at the La Union, NM monitor for the CAMx ERA (NAM) run. Also shown are date, observed MDA8 (ppb) and the model bias (ppb). Upper right panel: time series of observed (black) and modeled MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the La Union monitor. Lower right panel: Model bias in MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the La Union monitor.

NM_DONA_ANA_ERA_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	8/7/2011	48.63	81.38	32.75
2	8/2/2011	56.63	77.58	20.96
3	7/23/2011	53.63	77.48	23.85
4	7/25/2011	58.13	77.13	19.01
5	8/5/2011	57.63	77.07	19.45
6	7/21/2011	51.13	77.01	25.88
7	8/4/2011	61.63	76.63	15.01
8	7/8/2011	58.13	73.26	15.14
9	6/22/2011	64.25	73.20	8.95
10	6/27/2011	60.25	72.93	12.68

NM_DONA_ANA_NAM_4km				
Rank	Date	Obs_Average	Model_Average	Bias_Average
1	7/8/2011	58.13	76.66	18.54
2	7/7/2011	58.63	76.41	17.79
3	8/4/2011	61.63	76.19	14.56
4	8/3/2011	63.00	73.96	10.96
5	8/26/2011	45.88	73.81	27.93
6	8/9/2011	50.13	73.57	23.44
7	7/21/2011	51.13	73.31	22.18
8	7/9/2011	53.50	73.27	19.77
9	8/5/2011	57.63	73.15	15.53
10	6/27/2011	60.25	72.13	11.88



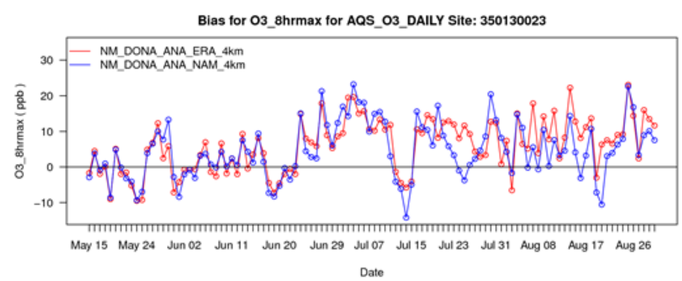


Figure 4-19. Upper (lower) left panel: Ranked list of the 10 days with the highest modeled values of modeled MDA8 ozone (ppb) at the Solano, NM monitor for the CAMx ERA (NAM) run. Also shown are date, observed MDA8 (ppb) and the model bias (ppb). Upper right panel: time series of observed (black) and modeled MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the Solano monitor. Lower right panel: Model bias in MDA8 ozone for the CAMx ERA (red) and CAMx NAM (blue) runs at the Solano monitor.

We summarize CAMx ERA and CAMx NAM model performance on the 10 highest modeled MDA8 ozone days at Doña Ana County monitors in Figure 4-20. The CAMx ERA run has slightly lower bias overall, but both runs consistently overestimate ozone on the 10 highest modeled days. Observed MDA8 ozone values are higher on the 10 highest modeled days using the ERA CAMx run.

Average Bias in MDA8 on 10 Highest Modeled MDA8 days (ppb)		
Monitor	CAMx: NAM WRF	CAMx: ERA WRF
Desert View	11.7	10.2
Sunland Park	14.6	13.9
La Union	18.3	19.4
Chapparal	16.4	15.9
Santa Teresa	12.4	11.3
Solano	12.1	11.0

Average Observed Value on 10 Highest Modeled Days (ppb)		
Monitor	CAMx: NAM WRF	CAMx: ERA WRF
Desert View	62.4	65.5
Sunland Park	58.4	61.3
La Union	56.0	57.0
Chapparal	56.2	59.6
Santa Teresa	61.5	63.8
Solano	58.9	61.7

Figure 4-20. Summary of CAMx ERA and CAMx NAM model performance on 10 highest modeled MDA8 days at Doña Ana County monitors. Left panel: average bias on the 10 highest modeled days. Right panel: average observed MDA8 value on the 10 highest modeled MDA8 days at Doña Ana County monitors.

For both CAMx runs, 10 highest MDA8 ozone days that will form the RRF for Doña Ana County monitors have significant regional overestimates of ozone, and most of the 10 highest modeled MDA8 ozone days did not have high observed ozone. It is therefore uncertain whether either model run will provide useful results for analyzing local emissions control strategies for Doña Ana County using the EPA MATS default RRF method. Local controls will not be predicted to reduce Dona Ana County ozone if the RRF is formed from days when modeled ozone is driven by an overestimated regional background.

Therefore, we propose to use an ozone model performance criterion in selecting days for making RRFs and DVF projections and using this procedure to determine whether the CAMx NAM or CAMx ERA run should be used as the 2011 base case in the SNMOS. We propose to use only modeled days in which the observed and modeled MDA8 ozone are within a specified % bias of each other. We will therefore form RRFs based on more days with observed high ozone and better model performance. Days on which the model performed poorly would not be used in the RRF. There are precedents for using an MPE filter in selecting days for use in RRFs in making future year ozone projections including modeling done in California (e.g. SCAQMD AQMP[2]).

To illustrate the procedure, we apply a ±10% bias criterion to the 10 highest modeled MDA8 ozone days at the Desert View monitor. If we were to apply the default MATS method to calculate the RRF, the days shaded in blue in Figure 4-21 would be selected. Only one of the top

[2] http://www.aqmd.gov/docs/default-source/clean-air-plans/air-quality-management-plans/2012-air-quality-management-plan/final-2012-aqmp-(february-2013)/appendix-v-final-2012.pdf

10 observed MDA8 ozone days (shaded yellow) at the Desert View monitor would be included using this method.

		MDA8 (ppb)		Bias	
Rank	Date	Observed	Modeled	(ppb)	(%)
1	8/5/2011	65.125	81.966	16.841	25.86%
2	8/7/2011	55	81.433	26.433	48.06%
3	7/21/2011	58.125	75.839	17.714	30.48%
4	8/4/2011	67.875	75.785	7.91	11.65%
5	6/22/2011	81.75	74.447	-7.303	-8.93%
6	7/9/2011	64.125	73.708	9.583	14.94%
7	7/20/2011	65.5	73.573	8.073	12.33%
8	7/25/2011	64.625	73.442	8.817	13.64%
9	7/8/2011	68	73.339	5.339	7.85%
10	8/30/2011	65.125	73.307	8.182	12.56%

Top 10 observed MDA8 days

Top 10 modeled MDA8 days

Figure 4-21. Desert View: default MATS method for selecting 10 highest modeled days for the RRF.

