Three-State Air Quality Modeling Study (3SAQS)

Final Modeling Protocol
2008 Emissions & Air Quality Modeling Platform

Prepared by:

University of North Carolina
Institute for the Environment
137 E. Franklin St., Room 665
Campus Box 6116
Chapel Hill, NC 27599-6116

ENVIRON International Corporation
773 San Marin Drive, Suite 2115
Novato, California, 94945

December 2013
Response to Comments April 2014

UNC | INSTITUTE FOR THE ENVIRONMENT

ENVIRON

CONTENTS

TABLES

FIGURES

1.0 Introduction

The University of North Carolina (UNC) at Chapel Hill Institute for Environment and ENVIRON International Corporation (ENVIRON), are performing the Three State Air Quality Study (3SAQS) through a Cooperative Ecosystems Study Unit (CESU) cooperative agreement with the National Park Service. The 3SAQS includes cooperators from U.S. Environmental Protection Agency (EPA), United States Forest Service (USFS), Bureau of Land Management (BLM), National Park Service (NPS), and the state air quality management agencies of Colorado, Utah, and Wyoming. The 3SAQS is intended to facilitate air resource analyses for federal and state agencies in the states of Wyoming, Colorado, and Utah toward improved information for the public and stakeholders as a part of the National Environmental Policy Act (NEPA) and potentially other studies. Funded by the Environmental Protection Agency (EPA), Bureau of Land Management (BLM), and the U.S. Forest Service (USFS) and with in-kind support from the National Park Service (NPS) and Colorado, Utah, and Wyoming state air agencies, by working closely with cooperators and overseeing the various agreements, the main focus of the 3SAQS is on assessing the environmental impacts of sources related to oil and gas development and production. In particular, the cooperators will use photochemical grid models (PGMs) to quantify the impacts of proposed oil and gas development projects within the 3SAQS region on current and future air quality, including ozone and visibility levels in the National Parks and Wilderness Areas. The objectives of the 3SAQS are as follows:

- Create a standard modeling database in the Three State Data Warehouse (3SDW) for use in NEPA Environmental Impact Assessment (EIA) modeling of oil and gas development projects in Colorado, Utah, and Wyoming.

- Engage oil and gas development stakeholders to participate in the NEPA EIA process through contributing and reviewing model input data, modeling results, and technical support documentation

- Periodically evaluate the air quality impacts of all known proposed development projects in the three state region

- Provide a modeling platform to address the next generation of air quality issues related to oil and gas development, including ozone, PM ($PM_{2.5}$ and PM_{10}, including both primary and secondary PM), visibility, nitrogen and sulfur (acid) deposition, air toxics, and greenhouse gases.

The goals of the 3SAQS include the following:

1. Incorporate all of the recent western modeling analyses into the 3SDW;
2. Perform a comprehensive model performance evaluation on a standardized modeling database for use in NEPA impact assessments;
3. Develop a modeling platform that can be used to conduct or as a starting point for NEPA EIA analyses in Colorado, Utah, and Wyoming;
4. Allow future evaluation of proposed oil and gas development activities in three state region; and
5. Provide a framework and recommendations for performing future analysis to address Ozone, PM, visibility, and deposition issues in the western U.S.

The 3SAQS is starting with 2008 as the base-case modeling year for assessing the impacts of oil and gas development on local and regional air quality. The year 2008 was selected for the 3SAQS to leverage work completed during the West-wide Jumpstart Air Quality Modeling Study (WestJumpAQMS).

Emission projections to the year 2020, which are based off of EPA National Emission Inventory (NEI) rulemaking data and projected oil and gas inventories, will be used for estimating the impacts of development in future years. This document is a protocol for the 3SAQS emissions and PGM modeling that will be conducted for the 2008 and 2020 base years. The protocol details the modeling inputs/outputs, modeling procedures, and evaluation procedures that will be used by UNC and ENVIRON for the 3SAQS 2008 and 2020 base-case modeling.

1.1 BACKGROUND

Air pollutant data analysis and modeling expertise and skills are integral needs of the 3SAQS participants to support routine application of PGMs by mid-2014. UNC and ENVIRON will assist the 3SAQS participants in developing the technical data needed to perform meteorology, emissions, and air quality modeling. A primary objective of the project is to populate the 3SDW with the best available data for conducting EIA modeling studies in the three state region (CO, UT, and WY). UNC and ENVIRON will work closely with the NPS and other cooperators to develop technical capacity and expertise needed to apply and evaluate PGMs for NEPA EIA applications. As needed, they will train NPS staff and other cooperators on key components of the data, modeling, and analysis systems.

1.2 AIR QUALITY STANDARDS AND AIR QUALITY RELATED VALUES

The United State (U.S.) Environmental Protection Agency (EPA) sets National Ambient Air Quality Standards (NAAQS) for six regulated air quality pollutants: ozone (O_3), particulate matter (PM), sulfur dioxide (SO_2), nitrogen dioxide (NO_2), carbon monoxide (CO) and lead (Pb). After promulgation of a NAAQS, EPA designates nonattainment areas (NAAs) and States are required to submit State Implementation Plans (SIPs) to EPA that contain emission control plans and a demonstration that the NAA will achieve the NAAQS by the required date.

In 1997, EPA promulgated the first 8-hour ozone National Ambient Air Quality Standard (NAAQS) with a threshold of 0.08 ppm (84 ppb). On March 12, 2008, EPA promulgated a more stringent 0.075 ppm (75 ppb) 8-hour ozone NAAQS. Figure 1-1 displays the locations of ozone nonattainment areas under the 2008 ozone NAAQS. EPA is currently re-evaluating the ozone NAAQS and will likely promulgate a new 8-hour ozone NAAQS in 2014 with a threshold that will likely be in the range of 0.060 ppm to 0.070 ppm. Under more stringent ozone NAAQS there would likely be many more areas in the U.S., including the western U.S., that would be in nonattainment.

On December 14, 2012, EPA revised the $PM_{2.5}$ primary NAAQS by lowering the annual $PM_{2.5}$ NAAQS threshold from 15.0 $\mu g/m^3$ to a 12.0 $\mu g/m^3$ range[1]. EPA is retaining the 24-hour $PM_{2.5}$ primary NAAQS at 35 $\mu g/m^3$. The 24-hour coarse PM NAAQS (PM_{10}) is also retained at 150 $\mu g/m^3$. EPA considered the adoption of a secondary $PM_{2.5}$ NAAQS to protect against visibility impairment in urban areas with a proposed threshold in the 28 to 30 deciview range and an averaging time in the range of 4 to 24 hours. However, EPA determined that the 35 $\mu g/m^3$ 24-hour $PM_{2.5}$ secondary NAAQS provides visibility protection equal to or better than a 30 deciview (dv) standard. Figure 1-2 displays counties that are violating the old 15.0 $\mu g/m^3$ annual $PM_{2.5}$ NAAQS and the additional counties that would violate a proposed 13.0 and the new 12.0 $\mu g/m^3$ annual $PM_{2.5}$ NAAQS based on 2008-2010 measurements. There would be no new $PM_{2.5}$ nonattainment counties in the western U.S. under the new annual $PM_{2.5}$ NAAQS 12 $\mu g/m^3$ level based on 2008-2010 air quality observations.

In February 2010 EPA issued a new 1-hour NO_2 NAAQS with a threshold of 100 ppb and a new 1-hour SO_2 NAAQS was promulgated in June 2010 with a threshold of 75 ppb. EPA has not yet designated the

---

[1] http://www.epa.gov/pm/actions.html#jun12

nonattainment areas for the 1-hour NO_2 and 1-hour SO_2 NAAQS. As of September 27, 2010 all NAAs for Carbon Monoxide have been redesignated as maintenance areas. A new lead NAAQS was issued in 2008 and, except for Los Angeles, all of the NAAs reside in the eastern or central U.S or Alaska.

The Clean Air Act Amendments (CAAA) designated 156 Class I areas consisting of National Parks and Wilderness Areas that are offered special protection for air quality and air quality related values (AQRVs). The Class I areas, compared to Class II areas, have lower Prevention of Significant Deterioration (PSD) air quality increments that new sources may not exceed, and are protected against excessive increases in several AQRVs including visibility impairment, acid (sulfur and nitrogen) deposition and nitrogen eutrophication. The Regional Haze Rule (RHR) has a goal of natural visibility conditions by 2064 at Class I areas, and States must submit RHR SIPs that demonstrate progress towards that goal. Figure 1-3 displays the locations of the 156 mandatory Class I areas, most of which are in the western U.S., including the states of Colorado, Utah and Wyoming.
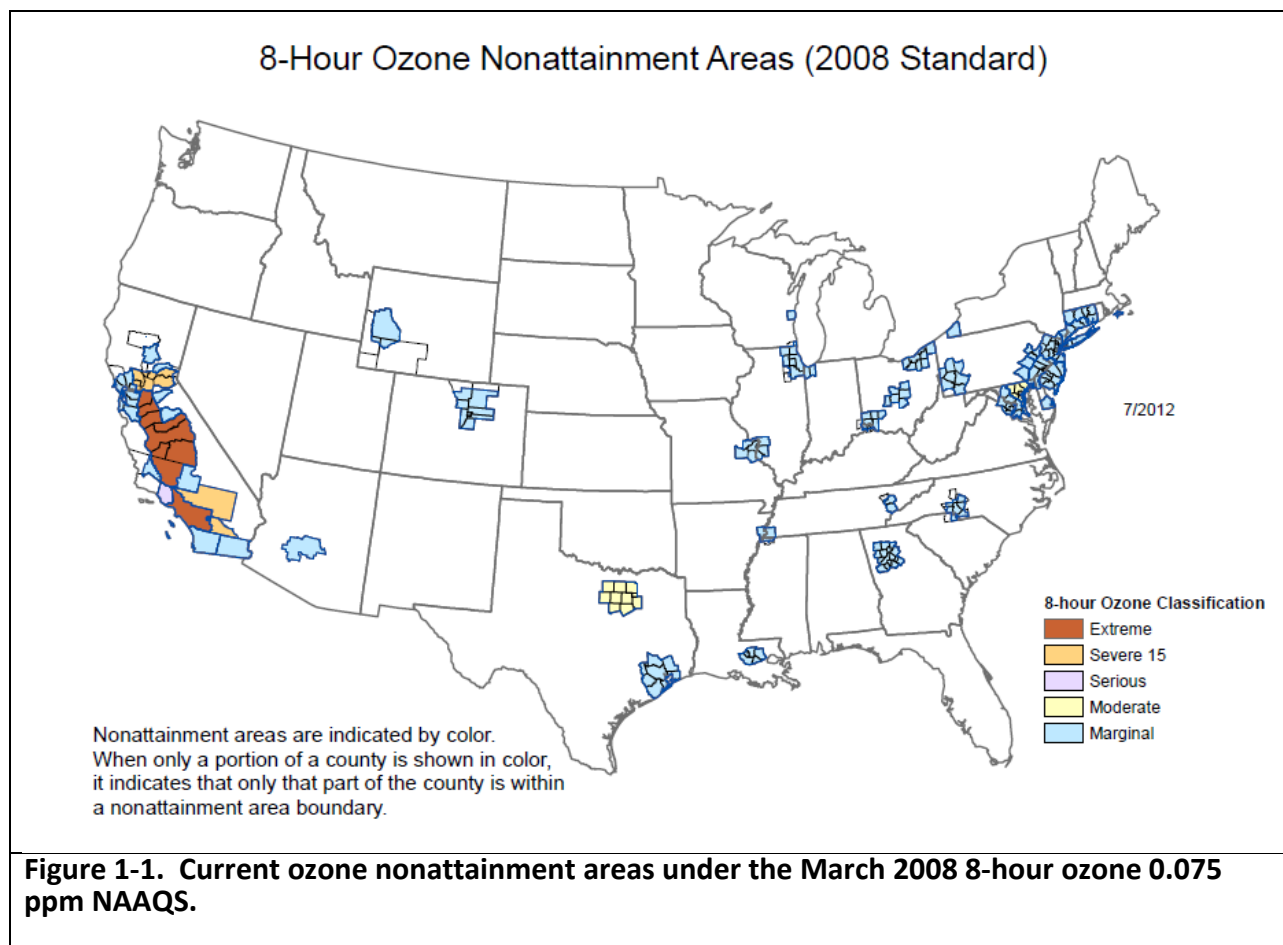
Figure 1-1. Current ozone nonattainment areas under the March 2008 8-hour ozone 0.075 ppm NAAQS.
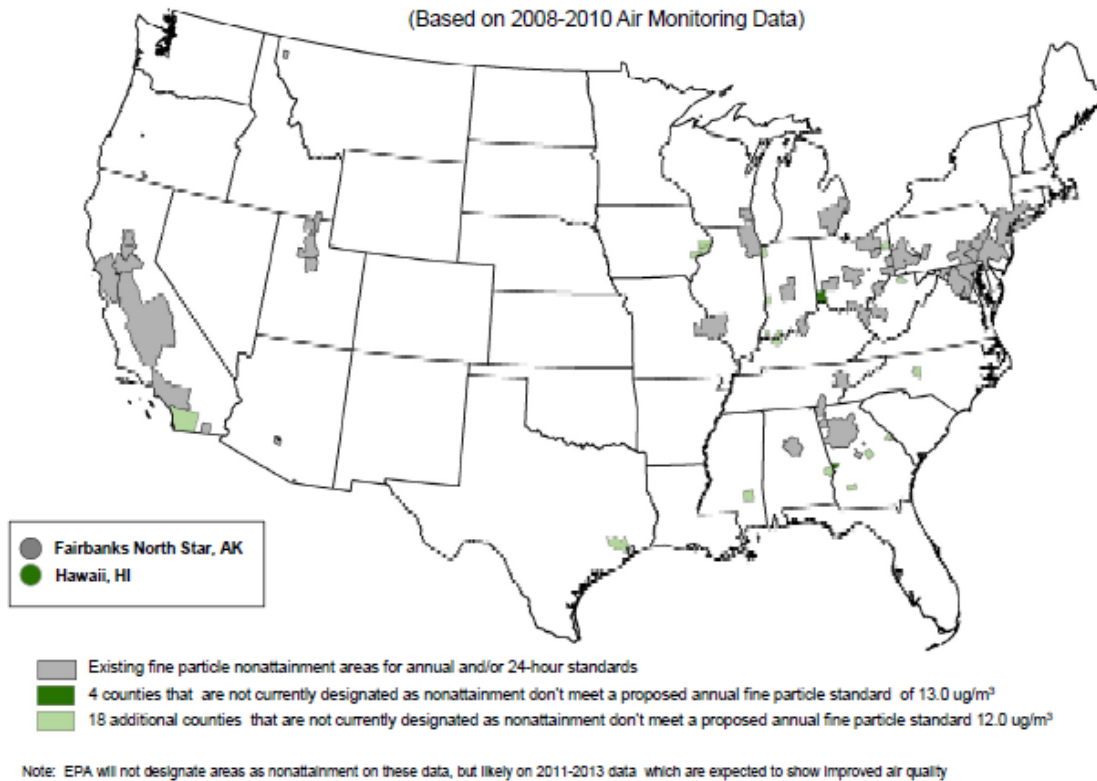
Figure 1-2. Counties that are violating the 1997 15.0 µg/m³ PM₂.₅ NAAQS and additional counties that would violate a 13.0 µg/m³ (dark green) and the new December 2012 12.0 µg/m³ PM₂.₅ NAAQS based on 2008-2010 observations (source: http://www.epa.gov/pm/actions.html#jun12).
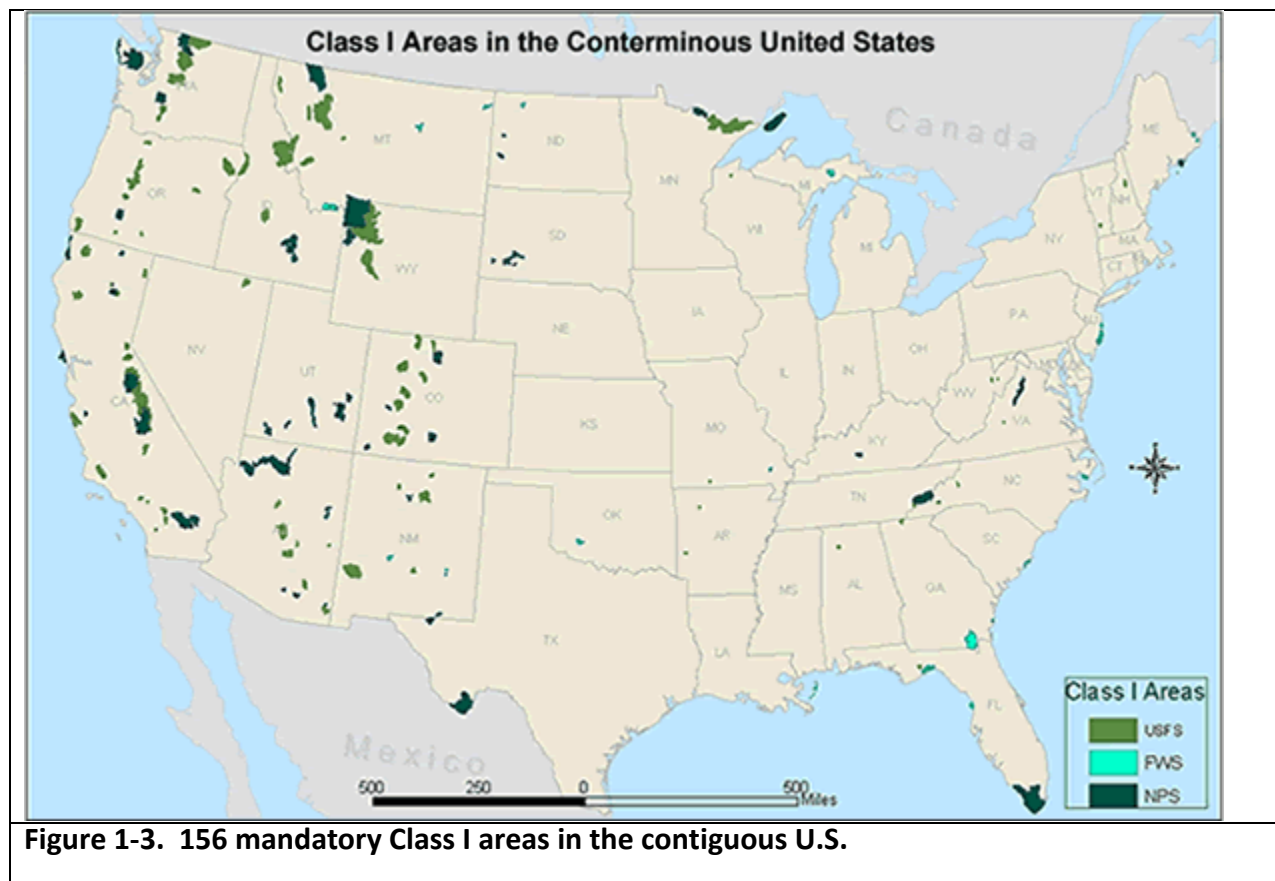
Figure 1-3. 156 mandatory Class I areas in the contiguous U.S.