		MDA8 (ppb)		Bias	
Rank	Date	Observed	Modeled	(ppb)	(%)
1	6/22/2011	81.75	74.447	-7.303	-8.93%
2	7/8/2011	68	73.339	5.339	7.85%
3	8/28/2011	69.125	72.483	3.358	4.86%
4	7/28/2011	72	71.9	-0.1	-0.14%
5	8/18/2011	66	71.665	5.665	8.58%
6	8/27/2011	73.375	70.966	-2.409	-3.28%
7	8/6/2011	66.375	70.191	3.816	5.75%
8	8/2/2011	68	69.984	1.984	2.92%
9	6/26/2011	68.75	68.794	0.044	0.06%
10	8/22/2011	67.5	68.517	1.017	1.51%

Top 10 observed MDA8 days

Top 10 modeled MDA8 days

Figure 4-22. Desert View: alternate method for selecting 10 highest modeled days for the RRF.

If we select only the top 10 modeled MDA8 ozone days on which the bias was < ±10%, we obtain a different population of days (Figure 4-22). The 10 days to be used in the RRF now include 4 of the 10 highest observed days at Desert View, and model performance is reasonably good on all days that would go into the RRF. Observed and modeled MDA8 values are now closer to the observed base year design value than would be the case using the default MATS method shown in Figure 4-21.

We tested this procedure using bias thresholds ranging from 5% to 20% for the CAMx ERA and CAMx NAM runs. For each bias threshold, we determined the number of modeled MDA8 ozone days in the RRF (top 10 days) that were also among the 10 highest observed MDA8 ozone days. The results are shown in Figure 4-23. For all values of the bias threshold, using the CAMx ERA run produced a higher number of days in the ranked list of the 10 highest modeled MDA8 ozone days that also corresponded to days that were among the top 10 observed MDA8 ozone days at the Doña Ana County monitors. Therefore, the CAMx ERA run is better suited for making future year ozone projections and for emissions control strategy development. The bias threshold that produced the highest number of top 10 observed MDA8 ozone days in the list of 10 highest modeled MDA8 ozone days was the 10% threshold, and we recommend that this threshold be used in making future year ozone projections in the SNMOS.

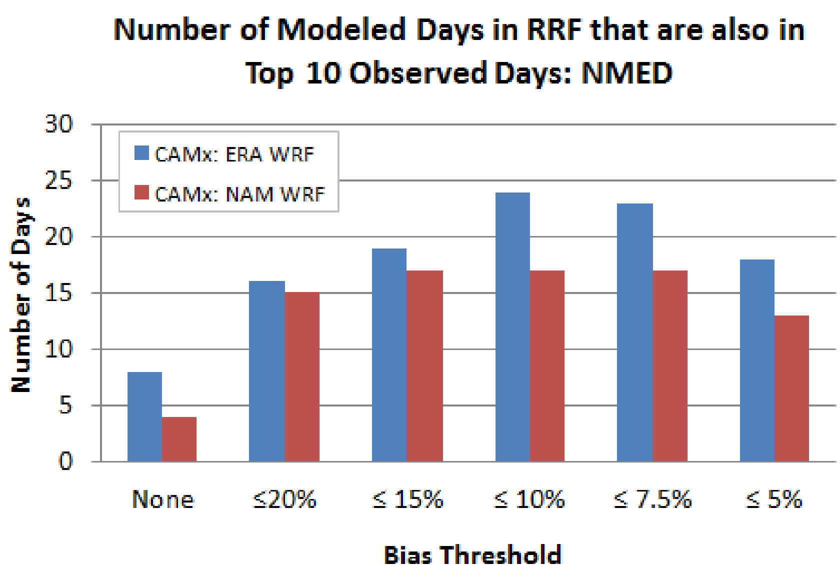


Figure 4-23. Comparison of bias thresholds for CAMx ERA and CAMx NAM runs

4.3 Summary of Ozone Model Performance

CAMx base year modeling of 2011 has been completed and model performance evaluated on the 12/4 km domains for two CAMx runs that used different meteorological inputs. For both CAMx runs, model performance for MDA8 ozone was acceptable based on comparison with EPA statistical performance benchmarks.

In both runs, CAMx had an overall high bias when all days were considered, but underestimated ozone on days with observed MDA8 ozone > 60 ppb. The CAMx run using ERA WRF meteorology performed slightly better than CAMx with NAM WRF meteorology when MDA8 ozone > 60 ppb. The CAMx NAM run performed slightly better when all days were considered.

For both CAMx runs, many of the 10 highest MDA8 ozone days that would be used to form an RRF for future year design value projections for Doña Ana County monitors have significant region-wide overestimates of ozone. Most of the 10 highest modeled MDA8 days did not have high observed MDA8 ozone. Future year projections based on these days would therefore not be useful for evaluating the impacts of local emissions control strategies in Doña Ana County.

We proposed an alternate method of making future year projections in which the model RRF is developed using a model performance criterion that selects only days when modeled ozone is high and model performance is within acceptable bias limits. This procedure produces a set of 10 days for the RRF that includes more of the 10 highest observed MDA8 ozone days than would the default MATS procedure of simply using the 10 highest modeled MDA8 ozone days. When this alternate procedure for developing RRFs is used, the CAMx ERA run has more of 10 highest observed days corresponding to high modeled MDA8 ozone days in the calculated RRF. In a perfect model run, the 10 highest model days would correspond to the 10 highest observed days, so we select the run that comes closest to this ideal.

We therefore select the CAMx ERA run as the SNMOS 2011 base year run due to its better performance within the 4 km and 12 km domain on days where observed MDA8 ozone > 60 ppb as well as the fact that RRFs formed with this run will have a better correspondence between high modeled and high observed MDA8 days.

4.4 Model Performance Evaluation for Ozone Precursors

We evaluated model performance in the CAMx ERA run for ozone precursor species CO and NO_2. The selection of species was based on data availability and completeness within AMET for the SNMOS episode.

A summary of the statistical evaluation of performance on the 4 km and 12 km domains is shown in Table 4-3 and Table 4-4, respectively. On the 4 km domain, the CAMx ERA run has a slight negative bias for NO_2 overall. Inspection of the spatial distribution of NO_2 FB by site (Figure 4-24) shows that sites within and near Doña Ana County had small positive or somewhat larger negative biases for NO_2. The same is true on the 12 km grid (Figure 4-25). Outside Doña Ana County and El Paso, NO_2 performance for FB was mixed, with positive and negative biases that were sometimes large (exceeding ±50%) depending on the site. The NO_2 performance showed large values of FE and NME. We note that NO_2 monitors are often influenced by local sources whose plumes are not well resolved at the model grid scale.

Table 4-3. 4 km domain NO_2 and CO performance indicators for the CAMx ERA run.

Species	Network	FB	FE	MB	ME	NMB	NME	R^2	RMSE
	Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)		(ppb)
NO_2	AQS Hourly	-13.3	80.1	-0.1	5.01	-1.62	81.4	0.19	7.79
CO	AQS Hourly	22.9	62.4	27.1	119	17.2	75.3	0.08	158

Table 4-4. 12 km domain NO_2 and CO performance indicators for the CAMx ERA run.

Species	Network	FB	FE	MB	ME	NMB	NME	R^2	RMSE
	Units	(%)	(%)	(ppb)	(ppb)	(%)	(%)		(ppb)
NO_2	AQS Hourly	-19.4	78.3	0.736	5.86	9.42	75.1	0.33	8.99
CO	AQS Hourly	4.01	56.3	-12.9	124	-6.26	60.2	0.08	175

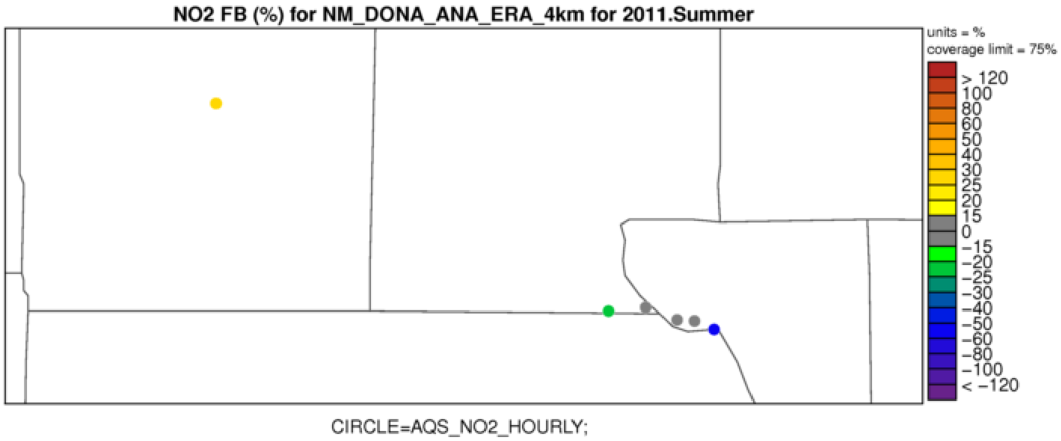


Figure 4-24. Spatial distribution of NO_2 fractional bias (%) within the 4 km grid.

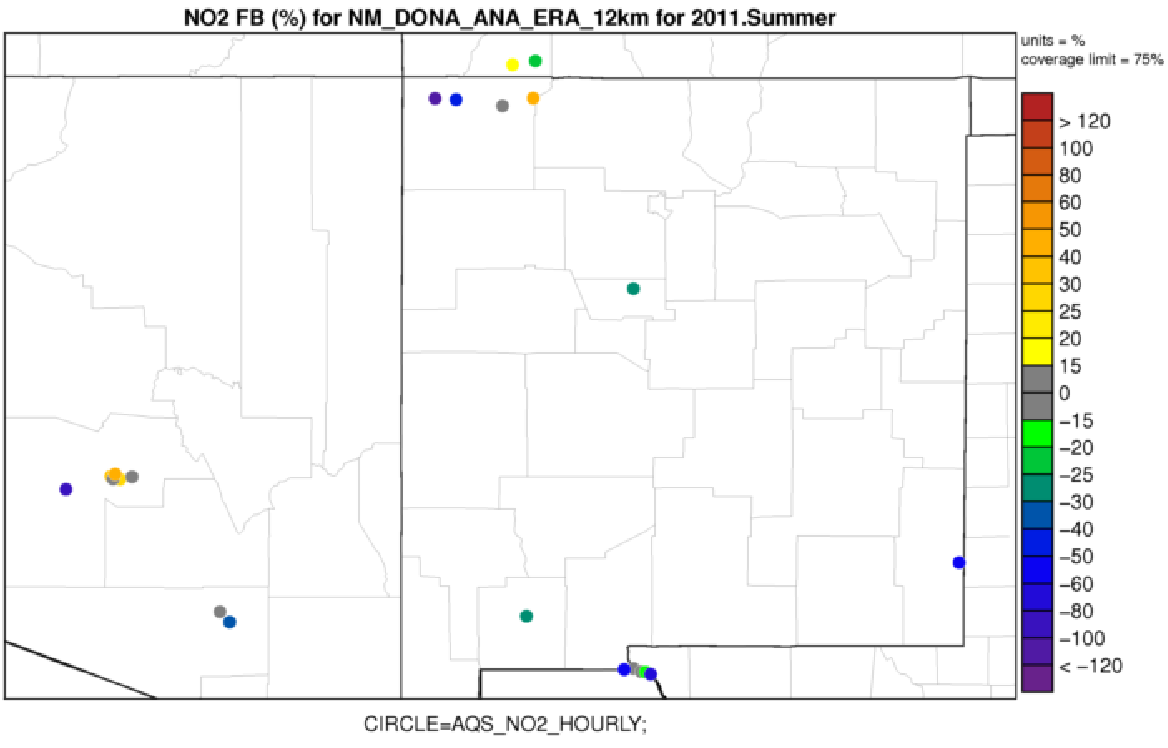


Figure 4-25. Spatial distribution of NO_2 fractional bias (%) within the 12 km grid.

Similar to NO_2, the CO performance in the CAMx ERA run was mixed across the 12 km and 4 km domains. The episode average statistical metrics shown in Table 4-3 and Table 4-4 show reasonably good performance for CO bias statistics, and much larger values of error metric as well as low values of R^2 indicating low levels of correspondence between the observed and modeled CO values. The spatial plots of CO FB (Figure 4-26, Figure 4-27) show no clear tendency toward domain-wide over- or under-prediction and reasonably good performance in the Doña Ana County. We conclude that NO_2 and CO performance are typical of simulations of