1.3 ORGANIZATION OF THE MODELING PROTOCOL

This document represents the 3SAQS Modeling Protocol for emissions and PGM modeling for the 2008 calendar year and 2020 future year. The 3SAQS modeling will leverage the meteorology and emissions data and configuration for 2008 conducted for the West-wide Jump-start Air Quality Modeling Study (WestJumpAQMS). Details of the WestJumpAQMS emissions technical approach can be found in the Modeling Protocol (ENVIRON, Alpine and UNC, 2013) and in a series of sixteen memos describing the data collection and processing activities for individual emissions categories (ENVIRON, Alpine, and UNC, 2013)[2]. The year 2008 WestJumpAQMS meteorology data are documented in the WestJumpAQMS WRF modeling final report (ENVIRON and Alpine, 2012). Although the 3SAQS modeling analysis is not currently being performed to fill any particular regulatory requirement, such as a State Implementation Plan (SIP) attainment demonstration, EIA, or Resource Management Plan (RMP) as part of the National Environmental Policy Act (NEPA), it is being conducted with the same level of technical rigor as a SIP-type analysis and may ultimately be used as a basis for regulatory air quality modeling. This 3SAQS emissions Modeling Protocol has the following sections:

1. Introduction: Presents a summary of the background, purpose and objectives of the study.
2. Model Selection: Introduces the models selected for the study
3. Episode Selection: Describes the modeling period for the study.

---

[2] http://www.wrapair2.org/WestJumpAQMS.aspx

4. <u>Modeling Domain Selection</u>: Presents the modeling domains and grid structure for the modeling study.
5. <u>WRF Meteorology</u>: Describes how the meteorological modeling was conducted and the WRF model evaluation.
6. <u>Emissions</u>: Describes the emissions input data, how the emissions modeling will be conducted, and the procedures for evaluating and validating the emissions processing results.
7. <u>Photochemical Modeling</u>: Describes the procedures for conducting the photochemical grid model including the model versions, inputs and options
8. <u>Model Performance Evaluation</u>: Provides the procedures for conducting the model performance evaluation of the photochemical grid models.
9. <u>Website:</u> web location for finding supporting project information
10. <u>Acronyms</u>: Definitions of acronyms used in this document
11. <u>References</u>: References cited in the document

1.5 PROJECT PARTICIPANTS

The 3SAQS is conducted by the states of Colorado, Utah and Wyoming, several Federal agencies including National Park Service, (NPS), United States Forest Service (USFS) and Bureau of Land Management (BLM) and several contractors. The 3SAQS year 2008 and 2020 emissions and air quality modeling is being conducted by UNC and ENVIRON. Key contacts and their roles in the 3SAQS are listed in Table 1-1.

Table 1-1. Key contacts in the 3SAQS meteorological modeling.

Name	Role	Organization/Contact
Tom Moore	Manager 3SAQS Data Warehouse	Western Regional Air Partnership (WRAP)/Westar c/o CSU/CIRA 1375 Campus Delivery Fort Collins, CO 80523 (970) 491-8837 tmoore@westar.org
Zac Adelman	UNC Lead	University of North Carolina Institute for the Environment 137 E. Franklin St, CB 6116 Chapel Hill, NC 27599-6116 (312) 533-4748 zac@unc.edu
Ralph Morris	ENVIRON Lead	ENVIRON International Corporation 773 San Marin Drive, Suite 2115 Novato, CA 94998 (415) 899-0708 rmorris@environcorp.com

1.6 RELATED STUDIES

There are numerous meteorological, emissions and air quality modeling and data analysis studies related to the 3SAQS modeling whose results will be incorporated into the study. In addition, EPA has promulgated several national rules that may affect emissions in the western states.

1.6.1 Federal Regional Regulatory Air Quality Programs

The federal government has implemented standards and actions to improve air quality across the entire country. These standards have largely involved mobile sources, whereas as many of the national rules address large stationary point sources. Federal standards include: the Tier 2 Vehicle Standards, the heavy-duty gasoline and diesel highway vehicle standards, the non-road spark-ignition engines and recreational engine standards, and the large non-road diesel engine rule. The federal government has also implemented regional control strategies for major stationary sources focusing on the eastern U.S. and intends to extend the program to the western U.S. The following is a list of federal regulatory actions that would likely lead to emission reductions in the western U.S.

- Tier 2 Vehicle Standards

- Heavy-duty Gasoline and Diesel Highway Vehicle Standards

- Non-Road Spark-ignition Engines and Recreational Engines Standards

- Large Non-Road Diesel Engine Rule

- Mercury and Air Toxics Standards (MATS)

- VOC MACT

- Federal Reformulated Gasoline

- Federal Non-Road Spark-Ignition Engines and Equipment

- Locomotive Engines and Marine Compression-Ignition Engines Final Rule

- Clean Air Act Title IV - Acid Rain Program

- Low-Sulfur Fuels

- Clean Air Visibility Rule (CAVR)

- Oil and Gas New Source Performance Standards (NSPS, August 16, 2012)

1.6.3 2008 Denver Ozone SIP Modeling

The 2008 Denver ozone SIP modeling used the MM5 meteorological, the CAMx photochemical grid model, and the SMOKE and CONCEPT models for emissions modeling. The CONCEPT model was interfaced with link-based Vehicle Miles Traveled (VMT) and other mobile source activity data (e.g., speeds, fleet mix, temporal variations, etc.) from a Traffic Demand Model (TDM) operated by DRCOG, on-road emission factors from the MOBILE6 model, and hourly meteorological data from MM5 to generate detailed on-road mobile source emissions for the DMA. Other emission inputs were generated using SMOKE. The MM5/SMOKE/CONCEPT/CAMx modeling system was applied to the June-July 2006 period and used to demonstrate that the DMA/NFR region would attain the 1997 8-hour ozone NAAQS by 2010. Details on the 2008 Denver 8-hour ozone SIP modeling can be found at:

1.6.4 Current Denver Modeling of a 2008 Episode

The RAQC is currently conducting a modeling study using the same WRF meteorological, SMOKE emissions and CAMx photochemical grid models as 3SAQS and the May through August 2008 portion of the 3SAQS 2008 modeling year. As in the 2008 Denver Ozone SIP, on-road mobile sources in the Denver area were estimated using CONCEPT MV with link-based TDM data, except the MOVES mobile source emissions factor

model was used instead of MOBILE6. The Modeling Protocol and preliminary model performance evaluation (MPE) results for the current 2008 Denver ozone modeling can be found at:

http://www.ozoneaware.org/postfiles/documentsandpresentations/modeling/documents/Denver_Model_Protocol_Draft3_080211.pdf

http://raqc.org/postfiles/ozone_modeling/modeling_forum/Denver_2008_Prelim_MPE_080912.pdf

1.6.5 WRAP Regional Modeling Center Modeling

In 2002, Five Regional Planning Organizations (RPOs) were formed to perform regional haze modeling using photochemical, ozone, and PM models, to support the development of regional haze SIPs due in December 2007. The Western Regional Air Partnership (WRAP) is the RPO for the western states.   The modeling was conducted by the WRAP Regional Modeling Center (RMC) that consisted of the University of California at Riverside (UCR), ENVIRON International Corporation, and the University of North Carolina (UNC). The RMC conducted modeling for the 2002 annual period, and continental U.S. using a 36 km grid and the MM5 meteorological (Kemball-Cook et al., 2005a), SMOKE emissions, and CMAQ and CAMx photochemical models. CMAQ was run for a 2002 base case, a 2018 future base-year, and a 2018 control scenarios to predict visibility projections in Federal Class I areas. The WRAP RMC has a website where modeling results can be obtained.   Some of the modeling results have been implemented in the WRAP Technical Support System (TSS) website where users can analyze data and modeling results. Pertinent WRAP RMC websites are at:

http://pah.cert.ucr.edu/aqm/308/index.shtml

http://vista.cira.colostate.edu/tss/

http://www.wrapair.org/

http://www.wrapair2.org/

1.6.6 Four Corners Air Quality Task Force

The Four Corners Air Quality Task Force (FCAQTF) conducted emissions and photochemical grid modeling for the four corners region to provide information regarding ozone, visibility, and deposition impacts in the region. The states of Colorado and New Mexico were active participants in the FCAQTF study. The MM5 meteorological, SMOKE emissions, and CAMx air quality models were applied for the 2005 year on a 36/12/4 km grid with the 4 km grid focused on northwest New Mexico, southwest Colorado and small portions of southeast Utah and northeast Arizona. This region not only includes the San Juan Basin oil and gas development area, but also several large coal-fired power plants (e.g., Four Corners and San Juan). The FCAQTF performed 2005 base case modeling, as well as 2018 future-year modeling and 2018 sensitivity modeling for several mitigation scenarios. More details on the FCAQTF modeling can be found at:

http://www.nmenv.state.nm.us/aqb/4C/PublicReview.html

1.67 Environmental Impact Statements (EISs) and Resource Management Plans (RMPs)

Photochemical grid models are also being applied in the Rocky Mountain States as part of the development of Environmental Impact Statements (EISs) for oil and gas development projects and Resource Management Plans (RMPs) for Bureau of Land Management (BLM) Field Offices. Most of these EIS/RMP studies have been or are being performed by the BLM under the National Environmental Policy Act (NEPA), although the United States Forest Service (USFS) and Tribes have also led some EISs. The main focus of these activities is on the air quality and air quality related value (AQRV; i.e., visibility and deposition) impacts due to oil and gas

development activities, although RMPs can also address mining, grazing, off-highway vehicles and other activities. Such EIS/RMP activities have occurred or are undergoing air quality modeling for projects in Colorado, New Mexico, Utah and Wyoming with more information found on the BLM websites:

http://www.blm.gov/co/st/en.html

http://www.blm.gov/nm/st/en.html

http://www.blm.gov/ut/st/en.html

http://www.blm.gov/wy/st/en.html

1.6.8 RoMANS

The National Park Service (NPS), CDPHE/APCD and others performed the Rocky Mountain Atmospheric Nitrogen and Sulfur Study (RoMANS) to study nitrogen deposition and potential mitigation scenarios at Rocky Mountains National Park (RMNP). The Rocky Mountain Initiative includes data collection, data analysis, modeling and the development of a nitrogen deposition reduction plan. Much of the analysis of RoMANS was for the 2006 period and they plan to do additional modeling for 2009. Details on the RoMANS study can be found at:

http://www.colorado.gov/cs/Satellite?c=Page&childpagename=CDPHE-AP%2FCBONLayout&cid=1251594862555&pagename=CBONWrapper

http://www.nature.nps.gov/air/studies/romans.cfm

1.6.9 WestJumpAQMS

The West-wide Jump-start Air Quality Modeling Study (WestJumpAQMS) is conducting meteorological, emissions and photochemical grid modeling of the western U.S. for the 2008 calendar year to investigate source-receptor relationships for ozone, particulate matter, visibility and deposition. WRF meteorological and SMOKE emissions modeling was conducted for a 36 km continental U.S., 12 km western U.S., and 4 km inter-mountain west domain. Ozone and PM source apportionment modeling was also conducted with CAMx to examine state-specific and source category-specific air quality impacts. Details on the WestJumpAQMS can be found at:

http://www.wrapair2.org/WestJumpAQMS.aspx

1.7 OVERVIEW OF MODELING APPROACH

The procedures for the 3SAQS 2008 modeling will follow those performed for the WestJumpAQMS and include updated data for sources in the three state study region. Unlike the WestJumpAQMS, a future year inventory will be simulated as part of the 3SAQS. The 3SAQS 2008 modeling platform will only be used to simulate 36- and 12-km modeling domains; there will be no 4-km modeling done for the 2008 3SAQS platform. The 3SAQS 2008 platform is a short shelf-life application that will serve as a bridge until the 2011 platform is available. As a temporary modeling platform, the 2008 simulations will only focus on CAMx performance in the three-state region for the 36-km and 12-km domains. There is currently no plan to run CMAQ, CAMx source apportionment tools, or to conduct targeted performance sensitivities for wintertime ozone using the 2008 platform. These extensions to the standard modeling platform will be considered in the 3SAQS 2011 modeling platform. A summary of the 3SAQS 2008 modeling approach is given below, with more details provided in the chapters of this modeling protocol.