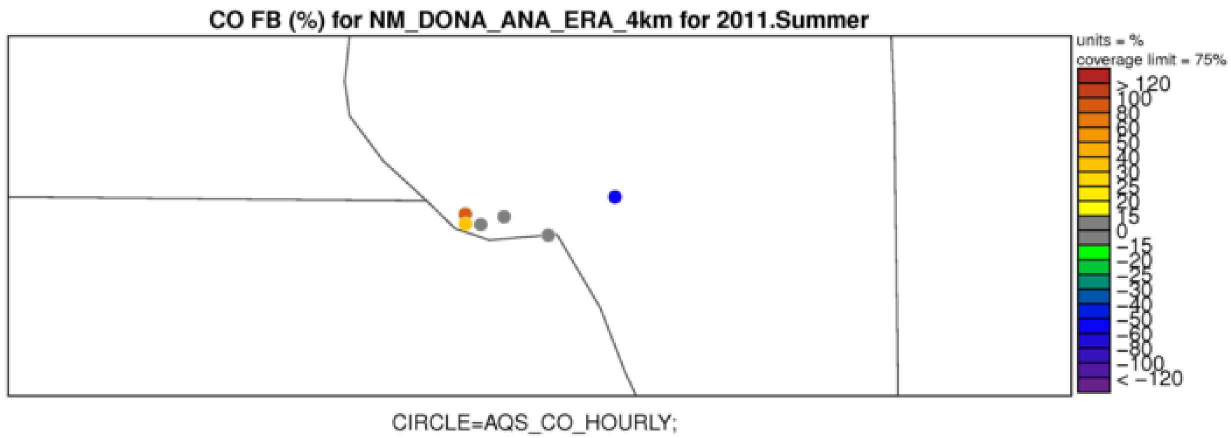


Figure 4-26. Spatial distribution of CO fractional bias (%) within the 4 km grid.

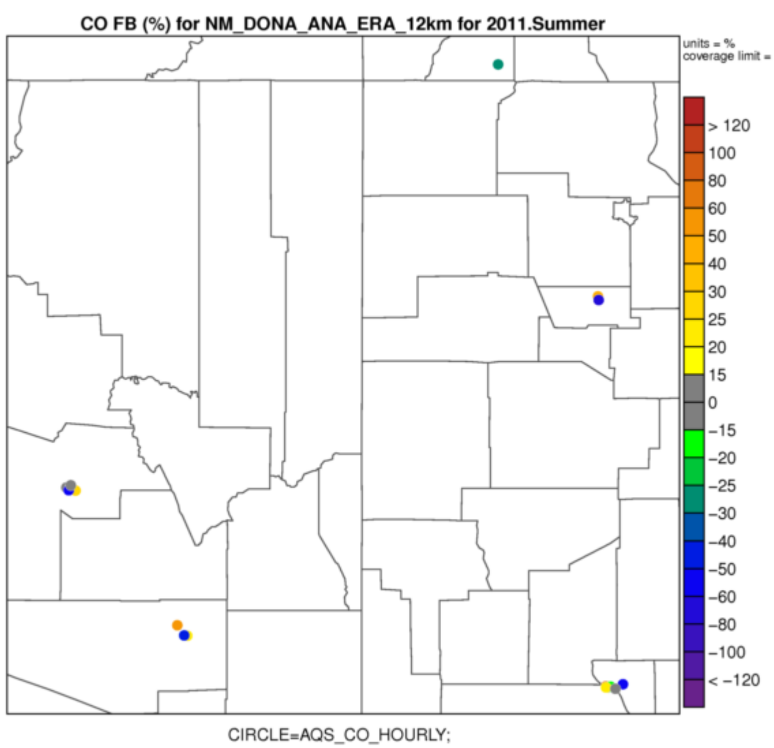


Figure 4-27. Spatial distribution of CO fractional bias (%) within the 12 km grid.

the Western U.S. and are comparable to performance observed in the WAQS 2011b modeling (Adelman et al., 2016) and the 3SAQS study (Adelman et al., 2015b). We conclude that model performance for ozone precursors NO_2 and CO is adequate for the SNMOS in the CAMx ERA run.

5.0 MODEL PERFORMANCE EVALUATION FOR PARTICULATE MATTER

Table 5-1 and Table 5-2 summarize episode average particulate matter (PM) performance by monitoring network at all sites in the 4 km and 12 km SNMOS modeling domains, respectively, for the CAMx ERA run. These results show that on annual domain-wide basis, CAMx misses the PM performance criteria for bias (≤ ±60%) on the 4 km grid for NO_3, NH_4, and $PM_{2.5}$ and misses the error (≤ ±75%) criteria NO_3 and NH_4. On the 12 km domain, CAMx misses the PM performance criteria for bias (≤ ±60%) and error (≤ ±75%) for NO_3 and NH_4.

Table 5-1. 4 km modeling domain Particulate Matter species performance indicators.

Species	Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod	RMSE	R^2
	Units	(%)	(%)	(µg/m³)	(µg/m³)	(%)	(%)	(µg/m³)	(µg/m³)	(µg/m³)	
SO_4	IMPROVE	-24.5	37.4	-0.27	0.40	-21.8	32.8	1.23	0.96	0.61	0.27
	CSN	-24.9	35	-0.23	0.34	-18.9	28	1.23	1.00	0.44	0.53
NO_3	IMPROVE	-190	190	-0.20	0.20	-94.1	94.1	0.22	0.01	0.25	0.10
	CSN	-184	186	-0.25	0.26	-89.9	93.7	0.28	0.03	0.28	0.12
EC	IMPROVE	-14.4	50.1	-0.01	0.07	-5.1	49.7	0.14	0.14	0.16	0.56
	CSN	-9.47	29.7	-0.08	0.15	-17.4	30.9	0.48	0.40	0.24	0.38
OC	IMPROVE	-42.8	65.3	-0.50	0.69	-41.8	57.9	1.20	0.70	1.12	0.19
	CSN	-32.9	54.6	-0.68	0.98	-37.4	53.7	1.82	1.14	1.55	0.00
NH_4	IMPROVE	-80	80.5	-0.29	0.30	-56.2	56.5	0.52	0.23	0.37	0.15
	CSN	-54.3	66.4	-0.16	0.20	-37.7	46.2	0.43	0.27	0.24	0.33
$PM_{2.5}$	IMPROVE	-71.3	72.7	-3.97	4.03	-55	55.9	7.22	3.25	5.24	0.04
	CSN	-69.9	71.1	-5.64	5.73	-53.7	54.5	10.50	4.87	6.96	0.02
TC	IMPROVE	-38.8	59.9	-0.51	0.71	-37.9	53.3	1.34	0.83	1.16	0.35
	CSN	-28.3	45.6	-0.77	1.07	-33.2	46.5	2.30	1.54	1.75	0.03

Table 5-2. 12 km modeling domain Particulate Matter species performance indicators.

Species	Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod	RMSE	R^2
	Units	(%)	(%)	(µg/m³)	(µg/m³)	(%)	(%)	(µg/m³)	(µg/m³)	(µg/m³)	
SO_4	IMPROVE	-20.9	40.1	-0.24	0.37	-25.2	39.4	0.94	0.71	0.52	0.26
	CSN	-28.3	44.1	-0.32	0.44	-28.1	38.6	1.14	0.82	0.57	0.20
NO_3	IMPROVE	-177	180	-0.17	0.17	-86.7	91	0.19	0.03	0.22	0.07
	CSN	-172	175	-0.23	0.25	-83.1	89	0.28	0.05	0.28	0.11
EC	IMPROVE	14.2	56.9	0.09	0.19	59.2	122	0.15	0.25	1.03	0.12

Species	Network	FB	FE	MB	ME	NMB	NME	Mean Obs	Mean Mod	RMSE	R^2
	Units	(%)	(%)	(µg/m³)	(µg/m³)	(%)	(%)	(µg/m³)	(µg/m³)	(µg/m³)	
	CSN	42.5	69.9	0.19	0.35	53.1	97.9	0.35	0.54	0.47	0.00
OC	IMPROVE	-14	55.6	-0.28	0.74	-25.8	68.8	1.07	0.80	2.46	0.08
	CSN	-2.67	45.2	-0.29	0.90	-17.5	53.9	1.66	1.37	2.01	0.00
NH_4	IMPROVE	-86.3	88.3	-0.25	0.26	-62.2	63.3	0.41	0.16	0.34	0.07
	CSN	-71.2	85.5	-0.19	0.23	-50.3	60.9	0.38	0.19	0.29	0.03
$PM_{2.5}$	IMPROVE	-53.6	60.9	-2.76	3.33	-45.9	55.4	6.00	3.25	5.68	0.07
	CSN	-25.9	48.6	-2.87	4.13	-32.8	47.1	8.77	5.90	6.66	0.00
TC	IMPROVE	-8.94	53	-0.19	0.89	-15.2	72.1	1.23	1.04	3.20	0.09
	CSN	7.51	49.2	-0.10	1.20	-5.18	59.3	2.02	1.91	2.32	0.00

Additional analyses of the spatial patterns in the CAMx PM model performance for the SNMOS base 2011 simulation are shown in this section. Model performance for SO_4 falls within the PM performance goals for bias (≤ ±30%) and error (≤ ±50%) on both the 4 km and 12 km grids (Table 5-1 and Table 5-2). The spatial distribution for FB in the 4 km and 12 km domains is shown in Figure 5-1 and Figure 5-2, respectively. The CAMx ERA run underestimates SO_4 at most sites across the 4 km and 12 km domains, but is within the performance goal for bias at all sites in the 4 km domain and all sites in the 12 km domain except the Great Sand Dune IMPROVE site in Colorado.

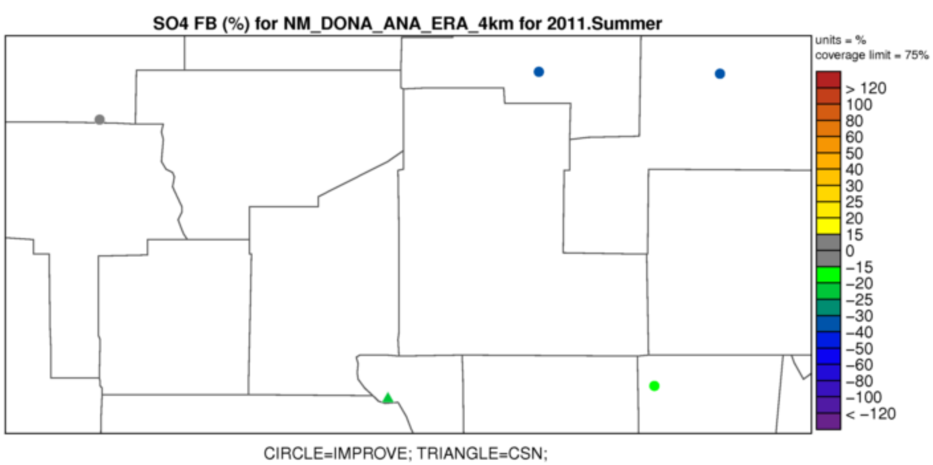


Figure 5-1. Spatial distribution of SO_4 fractional bias (%) within the 4 km grid.

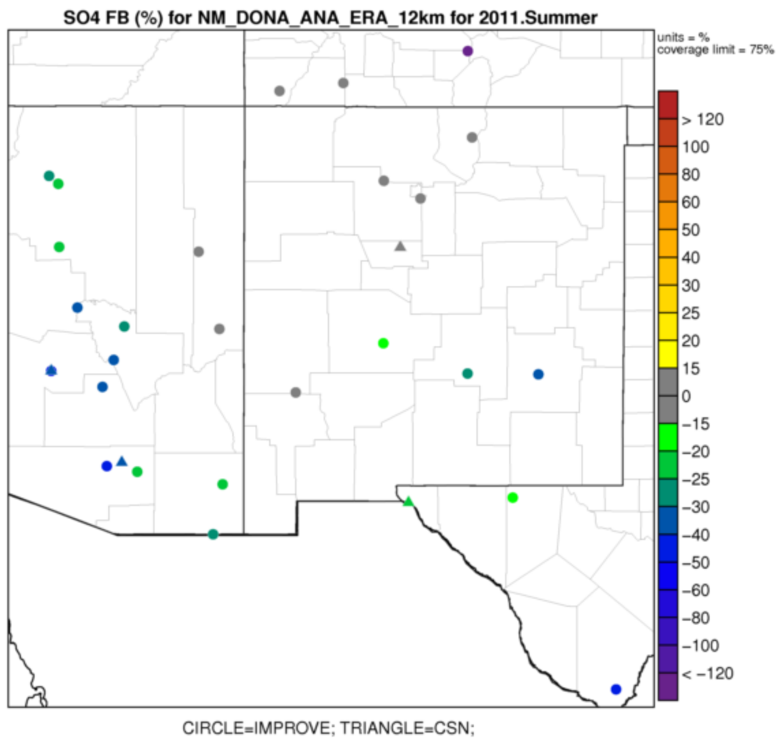


Figure 5-2. Spatial distribution of SO_4 fractional bias (%) within the 12 km grid.

The spatial plots of NH_4 FB on the 4 km and 12 km domains show a large underestimate of NH_4 at nearly all sites (Figure 5-3 and Figure 5-4) and the same is true for NO_3 (Figure 5-5 and Figure 5-6).