- The 2008 calendar year was selected for the 3SAQS emissions modeling period.

- Year 2008 and 2020 inventories will be used to estimate base and future year emissions for the 3SAQS

- A 36 km continental U.S. (CONUS) and 12 km western U.S. (WESTUS) domain that covers the 3SAQS region will be used.

- The WestJumpAQMS year 2008 Weather Research Forecasting (WRF) modeling results are being used to provide meteorology inputs to the 3SAQS.

- Emissions modeling is primarily conducted using the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system using mainly emissions data from the EPA 2008-based modeling platform (2007v5).

- Photochemical grid modeling is based on the Comprehensive Air-quality with extensions (CAMx) version 5.41.

- Boundary conditions (BCs) for the lateral boundaries of the 36 km CONUS domain are initially based on the MOZART global chemistry model.

- Model evaluation is being conducted for ozone, particulate matter (PM) mass and speciation and ozone and PM precursor and product species as well as for visibility and deposition.

2.0 Model Selection

This section discusses the emissions modeling software used for the 3SAQS. The modeling software selection methodology follows EPA's guidance for regulatory modeling in support of ozone and $PM_{2.5}$ attainment demonstration modeling and showing reasonable progress with visibility goals (EPA, 2007). EPA recommends that models be selected for regulatory ozone, PM and visibility studies on a "case-by-case" basis with appropriate consideration being given to the candidate models':

- Technical formulation, capabilities and features;

- Pertinent peer-review and performance evaluation history;

- Public availability; and

- Demonstrated success in similar regulatory applications.

All of these considerations should be examined for each class of models to be used (e.g., emissions, meteorological, and photochemical) in part because EPA no longer recommends a specific model or suite of photochemical models for regulatory application as it did twenty years ago in the first ozone SIP modeling guidance (EPA, 1991). Below we identify the most appropriate candidate models that we believe are best suited to the requirements of the 3SAQS, discuss the candidate model attributes and then justify the model selected using the four criteria above. The science configurations recommended for each model in this study are introduced in Chapter 5

2.1 JUSTIFICATION AND OVERVIEW OF SELECTED MODELS

The 3SAQS will be using three general types of models for simulating ozone, and other gaseous pollutants, particulate matter, visibility and deposition in the western U.S.:

- Meteorological Models (MM)

- Emissions Models (EM)

- Photochemical Grid Models (PGM)

These are not single models, but rather a suite of models or modeling systems that are used to generate PGM meteorological and emissions inputs and simulate air quality, visibility and deposition.

2.1.1 Meteorological Model

There are two prognostic meteorological models that are routinely used in the U.S. in photochemical grid modeling studies:

- The fifth generation Mesoscale Model (MM5); and

- The Weather Research Forecasting (WRF) model.

Both MM5 and WRF were developed by the community with the National Center for Atmospheric Research (NCAR) providing coordination and support. For many years the MM5 model was widely used by both the meteorological research as well as the air quality modeling community. Starting around the year 2000, the WRF model started to be developed as a technical improvement and replacement to MM5 and today NCAR no longer supports MM5. The 3SAQS is using 2008 meteorology fields developed for the WestJumpAQMS. Based on the four selection criteria, the WRF was selected as the WestJumpAQMS meteorological model for the following reasons:

- Technical: WRF is based on more recent physics and computing techniques and represents a technical improvement over MM5. WRF has numerous new capabilities and features not available in MM5 and, unlike MM5, it is supported by NCAR.

- Performance: Because it has been around longer MM5 has had a longer history of performance than WRF. However, WRF is being used by thousands of users and been subjected to a community peer-reviewed development process using the latest algorithms and physics. In general, it appears that the WRF is better able to reproduce the observed meteorological variables so performs better. WRF is amassing a rich publication and application history.

- Public Availability: WRF is publicly available and can be downloaded from the WRF website with no costs or restrictions[3].

- Demonstrated Success: The recent Denver ozone modeling of the 2008 episode using WRF has produced better meteorological and ozone model performance than achieved in past Denver ozone modeling efforts of 2002 and 2006 that used MM5 (Morris et al., 2012a,b).

More details on the selected WRF meteorological model are provided below.

WRF[4]: The non-hydrostatic version of the Advanced Research version of the Weather Research Forecast (WRF-ARW[5]) model (Skamarock et al. 2004; 2005; 2006; Michalakes et al. 1998; 2001; 2004) 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,

---

[3] http://wrf-model.org/users/users.php
[4] http://www.wrf-model.org/index.php
[5] All references to WRF in this document refer to the WRF-ARW

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. WRF-ARW has become the new standard model used in place of the older Mesoscale Meteorological Model (MM5) for regulatory air quality applications in the U.S. It is suitable for use in a broad spectrum of applications across scales ranging from hundreds of meters to thousands of kilometers.

2.1.2 Emissions Processing Systems

The following software will be used to prepare emissions inputs for the CAMx PGM used in the 3SAQS.

- Sparse Matrix Operator Kernel Emissions (SMOKE) processor, version 3.0 – software system that prepares emission inventory data for input to a PGM; primary functions include spatial, temporal, and chemical conversion of emission inventory data to the terms required by a PGM
- Model of Emissions of Gases and Aerosols from Nature (MEGAN), version 2.10[6] – biogenic emissions model; primary function is to estimate gridded gas-phase emissions from plants and soils
- WRAP Windblown Dust Model[7] - software to estimate wind-driven dust emissions

Emissions data for PGMs are prepared with a suite of data processing and modeling software. The basic component of the emissions modeling software suite is a processor to convert emission inventory data into PGM input files. Additional emissions modeling software target specific emissions sectors, including biogenic sources, on-road mobile sources, windblown dust, lightning, and sea spray. The three emissions processors that are routinely used in the U.S. in photochemical grid modeling studies:

- The Consolidated Community Emissions Processing Tool (CONCEPT);

- The Emissions Modeling System (EMS); and

- The Sparse Matrix Operator Kernel Emissions (SMOKE) system.

All of these software are considered emissions processors and not emissions models. The primary function of these tools is to convert emission inventory data to the spatial, chemical, and temporal terms required by a particular PGM. Based on the four selection criteria, the SMOKE system was selected as the 3SAQS emissions processor for the following reasons:

- Technical: SMOKE is undergoing the most active development and updates of all of the three processors listed above. It is updated annually to add new capabilities and features and to address bugs and inefficiencies. SMOKE is widely used for regulatory modeling studies and is the only emissions processor in use by EPA.

---

[6] Guenther, A. B., Jiang, X., Heald, C. L., Sakulyanontvittaya, T., Duhl, T., Emmons, L. K., and Wang, X.: The Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2.1): an extended and updated framework for modeling biogenic emissions, Geosci. Model Dev. Discuss., 5, 1503-1560, doi:10.5194/gmdd-5-1503-2012, 2012.
[7] http://12.45.109.3/forums/dejf/documents/WRAP_WBD_PhaseII_Final_Report_050506.pdf

- Performance: SMOKE is designed to be efficient in how it processes large quantities of data. It has been used in countless research and regulatory studies worldwide and is most likely the emissions processor in recently published regional modeling studies that used either the CMAQ or CAMx PGM.

- Public Availability: SMOKE is publicly available and can be downloaded from the Community Modeling and Analysis System Center with no costs or restrictions[8].

- Demonstrated Success: The RoMANS study, Denver 2008 SIP modeling, all of the EIS projects that used CMAQ or CAMx, and the WestJumpAQMS all used SMOKE for preparing the PGM emissions. While deficiencies in the modeling performance in all of these studies can be partially traced to flaws in the emissions data, SMOKE has proven to be a reliable system for processing the data.

SMOKE: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is a set of programs that is used by the U.S. EPA, Regional Planning Organizations (RPOs), and State environmental agencies to prepare emissions inventory data for input to PGMs. SMOKE converts annual, daily, or hourly estimates of emissions at the state or county level to hourly emissions fluxes on a uniform spatial grid that are formatted for input to either the CMAQ or CAMx PGMs. SMOKE integrates county-level emissions inventories with source-based temporal, spatial, and chemical allocation profiles to create hourly emissions fluxes on a predefined model grid. For elevated sources that require allocation of the emissions to the vertical model layers, SMOKE integrates meteorology data to derive dynamic vertical profiles. In addition to its capacity to simulate emissions from stationary area, stationary point, and on-road mobile sectors, SMOKE is also instrumented with the Biogenic Emissions Inventory System, version 3 (BEIS3) model for estimating biogenic emissions fluxes (U.S. EPA, 2004). The SMOKE-MOVES processor is an interface for the MOVES on-road mobile emissions model that prepares MOVES results for input to a PGM. SMOKE can additionally be used to calculate future-year emissions estimates, if the user provides data about how the emissions will change in the future.

SMOKE uses C-Shell scripts as user interfaces to set configuration options and call executables. SMOKE is designed with flexible QA capabilities to generate standard and custom reports for checking the emissions modeling process. After modeling all of the emissions source categories individually, SMOKE creates two files per day for input into CMAQ and CAMx: (1) an elevated point source file for large stationary sources, and (2) a merged gridded source file of low-level point, mobile, non-road, area, and biogenic emissions. The efficient processing of SMOKE makes it an appropriate choice for handling the large processing needs of regional and seasonal emissions processing, as described in more detail by Houyoux et al. (1996, 2000).

SMOKE is a software tool and not a set of data files; therefore, SMOKE relies on user-provided data files for emission inventories and factors to apply to those emissions. The factors assign the annual inventory data to the hours, grid cells, and model species and can be adjusted by the user in a way that is the most appropriate for the inventory sources included in the air quality modeling domain. In addition SMOKE requires meteorology data in the Input/Output Application Programmers Interface (I/O API) format to process meteorology-dependent emissions sectors. The temporal and spatial extents of the SMOKE modeling periods are dictated by the input meteorology. SMOKE can neither interpolate between different grid resolutions nor project/backcast to dates that are not covered in the input meteorology. SMOKE has strict requirements for the nature and formats of the inventory data that it can use.

---

[8] http://www.smoke-model.org

SMOKE primarily uses two types of input file formats: ASCII files and I/O API netCDF files. Input files are files that are read by at least one core SMOKE program, but are not written by a core program. SMOKE uses strict rules that define the format and content of the input files. These rules are explicitly laid out in the SMOKE Users Manual. All data input to SMOKE must be either formatted to one of the prescribed input file types or converted to an intermediate form, such as a gridded I/O API inventory file, before it can be input to SMOKE.

In general SMOKE requires an emissions inventory, temporal allocation, spatial allocation, and chemical allocation data to prepare emissions estimates for an air quality model. For some source categories, such as on-road mobile and stationary point sources, SMOKE also requires meteorology data to calculate emissions. SMOKE calculates biogenic emissions estimates with gridded land use, vegetative emissions factors, and meteorology data.

Upstream software and utilities are used to prepare many of the inputs to SMOKE. The Meteorology Chemistry Interface Processor (MCIP), which is part of the Community Multiscale Air Quality (CMAQ) model, is used to prepare MM5 and WRF meteorology data for input to SMOKE. A Geographic Information System (GIS), such as the open-source Spatial Allocator, is needed to create the spatial surrogates that map inventory data to modeling grids. The Speciation Tool is built on top of the SPECIATE database as an interface to create the chemical allocation profiles that convert inventory pollutants to PGM species. Temporal allocation profiles and the assignment files that associate the spatial/chemical/temporal profiles to inventory sources are all available through an ad-hoc database from the EPA Clearinghouse for Inventories and Emissions Factors. Other source-specific inputs, such as land use/land cover data for biogenic emissions and Motor Vehicle Emissions Simulator (MOVES) look up tables and ancillary files, are typically prepared for SMOKE on a project-specific basis. Details of the data used for the 3SAQS are provided in the next section.

MOVES[9]**:** The MOtor Vehicle Emission Simulator model (MOVES) is a multi-scale emissions modeling system that generates emission inventories or emission rate lookup tables for on-road mobile sources. MOVES is capable of creating inventories or lookup tables at the national, state, county, or project scales. MOVES was designed by EPA's Office of Transportation and Air Quality (OTAQ) and the latest release version is MOVES2010b in April 2012. MOVES is principally an emissions modeling system where emissions estimates are simulated from 'first principles' taking into account the effects of fleet age deterioration, ambient temperature and humidity, activity patterns, fuel properties, and inspection and maintenance programs on emissions from all types of motor vehicles. MOVES outputs can be input to emissions processing systems such as SMOKE.

MEGAN[10]**:** The Model of Emissions of Gases and Aerosols in Nature (MEGAN) is a modeling system for estimating the net emission of gases and aerosols from terrestrial ecosystems into the atmosphere (Jiang et al., 2012[11]; Wiedinmyer, Sakulyanontvittaya and Guenther, 2007[12]). Driving variables include landcover, weather, and atmospheric chemical composition. MEGAN is a global model with a base resolution of ~1 km and so is suitable for regional and global models. A FORTRAN code is available for generating emission estimates for the CMAQ and CAMx regional air quality models. Global distributions of landcover variables (Emission Factors, Leaf Area Index, and Plant Functional Types) are available for spatial resolutions ranging from ~ 1 to 100 km and in several formats (e.g., ARCGIS, netcdf). WRAP has

---

[9] http://www.epa.gov/otaq/models/moves/index.htm
[10] http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm
[11] http://acd.ucar.edu/~guenther/MEGAN/MEGANv2.10_beta/MEGAN2.1_User_Guide_05-07-2012.pdf
[12] http://acd.ucar.edu/~guenther/MEGAN/MEGANguideFORTRAN204.pdf

recently updated the MEGAN biogenic emissions models using western U.S. data and higher resolution inputs (Sakulyanontvittaya, Yarwood and Guenther, 2012[13]).

2.1.3 Photochemical Grid Model

There are two PGMs that are widely used for ozone, $PM_{2.5}$ and visibility planning in the U.S.:

- Community Multiscale Air Quality (CMAQ) modeling system; and

- Comprehensive Air-quality Model with extensions (CAMx).

CMAQ is developed by EPA and CAMx is developed by ENVIRON. Both models are publicly available and have adopted the "one-atmosphere" concept treating ozone, $PM_{2.5}$, air toxics, visibility and other air quality issues within a single platform. CMAQ has some more recent treatment in its aerosol modules, whereas CAMx has a more recent gas-phase photochemical mechanism.

- Technical: Both CMAQ and CAMx represent state-of-science one-atmosphere PGMs. CAMx was selected as the lead because it supports two-way grid nesting; a feature needed for the 3SAQS source apportionment modeling that is not present in CMAQ.

- Performance: A peer-review of the CAMx and CMAQ source apportionment algorithms found CAMx to be technically and operationally superior to CMAQ. CAMx also tends to run a little faster than CMAQ.

- Public Availability: CMAQ and CAMx are both publicly available.

- Demonstrated Success: Both CMAQ and CAMx have had many successful model performance applications. CAMx has been applied more frequently in the Rocky Mountain region for NEPA studies and the Denver ozone SIP modeling.

The CAMx and CMAQ models are summarized below.

CAMx[14]: The Comprehensive Air Quality Model with Extensions (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 (ENVIRON, 2011). 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, NO_X SIP Call, etc.).

CMAQ[15]: EPA's Models-3/Community Multiscale Air Quality (CMAQ) modeling system is also "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 (Byun and Ching, 1999). The CMAQ modeling system was designed to approach air quality as a whole by including state-of-the-science capabilities for

---

[13] http://wrapair2.org/pdf/WGA_BiogEmisInv_FinalReport_March20_2012.pdf

[14] http://www.camx.com/

[15] http://www.cmaq-model.org/

modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. CMAQ was also designed to have multi-scale capabilities so that separate models were not needed for urban and regional scale air quality modeling. The CMAQ modeling system contains three types of modeling components: (a) a meteorological module for the description of atmospheric states and motions, (b) an emission models for man-made and natural emissions that are injected into the atmosphere, and (c) a chemistry-transport modeling system for simulation of the chemical transformation and fate.

The CAMx PGM will be applied in the 3SAQS project. For consistency with the WestJumpAQMS, CAMx Version 5.41 (November 2012) was selected for the 3SAQS modeling. The WRF meteorological model Version 3.3 (April 2011) was applied for the selected modeling episode and grid structure. The WRF output was processed using the WRFCAMx program to generate meteorological inputs for the CAMx model.

Boundary Conditions (BCs) for the 36 km CONUS domain are based on output from a global chemistry model (GCM). The current plan is to initially use results from the MOZART GCM, however results from GEOS-Chem GCM will also be analyzed and considered. The interaction between the GCM with the regional models (CAMx and CMAQ) is performed through processors that perform the following activities:

- For each BC horizontal grid cell in the 36 km CONUS domain, identify the appropriate grid cell of the GCM where it resides.

- Mass consistent interpolation GCM species in the GCM vertical layer structure to the vertical layer structure used by CAMx/CMAQ.

- Mapping of species in the GCM chemical mechanism to the species used in CAMx or CMAQ.

3.0 EPISODE SELECTION

EPA's ozone, $PM_{2.5}$ and visibility SIP modeling guidance (EPA, 2007)[16] contains recommended procedures for selecting modeling episodes, while also referencing EPA's 1-hour ozone modeling guidance for episode selection (EPA, 1991)[17.] This Chapter presents the modeling period selected for performing the 3SAQS and the justification and rationale for its selection.

3.1 EPISODE SELECTION CRITERIA

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.

3.1.1 Primary Episode Selection Criteria

EPA's modeling guidance (EPA, 2007) identifies four specific criteria to consider when selecting episodes for use in demonstrating attainment of the 8-hour ozone or $PM_{2.5}$ NAAQS:

1. A variety of meteorological conditions should be covered, including the types of meteorological conditions that produce 8-hour ozone and 24-hour $PM_{2.5}$ exceedances in the western U.S.;
2. Choose episodes having days with monitored 8-hour daily maximum ozone and 24-hour $PM_{2.5}$ concentrations close to the ozone and $PM_{2.5}$ 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

---

[16] http://www.epa.gov/ttn/scram/guidance/guide/final-03-pm-rh-guidance.pdf

[17] http://www.epa.gov/ttn/scram/guidance/guide/uamreg.pdf

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 the absolute minimum.

3.1.2 Secondary 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 as possible.

EPA suggests that modeling an entire summer ozone season for ozone or an entire year for $PM_{2.5}$ would be a good way to assure that a variety of meteorological conditions are captured and that sufficient days are available to construct robust relative response factors (RRFs) for the 8-hour ozone and $PM_{2.5}$ Design Value projections.

3.2 EPISODE SELECTION RESULTS

The 3SAQS 2008 simulations are being built off of the WestJumpAQMS modeling. The 2008 calendar year was selected for the WestJumpAQMS modeling because it satisfied more of the 8 episode selection criteria listed above than other recent years:

1. Modeling the entire year of 2008 will capture a variety of conditions that lead to elevated ozone and $PM_{2.5}$ concentrations in the western U.S.
2. Of recent years, 2008 had the highest ozone concentrations of any year. 2009 was not only less conducive to photochemical production but emissions were also depressed due to the recession. 2010 ozone was also lower than 2008.
3. There is some special study data in 2008, including ozonesondes at two sites and a special study site in Erie, Colorado[18]. 2010 included the CalNex field study[19] that provides enhanced measurement data mainly in California. 2008 is also a National Emissions Inventory (NEI) update year that is an important database for modeling.
4. An annual simulation will assure sufficient days are available to analyze ozone and $PM_{2.5}$ impacts. Annual simulations also allow the assessment of annual AQ/AQRV issues such as sulfur and nitrogen deposition, annual average NAAQS and annual average evaluation using NADP, CASTNet and other observation networks.
5. 2008 is being used for other studies including several BLM Environmental Impact Statements (EISs) and Resource Management Plans (RMPs) as well as the Denver ozone SIP modeling being conducted by the Denver Regional Air Quality Council (RAQC) and the Colorado Department of Public Health and Environment (CDPHE).
6. The ozone Design Values used to make nonattainment area designations for the March 2008 ozone NAAQS were based on the 2008-2010 three-year period that includes 2008.
7. With an annual run, all weekend days in a year are included.
8. 2008 satisfies the most episode selection criteria of any recent year.

---

[18] http://esrl.noaa.gov/csd/groups/csd7/measurements/2008Erie/
[19] http://esrl.noaa.gov/csd/projects/calnex/

The decision to model for an entire calendar year rather than just for the summer ozone season is due to a need to address PM$_{2.5}$, visibility and deposition issues as well as recognition of the recent events in Wyoming and Utah that found elevated ozone concentrations in the winter. However, the model will not be configured to simulate the winter ozone events at this time, which requires more focused local-scale modeling of cold pooling. However, the 3SAQS modeling may be useful for providing the regional transport component (i.e., boundary conditions) to more focused finer-scale winter ozone modeling analysis in a future study.

4.0 DOMAIN SELECTION

This Chapter summarizes the model domain definitions for the 3SAQS photochemical grid modeling (PGM), including the domain coverage, resolution, map projection, and nesting schemes for the high resolution sub-domains. The modeling domains for the WRF meteorological modeling are defined slightly larger than the PGM domains and are given in Chapter 5 with more details provided in the WestJumpAQMS WRF Application/Evaluation Report (ENVIRON and Alpine, 2012).

4.1 HORIZONTAL MODELING DOMAIN

The WestJumpAQMS, and subsequently 3SAQS, modeling domains were selected as a trade-off between the need to have high resolution modeling for sources in the Inter-Mountain West versus ability to perform regional ozone and particulate matter source apportionment modeling among all of the western states. Where the WestJumpAQMS included a 4 km inner nest, the 3SAQS only simulated the 36 and 12 km domains for the 2008-based simulations. The WRF meteorological model requires use of an odd nesting ratio so the 36/12 km domains are using a 3:1 grid-nesting ratio. A Lambert Conformal Projection (LCP) was used for the 3SAQS 36/12 km horizontal modeling domains using the parameters in Table 4-1 with their extent defined in Figure 4-1.

- A 36 km continental U.S. (CONUS) domain that is the same as used by the RPOs (e.g., WRAP) and most other recent modeling studies (e.g., Denver Ozone SIP). It is defined large enough so that the outer boundaries are far away from our primary areas of interest (i.e., western states).

- A 12 km western U.S. (WESTUS) domain is larger than used in WRAP and contains all of the WRAP and adjacent states as well as extending into Canada and Mexico.

Figure 4-1 displays the 36 km CONUS and 12 km WESTUS processing domains and the definition of their extent. The SMOKE and MEGAN emissions modeling will be conducted on the 36/12 km domain grid structure shown in Figure 4-1. The 4km domain shown in Figure 4-1 is not being used for the 3SAQS.
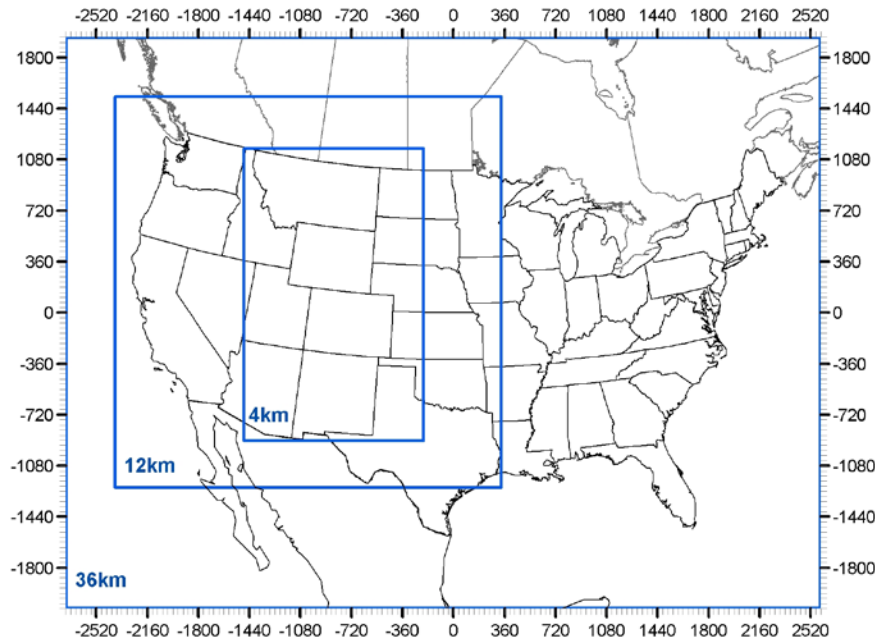
Modeling Domain

36km: 148 x 112 (-2736, -2088) to (2592, 1944)
12km*: 227 x 230 (-2388, -1236) to (336, 1542)
04km*: 317 x 515 (-1480, -904) to (-212, 1156)

* includes buffer cells

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

Table 4-1. Projection parameters for the 3SAQS modeling domains.

Parameter	Value
Projection	Lambert-Conformal
1st True Latitude	33 degrees N
2nd True Latitude	45 degrees N
Central Longitude	-97 degrees W
Central Latitude	40 degrees N

4.2 VERTICAL DOMAIN STRUCTURE

The CAMx vertical domain structure will depend on the definition of the WRF vertical layers structure. WRF was run with 37 vertical layer interfaces (36 vertical layers using CAMx definition of layer thicknesses) from the surface up to 50 mb (~19-km AGL) (ENVIRON and Alpine, 2012[20]). 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). A layer averaging scheme is adopted for the CAMx simulations

---

[20] http://www.wrapair2.org/pdf/WestJumpAQMS_2008_Annual_WRF_Final_Report_February29_2012.pdf

whereby multiple WRF layers are combined into one CAMx layer to reduce the air quality model computational time. Table 4-3 displays the approach for collapsing the WRF 36 vertical layers to 25 vertical layers in CAMx. In previous modeling for WRAP and the 2008 Denver ozone SIP, 19 vertical layers were used that resulted in some very thick vertical layers near the top of the modeling domain that contributed to the too rapid transport of high ozone concentrations of stratospheric ozone origin to the ground (Emery et al., 2009a,b).

The WRF layer collapsing scheme in Table 4-3 is collapsing two WRF layers into one CAMx layer for the lowest four layers in CAMx. In the past, the lowest layers of MM5/WRF were mapped directly into CAMx with no layer collapsing. However, in those applications the MM5/WRF layer 1 was much thicker (20-40 m) than used in this WRF application (12 m). Use of a 12 m lowest layer may trap emissions in a too shallow layer resulted in overstated surface concentrations. For example, NO_X emissions are caused by combustion so are buoyant and have plume rise that in reality could take them out of the first layer if it is defined too shallow. However, there is concern that layer collapsing of the lowest WRF layers may introduce uncertainties or errors in the modeling.

The Denver ozone SIP planning modeling of the May-August 2008 period used the same vertical layer structure as being used in 3SAQS and the same 36 WRF to 25 CAMx layer collapsing strategy. They conducted a no layer collapsing CAMx sensitivity test (36 vertical layers) and found it had essentially no effect on the afternoon and daily maximum 8-hour ozone concentration estimates (Morris et al., 2012a). The 36 layer CAMx sensitivity tests produced lower nighttime ozone at many sites, but it tended to degrade rather than improve ozone model performance. The 36 layer sensitivity tests also took 22% more time to run than the 25 vertical layer base case. The Allegheny County Health Department (ACHD) Liberty-Clairton $PM_{2.5}$ SIP modeling[21] also used the same 36 WRF to 25 CAMx layer collapsing strategy as used in the 3SAQS. ACHD also did a no layer collapsing sensitivity test and found essentially no difference in the CAMx-estimated $PM_{2.5}$ concentrations (Morris, Koo, Jung, Loomis and McNally, 2012). The BLM Continental Divide-Creston (CD-C) oil and gas development Environmental Impact Statement (EIS) study in southwestern Wyoming also performed a layer collapsing sensitivity test. Although CD-C layer collapsing strategy was slightly different than 3SAQS, as CD-C was collapsing 34 WRF to 21 CAMx vertical layers with the layer collapsing occurring in the upper layers. However, the rural southwestern Wyoming location of the focus of the CD-C modeling is similar to large expanses of the 3SAQS modeling. As seen in the Denver and ACHD layer collapsing sensitivity tests, the CD-C no layer collapsing sensitivity run produced essentially identical modeling results as was seen when layer collapsing was utilized (BLM, 2012). Based on these findings, it appears that when many layers are used (e.g., > 20) the effects of layer collapsing on the CAMx air quality modeling results are minimal.

---

[21] http://www.achd.net/air/index.php

Table 4-3. 37 Vertical layer interface definition for WRF simulations (left most columns), and approach for reducing to 25 vertical layers for CAMx by collapsing multiple WRF layers (right columns).

WRF Layer	Sigma	Pressure (mb)	Height (m)	Thickness (m)	CAMx Layer	Height (m)	Thickness (m)
37	0.0000	50.00	19260	2055	25	19260.0	3904.9
36	0.0270	75.65	17205	1850			
35	0.0600	107.00	15355	1725	24	15355.1	3425.4
34	0.1000	145.00	13630	1701			
33	0.1500	192.50	11930	1389	23	11929.7	2569.6
32	0.2000	240.00	10541	1181			
31	0.2500	287.50	9360	1032	22	9360.1	1952.2
30	0.3000	335.00	8328	920			
29	0.3500	382.50	7408	832	21	7407.9	1591.8
28	0.4000	430.00	6576	760			
27	0.4500	477.50	5816	701	20	5816.1	1352.9
26	0.5000	525.00	5115	652			
25	0.5500	572.50	4463	609	19	4463.3	609.2
24	0.6000	620.00	3854	461	18	3854.1	460.7
23	0.6400	658.00	3393	440	17	3393.4	439.6
22	0.6800	696.00	2954	421	16	2953.7	420.6
21	0.7200	734.00	2533	403	15	2533.1	403.3
20	0.7600	772.00	2130	388	14	2129.7	387.6
19	0.8000	810.00	1742	373	13	1742.2	373.1
18	0.8400	848.00	1369	271	12	1369.1	271.1
17	0.8700	876.50	1098	177	11	1098.0	176.8
16	0.8900	895.50	921	174	10	921.2	173.8
15	0.9100	914.50	747	171	9	747.5	170.9
14	0.9300	933.50	577	84	8	576.6	168.1
13	0.9400	943.00	492	84			
12	0.9500	952.50	409	83	7	408.6	83.0
11	0.9600	962.00	326	82	6	325.6	82.4
10	0.9700	971.50	243	82	5	243.2	81.7
9	0.9800	981.00	162	41	4	161.5	64.9
8	0.9850	985.75	121	24			
7	0.9880	988.60	97	24	3	96.6	40.4
6	0.9910	991.45	72	16			
5	0.9930	993.35	56	16	2	56.2	32.2
4	0.9950	995.25	40	16			
3	0.9970	997.15	24	12	1	24.1	24.1
2	0.9985	998.58	12	12			
1	1.0000	1000	0			0	

5.0 METEOROLOGICAL MODELING

The WRF meteorological model was applied for the 2008 calendar year using a 36/12/4 km domain structure; only the 36 and 12 km domains are being used for the 3SAQS. The WRF modeling results for the 2008 annual period were evaluated against surface meteorological observations of wind speed, wind direction, temperature and humidity and the WRF model performance was compared against meteorological modeling benchmarks and with past regional meteorological model performance evaluations (ENVIRON and Alpine, 2012). The WRF precipitation fields were also compared against analysis fields that were based on observations from the Climate Prediction Center (CPC).