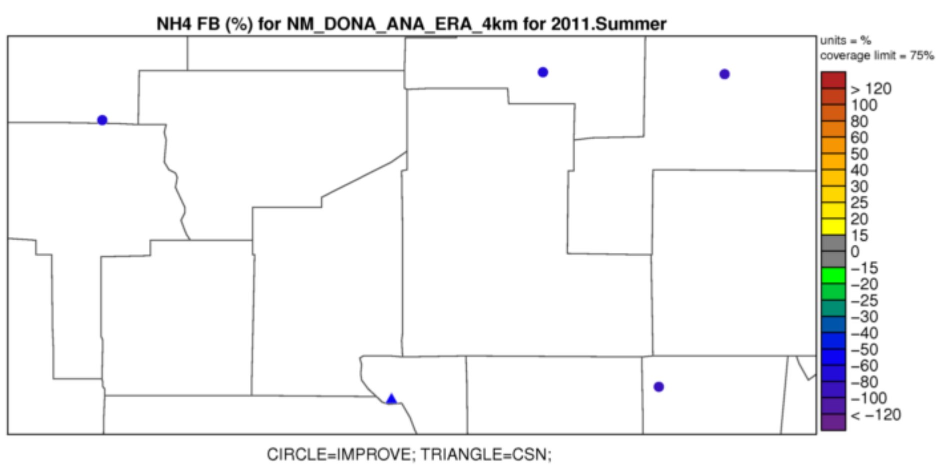


Figure 5-3. Spatial distribution of NH_4 fractional bias (%) within the 4 km grid.

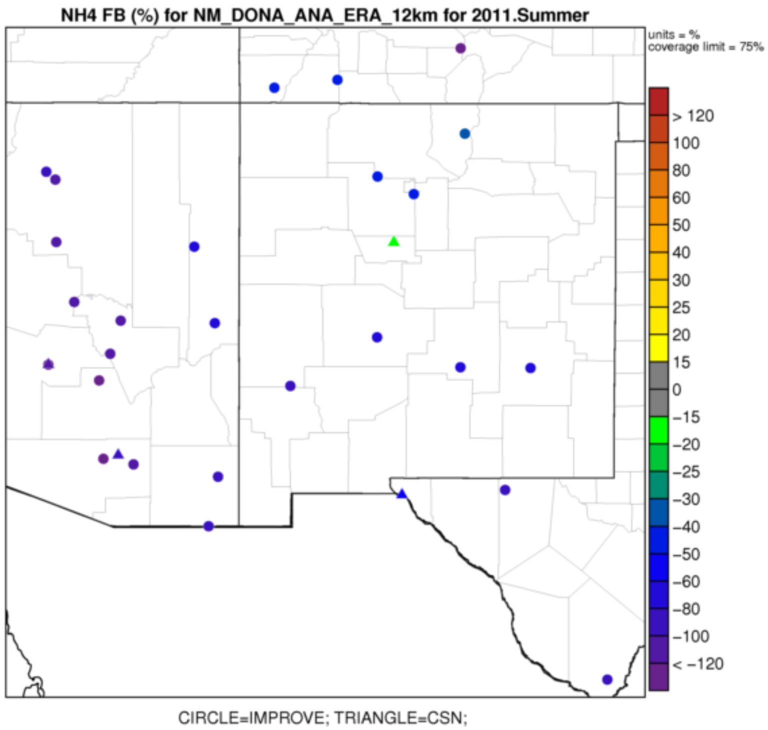


Figure 5-4. Spatial distribution of NH_4 fractional bias (%) within the 12 km grid.

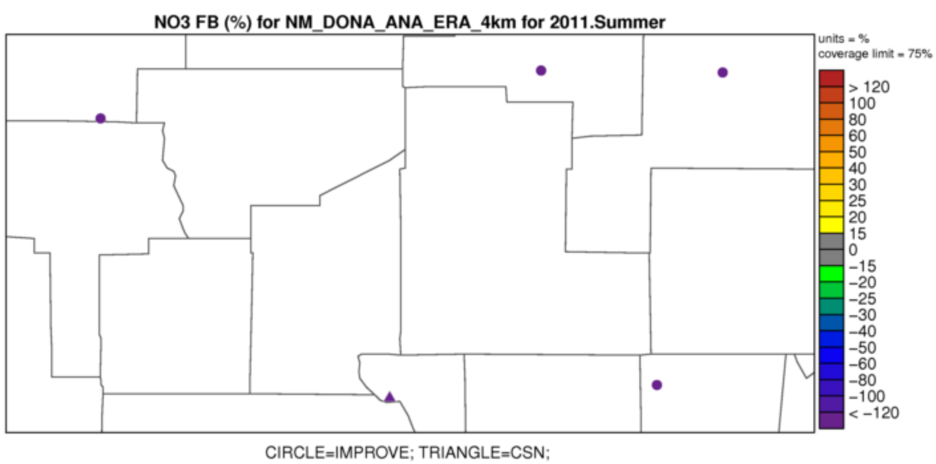


Figure 5-5. Spatial distribution of NO_3 fractional bias (%) within the 4 km grid.

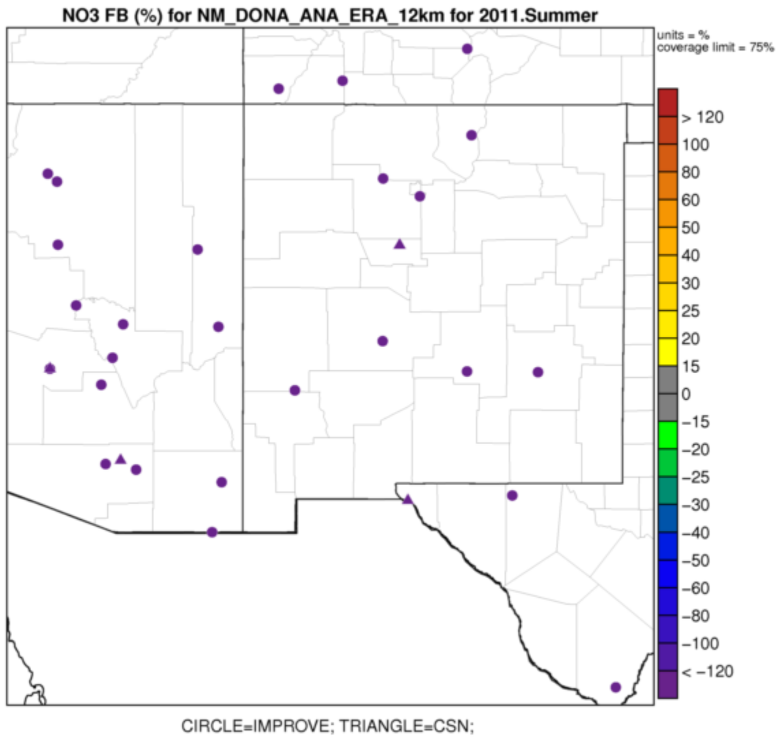


Figure 5-6. Spatial distribution of NO_3 fractional bias (%) within the 12 km grid.