5.1 MODEL SELECTION AND APPLICATION

The 3SAQS project is using the current publicly available version of WRF (version 3.3). The WRF preprocessor programs including GEOGRID, UNGRIB, and METGRID were used to develop model inputs.

5.2 WRF DOMAIN DEFINITION

The WRF computational grid was designed so that it can generate CAMx meteorological inputs for the 36 km CONUS and 12 km domains depicted in Figure 4-1 in Chapter 4. The WRF modeling domain was defined to be slightly larger than the CAMx PGM modeling domains to eliminate the occurrence of boundary artifacts in the meteorological fields used as input to CAMx. Such boundary artifacts can occur as the boundary conditions (BCs) for the meteorological variables come into dynamic balance with WRF's atmospheric equations and numerical methods. Figure 5-1 depicts the WRF horizontal modeling domain used in 3SAQS with the WRF 37 vertical layer structure presented previously in Table 4-2. The outer 36 km domain (D01) has 165 x 129 grid cells, selected to be consistent with existing Regional Planning Organization (RPO) and EPA modeling CONUS domain. The projection is Lambert Conformal with the "national RPO" grid projection pole of 40°, -97° with true latitudes of 33° and 45°. The 12 km has 256 x 253 grid cells with offsets from the 36 km grid of 15 columns and 26 rows. The nests were run together with continuous updating without feedback from the 12 km to 36 km or from the 4 km to 12 km domains.

5.3 TOPOGRAPHIC INPUTS

Topographic information for the WRF was developed using the standard WRF terrain databases available from the National Center for Atmospheric Research (NCAR)[22.] The 36 km CONUS domain was based on the 10 min. (~18 km) global data. The 12 km WESTUS domain was based on the 2 min. (~4 km) data.

5.4 VEGETATION TYPE AND LAND USE INPUTS

Vegetation type and land use information was developed using the most recently released WRF databases provided with the MM5 distribution. Standard WRF surface characteristics corresponding to each land use category were employed.

---

[22] http://dss.ucar.edu/
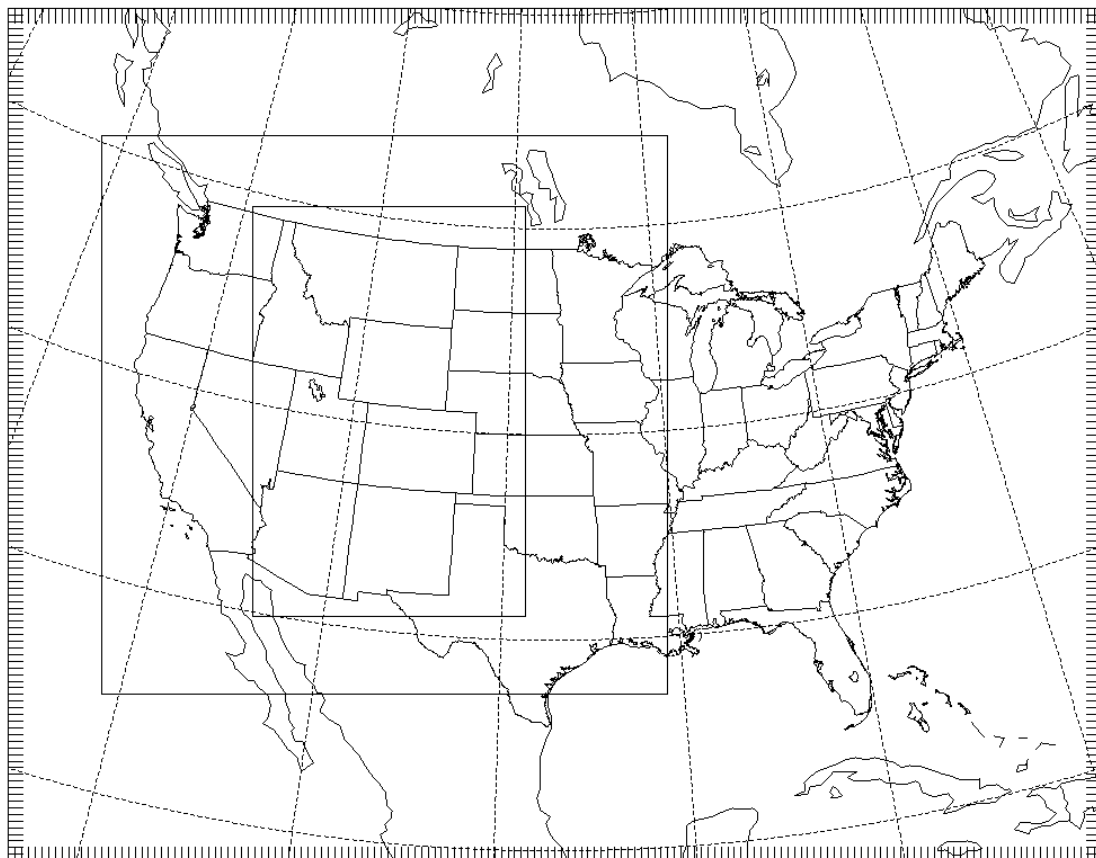
Figure 5-1. WRF 36/12/4 km grid structure for the WestJumpAQMS meteorological modeling. 3SAQS used the 36/12 km grids.

5.5 ATMOSPHERIC DATA INPUTS

The first guess fields were taken from the 12km (Grid #218) North American Model (NAM) archives available from the National Climatic Data Center (NCDC) NOMADS server.

5.6 WATER TEMPERATURE INPUTS

The water temperature data were taken from the NCEP RTG global one-twelfth degree analysis.

5.7 FDDA DATA ASSIMILATION

The WRF simulation used analysis nudging for the 36 and 12 km domains and observation nudging in the 4 km domain. For winds and temperature, analysis nudging coefficients of $5x10^{-4}$ and $3.0x10^{-4}$ were used on the 36 km and 12 km grids, respectively. For mixing ratio, analysis nudging coefficients of $1.0x10^{-5}$ were used for both the 36 km and 12 km grids. The nudging used both surface and aloft nudging with nudging for temperature and mixing ratio excluded in the boundary layer. Observation nudging was performed on the 4 km grid domain using the Meteorological Assimilation Data Ingest System (MADIS)[23] observation archive. The MADIS archive includes the National Climatic Data Center (NCDC)[24] observations and the National Data Buoy Center (NDBC) Coastal-Marine Automated Network C-MAN[25] stations. The observational nudging coefficients for winds, temperatures and mixing ratios were $1.0x10^{-4}$, $1.0x10^{-4}$, and $1.0x10^{-5}$, respectively and the radius of influence was set to 50 km.

5.8 WRF PHYSICS OPTIONS

The WRF model contains many different physics options. WRF physics options for an initial 2008 calendar year 36/12/4 km WRF simulation were based on our extensive experience with MM5 meteorological modeling and initial experience with WRF modeling of the Rocky Mountains and used the Pleim-Xu land-surface model (LSM), ACM2 planetary boundary layer (PBL) model and the Kain-Fritsch cumulus parameterization. An evaluation of the initial WRF 2008 36/12/4 km simulation identified performance issues related to overstated precipitation amounts over the western U.S. in the 36 km CONUS, 12 km WESTUS and 4 km IMWD domains. Numerous sensitivity simulations were conducted both for a winter (February) and summer (July) period in order to determine more optimal WRF physics options, including a run with no cumulus parameterization in the 36/12 km domains. The WRF sensitivity modeling identified the following physics options as producing improved meteorological fields over the western U.S. so were used in the final WestJumpAQMS 2008 36/12/4 km WRF simulation:

- WSM 3-class simple ice scheme (mp_physics=3)

- RRTMG long wave radiation (ra_lw_physics=4)

- RRTMG short wave radiation (rw_sw_physics=4)

- Monin-Obukhov surface layer (sf_sfclay_physics=1)

- Unified NOAH land-surface model (sf_surface_physics=2)

---

[23] Meteorological Assimilation Data Ingest System. http://madis.noaa.gov/
[24] National Climatic Data Center. http://lwf.ncdc.noaa.gov/oa/ncdc.html
[25] National Data Buoy Center. http://www.ndbc.noaa.gov/cman.php

- Kain-Fritsch cumulus parameterization in the 36/12 km domains and no cumulus parameterization (cu_physics=0) in the 4 km domain

- YSU planetary boundary layer (bl_pbl_physics=7)

5.9 APPLICATION METHODOLOGY

The WRF model was executed in 5-day blocks initialized at 12Z every 5 days with a 90 second time step. Model results were output every 60 minutes and output files were split at 24 hour intervals. Twelve (12) hours of spin-up was included in each 5-day block before the data were used in the subsequent evaluation. The model was run at both the 36 km and 12 km resolution from December 15, 2007 through January 4, 2009.

5.10 EVALUATION APPROACH

The WRF model evaluation approach was based on a combination of qualitative and quantitative analyses. The qualitative approach was to compare the spatial distribution of the model estimated monthly total precipitation with the monthly Center for Prediction of Climate (CPC) precipitation analysis using graphical outputs. The statistical approach was to examine tabulations and graphical displays of the model bias and error for surface wind speed, wind direction, temperature, and mixing ratio (humidity) and compare the performance statistics to benchmarks developed based on a history of meteorological modeling as well as past meteorological model performance evaluations.

Interpretation of bulk statistics over a continental or regional scale domain is problematic and it is difficult to detect if the model is missing important sub-regional features. For this analysis the statistics were performed on a state by state basis, a Regional Planning Organization (RPO) basis, and on a domain-wide basis for the 36 km CONUS, 12 km WESTUS and 4 km IMWD modeling domains. In addition, separate evaluation was also conducted for each IAD and DSAD domains that are the main focus of the WestJumpAQMS study.

The observed database for winds, temperature, and water mixing ratio used in this analysis was the National Oceanic and Atmospheric Administration (NOAA, Earth System Research Laboratory (ESRL) Meteorological Assimilation Data Ingest System (MADIS). The rain observations are taken from the NOAA Climate Prediction Center (CPC) retrospective rainfall archives available at http://www.cpc.ncep.noaa.gov/products/precip/realtime/retro.shtml.

5.11 REPORTING

The WestJumpAQMS application and evaluation is documented in a report prepared by ENVIRON and Alpine Geophysics, LLC (ENVIRON and Alpine, 2012[26]). The model evaluation was performed for winds, temperature, humidity and precipitation grouped by RPO region, western state and even down to the individual monitor for sites in the western U.S. Details are provided in the final WestJumpAQMS WRF Application/Evaluation report. No change was made to the WestJumpAQMS WRF results before using them for the 3SAQS.

6.0 EMISSIONS

The section presents the emissions database that we will compile for the 3SAQS 2008 base and future year modeling simulations. Emissions data fall into three broad categories:

---

[26] http://wrapair2.org/pdf/WestJumpAQMS_2008_Annual_WRF_Final_Report_February29_2012.pdf

- Inventory data – county total estimates of emissions from explicit source categories

- Gridded data – fluxes of emissions by grid cell or gridded data that are used to calculate emissions fluxes

- Ancillary data – non-inventory emissions data that characterize the spatial/chemical/temporal patterns of emissions

Descriptions of these three types of data used for the base year and future year 3SAQS emissions are described here.

6.1 BASE YEAR 2008 EMISSIONS

The modeling periods and domains for the 3SAQS that are described in the WestJumpAQMS 2008 WRF Modeling Protocol (ENVIRON and Alpine, 2012) dictate the temporal and spatial coverage requirements of the 3SAQS 2008 emissions. We will develop an emissions modeling platform, which consists of data and software, to estimate air emissions fluxes that best represent the conditions in the 3SAQS modeling domain and modeling period. The base 2008 modeling period is annual, starting with a model spin-up period on December 15, 2007 and ending December 31, 2008. The modeling domain includes a 36-km continental US (CONUS) domain with a 12-km nest over the western U.S. (Figure 4-1).

The following sectors will be used to represent air pollutant emissions for the 3SAQS:
- Inventory Data
    - Aircraft/locomotive/marine
    - Off-road mobile
    - On-road mobile
    - Non-point/Area (including agriculture and fugitive dust)
    - Area oil and gas
    - Point oil and gas
    - Continuous Emission Monitor (CEM) point
    - Non-CEM point
    - Offshore shipping
    - Fires
    - Canada and Mexico sources
- Gridded data
    - MEGAN biogenics
    - Windblown dust
    - Sea salt
    - Lightning

Details of the sources and nature of these emissions data are provided in the following sections.

6.1.1 Inventory Data

Anthropogenic emissions sources are inventoried as either point or non-point sources. Characteristics of point sources include a state/county code, plant/source/stack identifier, source classification code (SCC), and a latitude-longitude coordinate. Additional details in the point inventories are required if the sources are inventoried with Continuous Emissions Monitors (CEMs) or if they are fire sources. Characteristics of non-point sources include a state/county code and SCC. Non-point sources can further be broken down as either mobile or non-mobile sources, with special characteristics required for mobile sources. Descriptions of the different inventory sectors used for the 3SAQS modeling, including the sources of these data, are provided in this section.

All of the non-oil and gas (O&G) inventories for the 3SAQS are from the 2008 U.S. EPA National Emission Inventory (NEI). We will use the 2008-based 2007v5 platform[27] and the 2008v2 platform[28] inventories for representing the year 2008 emissions in the 3SAQS. EPA publically released the 2007v5 platform in December 2012 and the 2008v2 platform in April 2012. EPA developed and applied the 2007v5 platform for the Regulatory Impact Assessment (RIA) of the 2012 Final National Ambient Air Quality Standards (NAAQS) for particulate matter less than 2.5 microns ($PM_{2.5}$).

As many of the 3SAQS inventory sectors are based on the WestJump Air Quality Modeling Study (WestJumpAQMS) 2008 modeling platform, they are documented in a series of memos available as part of the WestJumpAQMS final report[29]. Table 6-1 lists the inventory sectors that we will simulate for the 3SAQS and includes the source of the data and other details about the inventory.

Table 6-1. 3SAQS inventory sectors

Sector	NEI Source	Type	Inventory Period	Description
Aircraft/ locomotive/ marine*	2008v2	Point and Nonpoint	Annual	The aircraft/locomotive/marine (ALM) sector is a subset of the non-point/area sector. It includes county-level emissions at airports (point), line haul locomotives (nonpoint), train yards (point), and class 1 and 2 in- and near-shore commercial marine
Off-road mobile*	2008v2	Nonpoint	Monthly	NONROAD2008 county-level inventories for recreational vehicles, logging equipment, agricultural equipment, construction equipment, industrial equipment, lawn and garden equipment, leaf and snow blowers, and recreational marine
On-road mobile	2007v5	MOVES	Annual and Daily	EPA ran MOVES for 2008 in emissions factor mode. The MOVES lookup tables include on-network (RPD), on-network refueling (RPDrfl), off-network starts/stops (RPV), off-network starts/stops refueling (RPVrfl), and off-network vapor venting (RPP) sources. These data include the reference county and reference fuel month assignments that EPA used for the MOVES simulation.
Non-point/ Area*	2008v2	Nonpoint	Annual	County-level emissions for sources that individually are too small in magnitude or too numerous to inventory as individual point sources. Includes small industrial, residential, and commercial sources; agricultural sources; and fugitive dust sources
Area Oil & Gas*	WRAP P3 and 2008v2	Nonpoint	Annual	The non-point O&G sector consists of the WRAP Phase III 2006 inventory grown to 2008, a 2008 Permian basin inventory, and the NEI08v2 inventory for all areas outside of the WRAP Phase III inventory coverage area
Point Oil &	WRAP P3	Point	Annual	The point O&G sector consists of the WRAP Phase III

[27] http://www.epa.gov/ttn/chief/emch/index.html - 2008
[28] ftp://ftp.epa.gov/EmisInventory/2008dev/README.txt
[29] http://www.wrapair2.org/WestJumpAQMS.aspx

Gas*	and 2008v2			2006 inventory grown to 2008, a 2008 Permian basin inventory, and the NEI08v2 inventory for all areas outside of the WRAP Phase III inventory coverage area
CEM Point*	2008v2 and CAMD	Point	Hourly	2008 Clean Air Markets Division (CAMD) hourly Continuous Emissions Monitor (CEM) data
non-CEM Point*	2008v2	Point	Annual	Elevated and low-level combustion and industrial sources, airports, and offshore drilling platforms.
Offshore Shipping*	2008v2	Point	Annual	Elevated point C3 commercial marine sources in offshore commercial shipping lanes
Fires*	DEASCO3	Point	Hourly	Hourly agricultural, prescribed, and wildfire sources with pre-computed plume parameters and speciated PM.
Canada Sources*	NPRI2006	Nonpoint and Point	Annual	Canadian 2006 National Pollutant Release Inventory
Mexico Sources*	MNEI99	Nonpoint and Point	Annual	Mexican NEI 1999 grown to 2008

* Taken directly from the WestJumpAQMS 2008 modeling platform and documented in the WestJumpAQMS emissions modeling memos

6.1.2 Gridded Data

Several gridded datasets are used for either directly estimating air emissions or as ancillary data for processing/adjusting the emissions data. The following datasets are key gridded data used for the 3SAQS.

Biogenic Emissions Model Inputs

The major components of biogenic emissions models include:

- Leaf Area Index (LAI)

- Plant Functional Type (PFT)

- Plant specific species composition data and averaging

- Emissions factors, including the effects of temperature and photosynthetically active radiation (PAR)

The gridded data for input the MEGANv2.10 biogenic model used to estimate 2008 biogenic emissions for the WestJumpAQMS and adopted directly for used in the 3SAQS include the following:

Leaf Area Index (LAI): A gridded dataset of 46 8-day files for North America were generated for 2008 at 1-km resolution

Plant Functional Type (PFT): A gridded dataset of 9 PFTs were developed at both 1-km and 56-m resolutions across the modeling domains.

Photsynthetically Active Radiation (PAR): Satellite PAR gap-filled with WRF solar radiation fields scaled by a factor of 0.45

Additional details on the development and evaluation of the gridded data used for the WestJumpAQMS and 3SAQS are available in the final report on the WRAP Biogenic Emissions Study[30].

Land use/Land cover Data for Estimating Windblown Dust (WBD) Emissions

The major components of the WRAP WBD model include:

- Land use/land cover (LULC)

- Soil characteristics

- Surface roughness lengths

- Meteorology (wind-speeds and friction velocities)

The gridded data for input to the WRAP WBD Model used to estimate 2008 emissions for the WestJumpAQMS and adopted directly for used in the 3SAQS include the following:

Land use/Land cover (LULC): Gridded dataset of 1-km year 2000 North American Land Cover (NALC) regridded to the WestJump modeling domains

Soil characteristics: Gridded 12-category State Soil Geographic Database (STATSGO) mapped to the 4-category classification used in the WRAP WBD

Surface roughness lengths: Values reported in the literature as of 2006 were mapped to the land use categories in the NALC

Additional details on the development and evaluation of the gridded data used for the WestJumpAQMS and 3SAQS are available in the final report on the WRAP WBD[31].

Fugitive Dust Transport Factors

Transport factors are applied to the primary dust emissions estimates to adjust the emissions for vegetative scavenging. The dust models and emissions factors are based on soil characteristics and do not account for the presence of vegetation, which has a mitigating effect on both winds and dust emissions. An ad-hoc approach of adjusting dust emissions estimates has been developed that uses gridded land cover data to simulate the impacts of vegetation cover on dust.

For the 3SAQS 2008 modeling platform we will use the dust transport factors collected for the WestJumpAQMS. WestJumpAQMS implemented fugitive dust correction factors that are derived from the Biogenic Emission Landuse Database version 3 (BELD3)[32]. Following the approach of Pouliot et al.[33] we adjusted the fugitive and road dust emissions as a post-processing step after the emissions data were output from SMOKE. We used transport factors gridded to each of the

---

[30] http://www.wrapair2.org/pdf/WGA_BiogEmisInv_FinalReport_March20_2012.pdf

[31] http://www.wrapair.org/forums/dejf/documents/WRAP_WBD_PhaseII_Final_Report_050506.pdf

[32] Vukovich, J. and T. Pierce (2002) "The Implementation of BEIS3 within the SMOKE Modeling Framework", In Proceedings of the 11th International Emissions Inventory Conference, Atlanta, Georgia, April 15-18, 2002. Available online: http://www.epa.gov/ttn/chief/conference/ei11/modeling/vukovich.pdf

[33] Pouliot, G. et al. (2010) "Assessing the Anthropogenic Fugitive Dust Emission Inventory and Temporal Allocation Using an Updated Speciation of Particulate Matter", In Proceedings of the 19th International Inventory Conference, San Antonio, TX, September 27-30, 2010. Available online: http://www.epa.gov/ttn/chief/conference/ei19/session9/pouliot.pdf.

WestJumpAQMS modeling domains to reduce the dust emissions. The values of the transport factors associated with each BELD3 land cover category are available in Pouliot et al.

6.1.3 Ancillary Emissions Data

Ancillary emissions data includes all of the factors and support files required to convert inventory and gridded data to the input formats and terms expected by a PGM, including:

- **Spatial data.** All anthropogenic non-point inventory data, including on-road and non-road mobile sources, are estimated at the county level. Data files called spatial surrogates are used to map the county-level emission inventories to the model grid cells. Spatial surrogates are generated from Geographic Information System (GIS) Shapefiles using software that calculates the fractions of county-level different geospatial attributes in a model grid cell. For example, a Shapefile of the housing distribution in Los Angeles County is combined with a description of a modeling grid to calculate the percentage of L.A. County housing assigned to each grid cell. This information is then used to allocate county-level emission inventory sources that are associated with housing (e.g. residential wood combustion) to the modeling grids.

  Spatial surrogates require cross-referencing data that assign a spatial surrogate to specific categories of inventory sources. Spatial cross-reference files assign surrogates to inventory sources using country/state/county codes (FIPS) and source classification codes (SCCs).

- **Temporal data.** Air quality modeling systems, such as CMAQ and CAMx, require hourly emissions input data. With the exception of a few source types (e.g. Continuous Emissions Monitoring data, biogenic emissions and some fire inventories), most inventory data include annual or daily emission estimates. Temporal profiles are used to compute hourly emissions from the annual or daily inventory estimates. The SMOKE model, which is being used to process emission for the 3SAQS, uses three types of temporal profiles:

  1. Monthly profiles: Convert annual inventory to monthly emissions accounting for seasonal and other effects.

  2. Daily profiles: Convert monthly emissions to daily emissions accounting for day-of-week and other effects.

  3. Hourly profiles: Convert daily emissions to hourly emissions accounting for the diurnal variation in emissions (e.g., work schedules and commute times).

  Temporal profiles are assigned to inventory sources using cross-referencing data that match the profiles and inventory sources using country/state/county (FIPS) and source classification codes (SCCs).

- **Chemical speciation data.** Emissions inventories have limited chemical composition information. The emissions inventories for the 3SAQS include 6 criteria pollutants: carbon monoxide (CO), nitrogen oxides (NO_X), volatile organic compounds (VOC), ammonia (NH_3), sulfur dioxide (SO_2), particulate matter with a mean diameter < 10 micrometers (PM_{10}), and particulate matter with a mean diameter < 2.5 micrometers ($PM_{2.5}$). Chemical speciation profiles are used to describe the chemical compositions of the effluent from particular emissions sources. The exact specification of the source-specific emissions species is determined by the chemistry mechanism selected for the AQM simulation. Speciation profiles convert the inventory pollutants to more detailed source-specific species in terms required by the AQM chemistry mechanism. For example, there is a speciation profile that converts the inventory pollutant

NO$_X$ to the AQM input species NO, NO$_2$, and HONO. Speciation profiles are required to convert inventory NO$_X$, VOC, SO$_2$, and PM$_{2.5}$ into AQM species. For the 3SAQS SMOKE emissions modeling the CB05 chemical mechanism will be utilized and VOC will be speciated using source specific speciation profiles developed using the SPECIATE 4.3 database[34].

Chemical speciation profiles are assigned to inventory sources using cross-referencing data that match the profiles and inventory sources using country/state/county (FIPS) and source classification codes (SCCs).

The base set of ancillary data for 3SAQS will be taken directly from the EPA 2008v2 modeling platform. These were the same data used for the WestJumpAQMS and are detailed in WestJumpAQMS Final Emissions Modeling Parameters Technical Memo[35]. For the 3SAQS, we made targeted improvements to the ancillary files for counties in the 3-state study region (Figure 6-1). We focused the improvements on the assignments of spatial/chemical/temporal profiles to inventory sources and on developing profiles that best represent the emissions patterns in the 3-state study region.
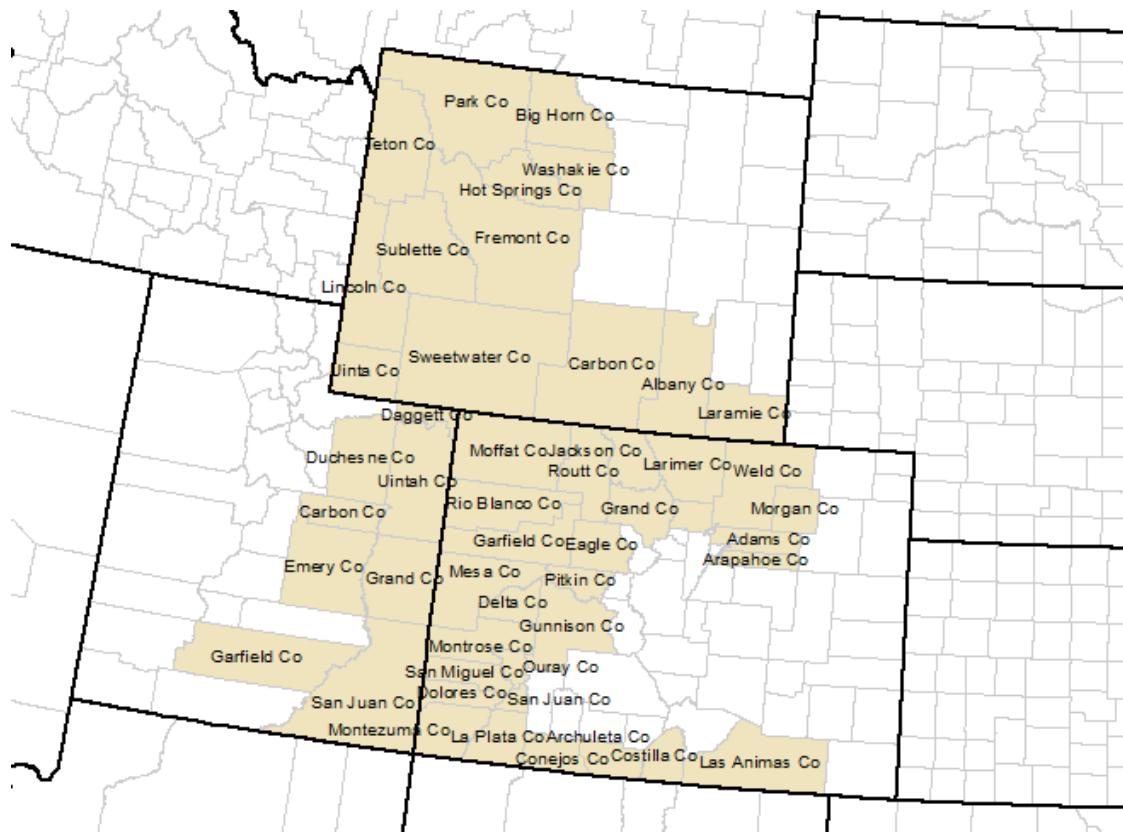
Figure 6-1. Preliminary list of counties in the 3-state study region

By targeting the largest emitters (top 90% of annual NOx and VOC emitters) in the three state region, we maximized the improvement effort by limiting the number of sources to those with the largest impact on air quality. The results of this effort were presented to the states of Utah, Colorado, and Wyoming in a series of

---

[34] http://www.epa.gov/ttnchie1/software/speciate/
[35] http://www.wrapair2.org/pdf/Memo13_Parameters_Sep30_2013.pdf

3SAQS workshops during January 2013. The improvements that we made for the CO/UT/WY counties include the following:

Utah

Updated the NEI08v2 spatial surrogates for land cover and building square footage with NLCD2006 and FEMA-HAZUS data

Changed the ATV/ORV/Snowmobile surrogate assignment from rural land area to forest land

Changed the livestock surrogate assignment from total agricultural land to pasture land

Changed the fertilizer surrogate assignment from total agricultural land to crop land

Created a state-specific, year 2008 monthly temporal profile for residential natural gas heating fuel use with Energy Information Administration data (Figure 6-2).

Colorado

Updated the NEI08v2 spatial surrogates for land cover and building square footage with NLCD2006 and FEMA-HAZUS data

Changed the ATV/ORV/Snowmobile surrogate assignment from rural land area to forest land

Changed the livestock surrogate assignment from total agricultural land to pasture land

Changed the fertilizer surrogate assignment from total agricultural land to crop land

Created a state-specific, year 2008 monthly temporal profile for residential natural gas heating fuel use with Energy Information Administration data (Figure 6-2).

Developed 2008 vehicle miles traveled (VMT)-based spatial surrogates for on-road mobile sources. Figure 6-3 compares the U.S. Census year 2010 TIGER line roadway data with link-based VMT data from CO.