For EC, the model performs well on the 4 km domain, with FB meeting the PM performance goal of FB < ±15% for all sites (Figure 5-7). On the 12 km domain (Figure 5-8), performance within New Mexico is good, with all sites meeting the PM performance goals; however, outside New Mexico, model performance is mixed. There are sites in Arizona and Colorado for which the FB exceeds the PM performance criteria. This is likely related to the intense fire activity during this model episode.

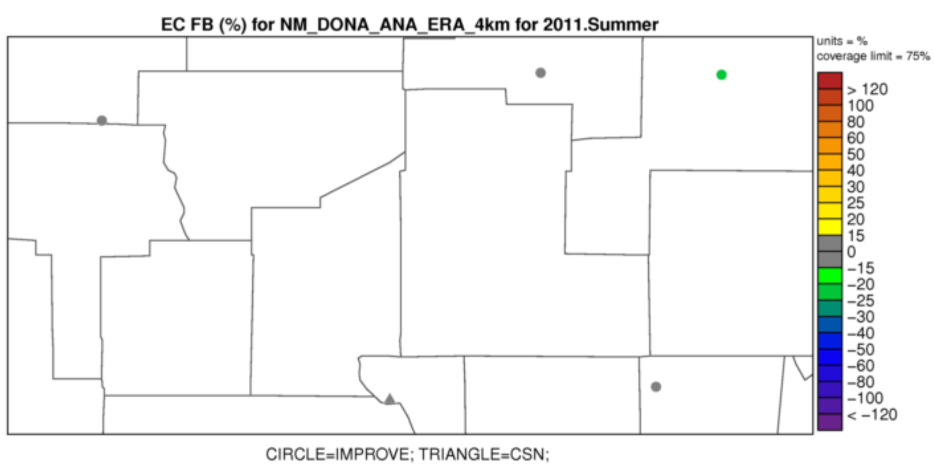


Figure 5-7. Spatial distribution of EC fractional bias (%) within the 4 km grid.

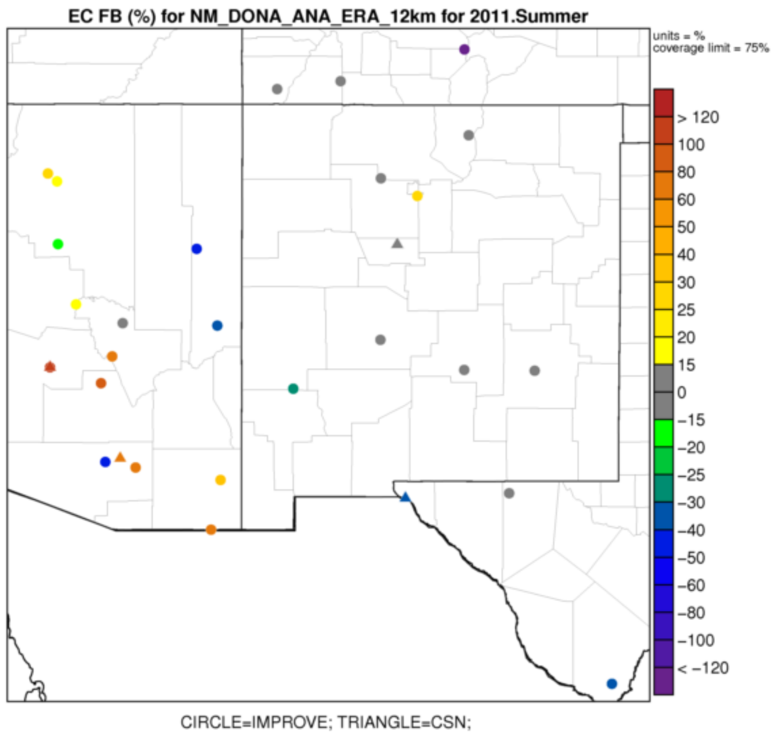


Figure 5-8. Spatial distribution of EC fractional bias (%) within the 12 km grid.

OC performance for FB on the 4 km grid showed an underestimate of OC at all sites (Figure 5-9). Across the 12 km domain (Figure 5-10), the model also underestimated OC at most sites except those in Arizona that also had a strong positive EC bias. Model errors in simulating EC and OC in the vicinity of large fires reflect uncertainty in emissions from fires as well as in the model's simulation of the fire plume and the chemical evolution of emitted species within the plume as it travels away from the active fire location.

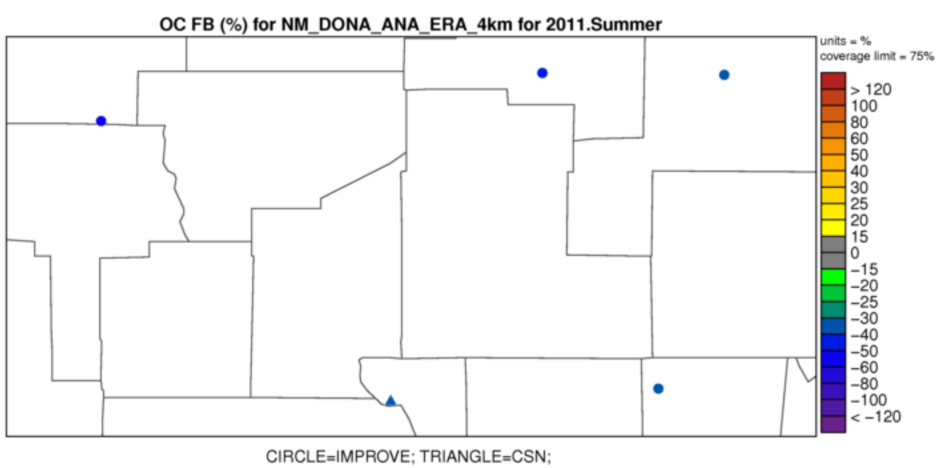


Figure 5-9. Spatial distribution of OC fractional bias (%) within the 4 km grid.

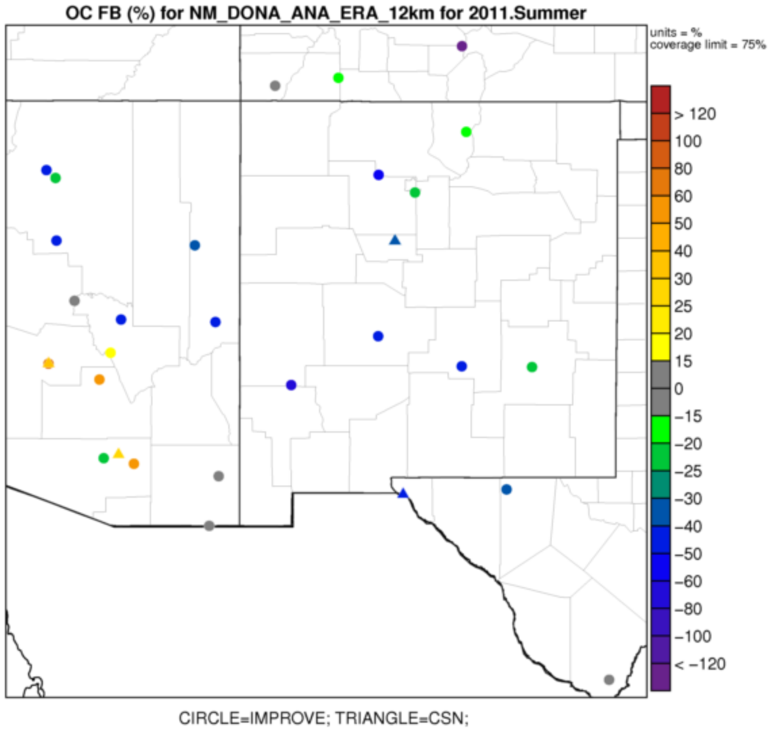


Figure 5-10. Spatial distribution of OC fractional bias (%) within the 12 km grid.

The spatial distribution of FB in total $PM_{2.5}$ across the 4 km and 12 km domains is shown in Figure 5-11 and Figure 5-12, respectively. Given the underestimate in many of the component species of $PM_{2.5}$ across the two modeling domains, it is not surprising that total $PM_{2.5}$ is consistently underestimated across the 4 km and 12 km domains. Several sites in both domains exceed the PM performance criteria for FB. Performance indicators for $PM_{2.5}$ in the SNMOS were roughly comparable to the $PM_{2.5}$ indicators for the WAQS and 3SAQS.

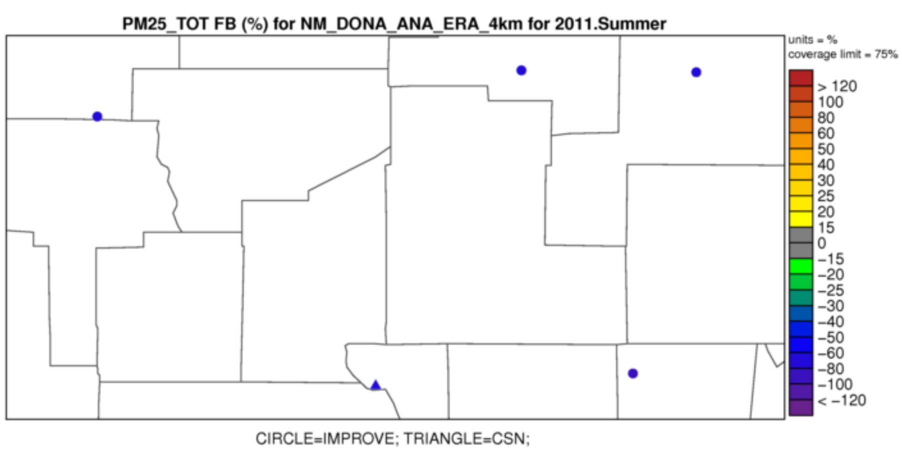


Figure 5-11. Spatial distribution of $PM_{2.5}$ fractional bias (%) within the 4 km grid.

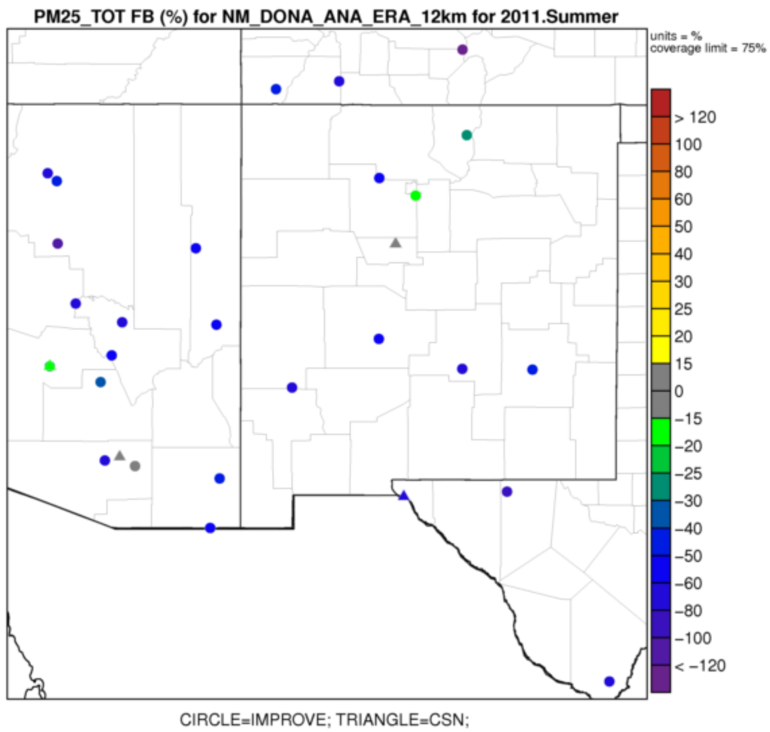


Figure 5-12. Spatial distribution of $PM_{2.5}$ fractional bias (%) within the 12 km grid.

While there are shortcomings in model performance for the CAMx ERA simulation of $PM_{2.5}$ and its component species, performance is similar to that of other similar studies in the western U.S. PM performance is not the main focus of this study, and so no effort was expended to try to diagnose and improve model performance for PM. We note the reasonable model performance and conclude that the CAMx model is functioning as expected.

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APPENDIX A

CAMx Post-Processing

Appendix A. CAMx Post-Processing

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
	ppbV	1000.0*
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++PAN)
NOY	ppbV	1000.0*(NO++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
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 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 Unit**	**CAMx/Combine Species**	**Output Unit**	**Output 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
	ppb	+PAN+PANX+HNO3	ppb	
NOX	ppb	NO++PAN+PANX+HNO3	ppb	NOX
CO	ppb	CO	ppb	CO
SO2	ppb	SO2	ppb	SO2
PM25	ug/m3	PM25_TOT	ug/m3	PM25_TOT