Wyoming

Updated the NEI08v2 spatial surrogates for land cover and building square footage with NLCD2006 and FEMA-HAZUS data

Changed the ATV/ORV/Snowmobile surrogate assignment from rural land area to forest land

Changed the livestock surrogate assignment from total agricultural land to pasture land

Changed the fertilizer surrogate assignment from total agricultural land to crop land

Created a state-specific, year 2008 monthly temporal profile for residential natural gas heating fuel use with Energy Information Administration data (Figure 6-2).

Developed confined animal feeding operation (CAFO) spatial surrogates for livestock sources. Figure 6-4 shows the locations of the CAFOs provided by WY. We converted these data to a point Shapefile and then generated WY livestock surrogates for cattle and swine for 3SAQS.
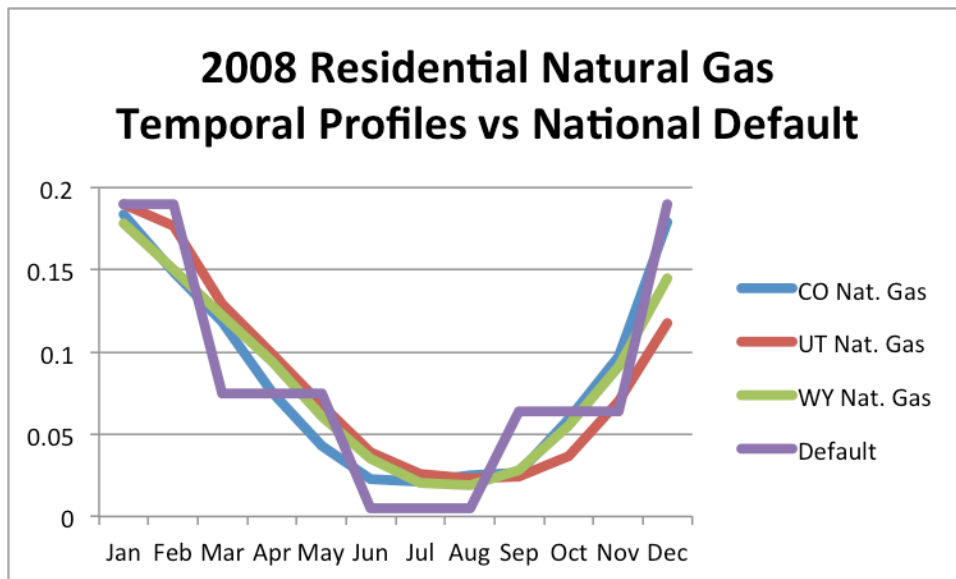
Figure 6-2. 3SAQS 2008 residential natural gas consumption monthly temporal profiles
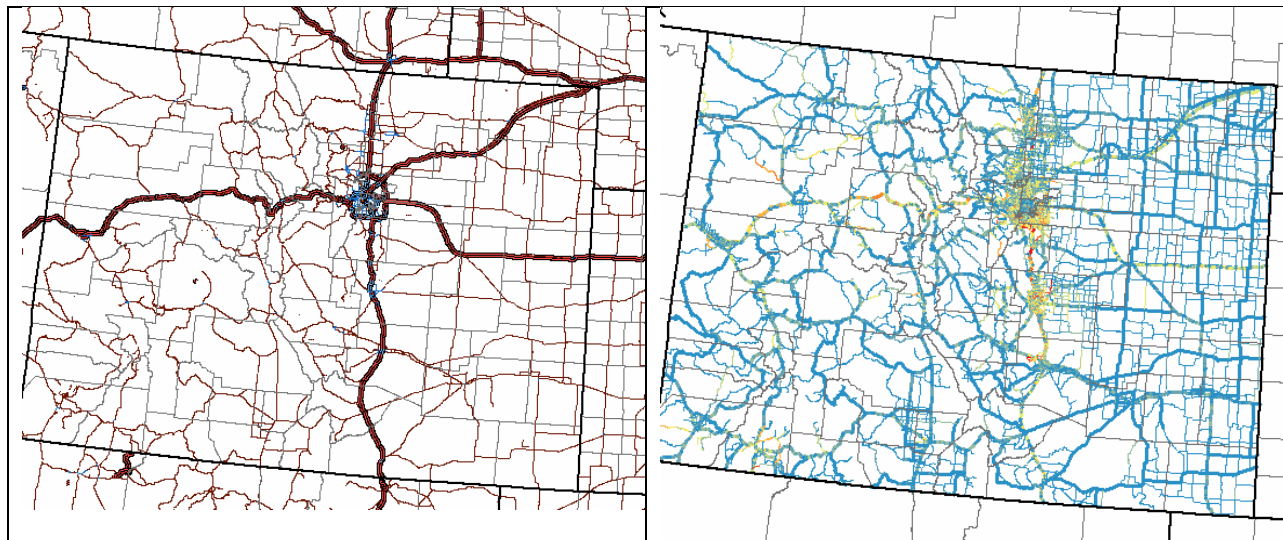
Figure 6-3. Colorado roadway spatial data improvement plots. Left: TIGER 2010 Shapefile of urban/rural primary/secondary roads. Right: CO 2008 VMT-based roadways
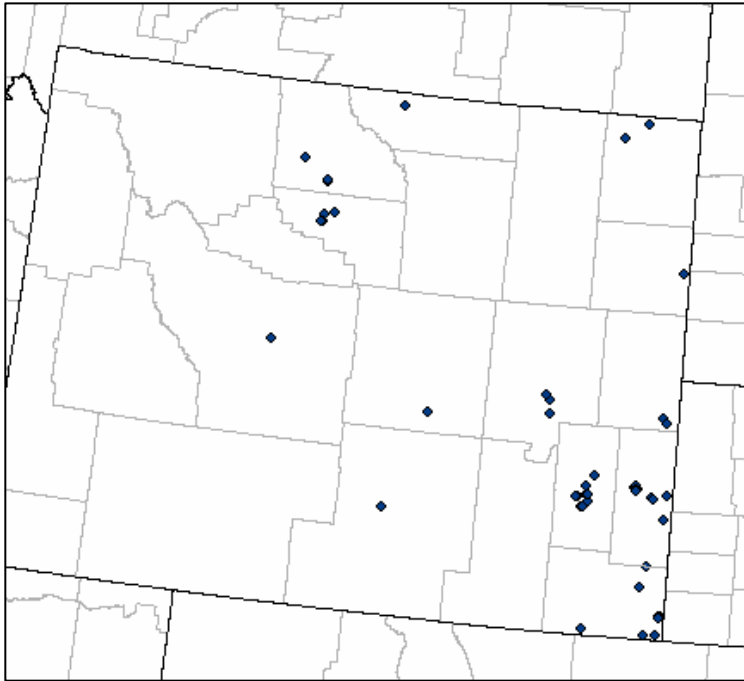
Figure 6-4. Wyoming CAFO locations

6.2 FUTURE YEAR 2020 EMISSIONS

We will prepare a future year modeling platform with inventories projected to 2020 using information on emissions growth and controls between the year 2008 and 2020. The inventory data for the 3SAQS 2020 emissions modeling platform will come primarily from the three sources:

• NEI08 (2007v5 modeling platform)

• 3SAQS 2008 → 2020 oil and gas inventory projections

• WestJumpAQMS

6.2.1 Non-Oil and Gas Future-Year Emissions Data

For all of the inventory sectors except oil & gas, biogenics, windblown dust, seasalt, and lightning, the 2020 inventory and ancillary emissions data will be taken directly from the EPA 2007v5 modeling platform. Developed by EPA for use in the PM$_{2.5}$ NAAQS RIA, the 2020 inventory represent the best estimate of future year emissions without the implementation of any new controls necessary to attain the current PM$_{2.5}$ annual and 24-hr (35 µg/m^3 and 15 µg/m^3) and ozone 8-hr (75 ppb) standards (EPA, 2012). These emissions reflect rule promulgated or under reconsideration as of July 2012.

A summary of the 2007v5 modeling platform 2020 inventory is provided below and additional details are available from EPA (2012).

• CEM Point: Unit-specific estimates from IPM, version 4.10 with CSAPR and Final MATS.
• Non-CEM Point: Projection factors and percent reductions reflect Cross-State Air Pollution Rule (CSAPR) comments and emission reductions due to national rules, control programs, plant closures, consent decrees and settlements and 1997 and 2001 ozone State Implementation Plans in NY, CT, and VA. EPA used projection approaches for corn ethanol and biodiesel plants, refineries and

upstream impacts from the Energy Independence and Security Act of 2007 (EISA). Terminal area forecast (TAF) data aggregated to the national level were used for aircraft to account for projected changes in landing/takeoff activity.

- Nonpoint/Area: Agricultural sector projection factors for livestock estimates based on expected changes in animal population from 2005 Department of Agriculture data, updated based on personal communication with EPA experts in July 2012; fertilizer application NH3 emissions projections include upstream impacts EISA. Fugitive dust projection factors for dust categories related to livestock estimates based on expected changes in animal population and upstream impacts from EISA. Other nonpoint source projection factors that implement Cross State Air Pollution Rule comments and reflect emission reductions due to control programs. Residential wood combustion projections are based on growth in lower-emitting stoves and a reduction in higher emitting stoves. PFC projection factors reflecting impact of the final Mobile Source Air Toxics (MSAT 2) rule. Upstream impacts from EISA, including post-2007 cellulosic ethanol plants are also reflected.
- Off-road Mobile: Other than for California, this sector uses data from a run of NMIM that utilized NONROAD2008a, using future-year equipment population estimates and control programs to the year 2020 and using national level inputs. Final controls from the final locomotive-marine and small spark ignition OTAQ rules are included. California-specific data were provided by CARB.
- Aircraft/locomotive/marine: For all states except California, projection factors for Class 1 and Class 2 commercial marine and locomotives, which reflect final locomotive-marine controls. California projected year-2020 inventory data were provided by CARB.
- Offshore shipping: Base-year 2007 emissions grown and controlled to 2020, incorporating controls based on Emissions Control Area (ECA) and International Marine Organization (IMO) global NOX and SO2 controls.
- On-road Mobile, not including refueling: MOVES2010b emissions factors for year 2020 were developed using the same representative counties, state-supplied data, meteorology, and procedures that were used to produce the 2007 emission factors. California-specific data were provided by CARB. Other than California, this sector includes all non-refueling on-road mobile emissions (exhaust, evaporative, evaporative permeation, brake wear and tire wear modes).
- On-road Refueling: Uses the same projection and processing approach as the on-road sector, except for California where EPA projected using MOVES2010b and did not include CARB data.
- Canada Sources: Held constant and 2006 levels
- Mexico Sources: Projections from 1999 to 2018

We will not make any changes to the ancillary emissions data (spatial/temporal/chemical) for the 2020 future year emissions. These data will be held constant at the 2008 values when preparing the 2020 emissions for CAMx.

3.2.2 O&G Future-Year Emissions Data

Future year O&G inventories for the states of Colorado, Wyoming, and Utah will be based off the 2008 WestJumpAQMS data and projected to 2020. We will first project the 2008 inventories to 2011 and then from 2011 to 2020. If 2011 inventories or permitted source data already exist (i.e. Wyoming, Colorado APENs data, Utah permit data), we will use these. For the basins in which 2011 inventories don't already exist, we will project the production to 2011 levels and factor in all state and federal regulatory requirements. We will develop new 2011 baseline O&G inventories for the following WRAP Phase III basins:

- Piceance

- Denver-Julesburg
- South San Juan
- North San Juan
- Southwest Wyoming
- Powder River
- Uintah
- Wind River
- Permian

We will also collect 2011 O&G inventory data for the following basins:
- Big Horn – data will come directly from Wyoming DEQ detailed operator surveys and permit database for all sources
- Raton – data will come from CDPHE APENs database for all sources
- Paradox – data will come from any major and minor source permits available from Utah DEQ

After developing the 2011 baseline O&G inventory, will well project these data to 2020 based on controls analysis and activity growth and decline. The activity projections will be developed from a linear fitting of trend-lines based on an analysis of historic production statistics in the IHS database through 2012. IHS production history of well counts, spud counts, and production by type (gas, condensate, oil) will be mined for developing the trend-lines. We will forecast the historic trend-lines to 2020. For forecasts that indicate a decline in production, we will continue the decline toward 2020 without allowing the productions to drop to zero. For forecasts that indicate an increase, we will continue the increase toward 2020 but use literature reviews to determine whether we should apply a cap on the upward trend. We will seek information on reservoir analyses, well spacing, and the allowable number of operating rigs to determine future year production caps. For forecasts that indicate relatively flat trends, we will hold the emissions constant at 2011 levels. Once we have developed the trend-lines for each basin, we will use these to develop scaling factors (2020 activity/2011 activity) and then apply these factors to generate uncontrolled 2020 inventories for each basin.

For each basin in Colorado, Utah, and Wyoming we apply controls based on both state and federal regulatory requirements. If redundant controls are found in a comparison of the state and federal rules by year and source category, we will apply the more stringent control to the inventory. Determining the impacts of some controls will require a year-to-year controls analysis, while others can be applied directly to the projected 2020 inventory. Our control analysis will include all source categories subject to regulations that are currently promulgated, but not controls that are under consideration. We will also be using a "no turnover" assumption in developing the control scenarios, which speculates that existing equipment in use in the basins are unlikely to be replaced with newer technologies before 2020. We also assume that the existing equipment are subject only to regulations that existed at the time of their installation.

We will apply the control data for each basin to the 2020 uncontrolled forecasted O&G inventories to develop the future year inventories for use in the 3SAQS.

We will not make any changes to the spatial patterns or chemical profiles of the O&G emissions for the 2020 projections. The basin-specific spatial surrogates and VOC speciation profiles for 2008 will be applied to the 2020 inventories to estimate 2020 model-ready emissions.

6.3 EMISSIONS PROCESSING

We will use SMOKE version 3.0 (October, 2012 release) for the 3SAQS. SMOKE will be used to process all of the emissions sectors other than biogenics, wind blown dust, sea salt, and lightning. The primary steps in the SMOKE processing sequence, with the name of the SMOKE program, are listed below. We provide the significant SMOKE configuration options along with each step.

6.3.1 SMOKE Processing

- Import (Smkinven) – read raw inventory files

    - Calculate coarse mode primary particulate matter (PMC) emissions, where SMKINVEN_FORMULA: PMC = PM10-PM2.5

    - For the hourly CEM inventories, set to read hourly data, where HOUR_SPECIFIC_YN = Y

    - Do NOT normalize weekly emissions by weekdays only, where WKDAY_NORMALIZE = N

    - Do NOT process hazardous air pollutant emissions, where SMK_PROCESS_HAPS = N

- Grid (Grdmat) – read and match spatial surrogates to inventory sources and assign the emissions to PGM grid cells

    - For all sources other than agriculture, use population as the fallback surrogate, where SMK_DEFAULT_SRGID = 100

    - For livestock and fertilizer, use rural land area as the fallback surrogate, where SMK_DEFAULT_SRGID = 400

    - Process all sources on a normal sphere with radius 6,370,000 m, where IOAPI_ISPH = 20

- Speciation (Spcmat) – read and match VOC and PM chemical profiles to inventory sources and calculate emissions in terms of PGM species

    - Convert inventory VOC to total organic gases (TOG) for consistency with the NEI SPECIATE speciation profiles, where POLLUTANT_CONVERSION = Y

- Temporal (Temporal) – read and match monthly/week/hourly temporal profiles to inventory sources and estimate hourly emissions

    - Renormalize the temporal profiles, where RENORM_TPROF = Y

    - Do NOT force all temporal profiles to be flat, where UNIFORM_TPROF_YN = N

    - Output emissions on the GMT timezone, where OUTZONE = 0

- Select elevated sources (Elevpoint) – read criteria for specifying elevated point sources

    - Use a configuration file to select elevated sources, where SMK_ELEV_METHOD = 1

    - All point sources for the 3SAQS are considered elevated if the effective stack height is greater than 20m

- Create PGM-ready emissions by sector (Smkmerge) – combine all of the intermediate steps above to create a low-level emissions file for each inventory sector and an elevated file for the elevated point sectors

    - Combine gridding, temporal, and speciation intermediates to create PGM-ready emissions, where MRG_GRDOUT_YN = MRG_TEMPORAL_YN = MRG_SPCMAT_YN = Y

- o Output an elevated file that includes the emissions for elevated sources, where SMK_ASCIIELEV_YN = Y

- o Output emissions in CAMx units, where MRG_GRDOUT_UNIT = moles/hr

- Estimate On-Road Mobile Emissions from MOVES (MOVESMrg) – input mobile activity data and MOVES emission factor look up tables to generated gridded, speciated, hourly emissions

  - o Process MOVES emissions, where SMK_EF_MODEL = MOVES

  - o Use 2-m temperatures for processing the on-road mobile emissions, where TVARNAME = TEMP2

  - o Extend a 10 degree temperature buffer on either side of the emissions factor look up tables, where TEMP_BUFFER_BIN = 10

- Final merge (Mrggrid) - Merge the low-level sector emissions to a single file per day

- Create CAMx-ready binary files (Smk2emis) – convert netCDF SMOKE outputs to UAM-formatted data for CAMx

- Merge elevated source (Mrgelev) – combine elevated files to a single file per day and convert to UAM-formatted data for CAMx

We will define a series of emissions processing categories for the 3SAQS project to facilitate the modeling and quality assurance of the inventory data. While there are four main types of inventory data (point, nonpoint, mobile, and biogenic), it is necessary to refine these categories to support special emissions modeling approaches or to provide flexibility for tagging emissions categories in source apportionment air quality modeling.

Efficiencies in the emissions modeling process are gained through consideration of the temporal variability in the emissions sources. If a processing category includes only sources that use a flat temporal profile throughout the year, meaning that the emissions are the same on every hour of every day of the year, it is possible to process a single day for that category and recycle the emissions on each day of the air quality modeling simulation. Both processing time and disk space are conserved by not producing 365 files that all contain the exact same information. Other types of temporal processing configurations that may be used for the 3SAQS project include:

- Single day per year (aveday_yr)
- Single day per month (aveday_mon)
- Typical Monday, Weekday, Saturday, Sunday per year (mwdss_yr)
- Typical Monday, Weekday, Saturday, Sunday per month (mwdss_mon)
- Emissions estimated for each model simulation day (daily)
- Emissions estimated for each model simulation day with temporal profiles generated with average daily meteorology (daily met)
- Emissions estimated for each model simulation day with temporal profiles generated with hourly meteorology (hourly met)

Table 6-2 defines the emissions categories that we will define for the 3SAQS project. The "Temporal" column in Table 6-2 refers to the temporal configuration that will be used for each category.

Table 6-2. 3SAQS emissions processing categories

No.	Emissions Processing Category (Abbr)	Inventory Year	Inventory Source	Temporal	Processing Comments
1	Nonpoint/Area (nonpt)	2008	NEI08v2	mwdss_mon	Remove oil & gas, agricultural NH3, and dust,; includes commercial marine and rail
2	Livestock NH3 (lv)	2008	NEI08v2	mwdss_mon	Do not apply met-based temporal profiles; separate out for possible sensitivity later
	Fertilizer NH3 (ft)	2008	NEI08v2	mwdss_mon	Group with lv as a full agricultural NH3 sector (ag)
3	Fugitive and Road Dust (fd)	2008	NEI08v2	mwdss_mon	Includes paved and unpaved road dust; apply transport factors but not met factors
4	Residential Wood Combustion (rwc)	2008	NEI08v2	mwdss_mon	Do not apply met-based temporal profiles; separate out for possible sensitivity later
5	Area Oil & Gas (og)		IPAMS	mwdss_mon	Basin specific speciation profiles and spatial surrogates
6	Nonroad mobile (nr)	2008	NEI08v2	mwdss_mon	Includes NMIM commercial marine and rail
7	MOVES RPD (rpd)	2008	NEI08/MOVES2010b	hourly met	Daily emissions factor lookup tables
8	MOVE RPD Refueling (rpd_rfl)	2008	NEI08/MOVES2010b	hourly_met	Daily emissions factor lookup tables
9	MOVES RPP (rpp)	2008	NEI08/MOVES2010b	hourly met	Daily emissions factor lookup tables
10	MOVES RPV (rpv)	2008	NEI08/MOVES2010b	hourly met	Daily emissions factor lookup tables
11	MOVES RPV Refueling (rpv_rfl)	2008	NEI08/MOVES2010b	hourly_met	Daily emissions factor lookup tables
12	CEM Point (ptcem)	2008	NEI08v2/CAMD	daily	Anomalies removed from 2008 CAMD data
13	Non-CEM Point (ptncem)	2008	NEI08v2	mwdss_mon	Removed oil & gas sources and transferred to ptog sector; includes point aircraft and ports
14	Point Oil & Gas (ptog)		IPAMS	mwdss_mon	Combination of WRAP Phase III inventory and NEI08v2 for areas not covered by WRAP EI
15	Point Fires (ptfire)	2008	DEASCO3	daily	Pre-computed plume rise, processing outside of SMOKE

16	Commercial Marine (ptseca)	2008	NEI08v2	aveday_mon	
17	Canada/Mexico Area (nusar)	Can2006/Mex2008	Canada NPRI Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2008
18	Canada/Mexico Point (nuspt)	Can2006/Mex2008	Canada NPRI Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2008
19	Canada/Mexico Mobile (nusmb)	Can006/Mex2008	Canada NPRI Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2008
20	Lightning NOx (lnox)	N/A		hourly met	Gridded monthly NLCD lightning flash counts converted to hourly, gridded NO emissions with WRF convective rainfall
21	Sea salt (ss)	N/A		hourly met	Surfzone and open ocean PM emissions
22	Windblown Dust (wbd)	N/A	WRAP WBD Model	hourly met	
23	MEGAN Biogenic (bg)	N/A	MEGAN2.1	hourly met	Use new versions of MEGAN V2.10 updated by WRAP for the western U.S.

6.3.2 MEGAN Biogenic Modeling

For the 3SAQS, we will use the MEGAN biogenic emissions prepared for the WestJumpAQMS. Details on the model inputs, software, and configuration are available in the [Improved Biogenic Emission Inventories Across the West Final Report](#) (ENVIRON, 2012c).

6.3.3 Windblown Dust Processing

For the 3SAQS, we will use the windblown dust emissions prepared for the WestJumpAQMS. Details on the model inputs, software, and configuration are available in the Final Dust Emissions Technical Memo[36].

6.3.4 Seasalt and Lightning Emissions Processing

For the 3SAQS, we will use the seasalt and lightning emissions prepared for the WestJumpAQMS. Details on the model inputs, software, and configuration are available in the Final Seasal and Lightning Emissions Technical Memo[37].

6.4 QUALITY ASSURANCE AND QUALITY CONTROL

The emissions will be processed by major source category in several different "streams" of emissions modeling. This is done in order to assist in the quality assurance (QA) and quality control (QC) of the emissions modeling. Each stream of emissions modeling generates a pre-merged CAMx-ready emissions model input with all pre-merged emissions inputs merged together to generate the final CAMx-ready two-dimensional gridded low-level (layer 1) and point source emission inputs. Table 6-3 lists the separate streams of emissions modeling by source category to be used in the 3SAQS project. Also shown in Table 6-2 are the source of the emissions, processing comments and the temporal allocation strategy whose options are as follows:

- Single day per year (aveday_yr)
- Single day per month (aveday_mon)
- Typical Monday, Weekday, Saturday, Sunday per year (mwdss_yr)
- Typical Monday, Weekday, Saturday, Sunday per month (mwdss_mon)
- Emissions estimated for each model simulation day (daily)
- Emissions estimated for each model simulation day with temporal profiles generated with average daily meteorology (daily met)
- Emissions estimated for each model simulation day with temporal profiles generated with hourly meteorology (hourly met)

7.0 PHOTOCHEMICAL MODELING

The 3SAQS project will conduct photochemical modeling using the CAMx photochemical grid model (PGM) version 5.41.

---

[36] http://www.wrapair2.org/pdf/Memo6_Dust_Mar11_2013review_draft.pdf
[37] http://www.wrapair2.org/pdf/Memo_12_SeaSalt_Lightning_June25_2012_final.pdf

Three types of PGM model simulations will be conducted:

- 2008 base case modeling that is used in the model performance evaluation.

- 2020 future year modeling for estimating the change to air quality under future year emissions conditions

The 3SAQS photochemical modeling will provide the framework for 2008-based NEPA EIA modeling for the three state region. This Chapter describes the model configurations for the CAMx 2008 and 2020 base case simulations, whereas Chapter 8 describes the model performance evaluation procedures for the 2008 simulation.

7.1 CAMX SCIENCE AND INPUT CONFIGURATIONS

Table 7-1 summarizes the CAMx science configurations and options to be used for the 2008 and 2011 base case simulations. CAMx Version 5.41 (released November 2012) will be used. CAMx V5.41 includes several recent updates that will be used in the 3SAQS such as the new CB05 chemical mechanism. The model will be configured to predict both ozone and PM species.

We will use the PPM advection solver for horizontal transport (Colella and Woodward, 1984) along with the spatially varying (Smagorinsky) horizontal diffusion approach. CAMx will use K-theory for vertical diffusion using the CMAQ-like vertical diffusivities from WRFCAMx. The CB05 gas-phase chemical mechanism is selected for CAMx because it includes the very latest chemical kinetic rates and represents improvements over the other alternative CB05 and SAPRC chemical mechanisms. Additional CAMx inputs will be as follows:

Meteorological Inputs: The WRF-derived meteorological fields will be processed to generate CAMx meteorological inputs using the WRFCAMx processor, as descried in Chapter 5.

Initial/Boundary Conditions: The boundary conditions (BCs) for the 36 km CONUS domain simulation will be based on the MOZART[38] global chemistry model. Considerations were also given to generating the 2008 36 km CONUS domain BCs using output from the GEOS-Chem[39] or AM3[40] global chemistry models. However, at this time we only have access to the 2008 MOZART global chemistry model output. Existing programs will be used to interpolate from the MOZART horizontal and vertical coordinate system to the CAMx LCP coordinate system and vertical layer structure and to map the MOZART chemical species to the chemical mechanisms being used by CAMx.

Photolysis Rates: The modeling team will prepare the photolysis rate inputs as well as albedo/haze/ozone/snow inputs for CAMx. Day-specific ozone column data will based on the Total Ozone Mapping Spectrometer (TOMS) data measured using the satellite-based Ozone Monitoring Instrument (OMI[41]). Albedo will be based on land use data. For CAMx there is an ancillary snow cover input that will override the land use based albedo input. Average values for typical snow cover will be utilized; note that this is in contrast to the more highly reflective white snow that typically occurs during winter high ozone events in southwest Wyoming and the Uinta Basin in Utah. For CAMx, the TUV[42] photolysis rate processor will be used. If there are periods of more than a couple of days where daily TOMS data are unavailable, the TOM measurements will be interpolated between

---

[38] http://www.acd.ucar.edu/wrf-chem/mozart.shtml
[39] http://acmg.seas.harvard.edu/geos/
[40] http://www.gfdl.noaa.gov/atmospheric-model
[41] http://ozoneaq.gsfc.nasa.gov/
[42] http://cprm.acd.ucar.edu/Models/TUV/

the days with valid data; in the case large periods of TOMS data are missing monthly average TOMS data will be used. CAMx will also be 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 may be especially important in adjusting the photolysis rates due to the occurrence of PM concentrations associated with emissions from fires.

Landuse: The team will generate landuse fields based on USGS GIRAS data.

Spin-Up Initialization: A minimum of ten days of model spin up (e.g., December 21-31, 2007) will be used on the 36 km CONUS domain before adding the 12 nested domain for the last two days of 2007 before the start of the 2008 calendar year (January 1, 2008).

Table 7-1. CAMx (Version 5.41) model configurations for 3SAQS

Science Options	Configuration	Details
Model Codes	CAMx V5.41 – November 2012 Release	Newer version may become available during the course of the study and will be considered for use at that time.
Horizontal Grid Mesh	36/12 km	Many CAMx runs done using just 36/12 km grids
36 km grid	148 x 112 cells	36 km CONUS domain
12 km grid	239 x 206 cells	12 km WESTUS domain
Vertical Grid Mesh	25 vertical layers, defined by WRF	Layer 1 thickness ~24- m. Model top at ~19-km above MSL
Grid Interaction	36/12 km two-way nesting for CAMx	
Initial Conditions	10 day spin-up on 36 km grid	Clean initial conditions
Boundary Conditions	36 km from global chemistry model	Currently only MOZART data available for 2008.
Emissions		
Baseline Emissions Processing	SMOKE, MOVES and MEGAN	
Sub-grid-scale Plumes	Plume-in-Grid for major NO_X sources in CAMx	
Chemistry		
Gas Phase Chemistry	CB05 in CAMx	
Meteorological Processor	WRFCAMx	Compatible with CAMx V5.4
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	
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	
Integration Time Step	Wind speed dependent	~0.1-1 min (4 km), 1-5 min (1 -km), 5-15 min (36 km)

8.0 MODEL PERFORMANCE EVALUATION

This chapter describes the general model performance evaluation procedures that are designed to estimate the reliability of the CAMx model for simulating air quality, visibility and deposition in the western U.S. for the 2008 modeling period. An initial model performance evaluation would be conducted for ozone and fine particulate matter ($PM_{2.5}$) and if the ozone and $PM_{2.5}$ model performance seems reasonable, a more detailed model performance evaluation would be conducted that also includes: ozone/$PM_{2.5}$ precursor, product and indicator species; visibility; sulfur and nitrogen deposition; and comparisons against special study data such as the ozonesonde measurements to evaluate the model for ozone aloft.

8.1 OVERVIEW OF MODEL PERFORMANCE EVALUATION

Using the inputs and model configurations described in this Modeling Protocol, an initial CAMx base case simulation will be conducted for the 36/12 km domains and the 2008 calendar period. The initial 2008 base case ozone, total $PM_{2.5}$ mass and speciated $PM_{2.5}$ concentrations would be evaluated against concurrent measured ambient concentrations using graphical displays of model performance and statistical model performance measures that would be compared against established model performance goals and criteria. The CAMx performance evaluation will follow the procedures recommended in EPA's photochemical modeling guidance documents (e.g., EPA, 1991; 2007). Note that EPA is currently updating their modeling guidance, but the basic features on how to evaluate a photochemical grid model is expected to be similar.

After an initial overview of the model performance evaluation focusing on ozone and $PM_{2.5}$ is performed, a more detailed model performance evaluation will be conducted that also includes ozone/$PM_{2.5}$ precursor species (e.g., NO, NO_2, NO_X and SO_2), related species (e.g., HNO_3), visibility and deposition. The more detailed evaluation will also include more subregional evaluations and evaluations for specific episode periods of interest.
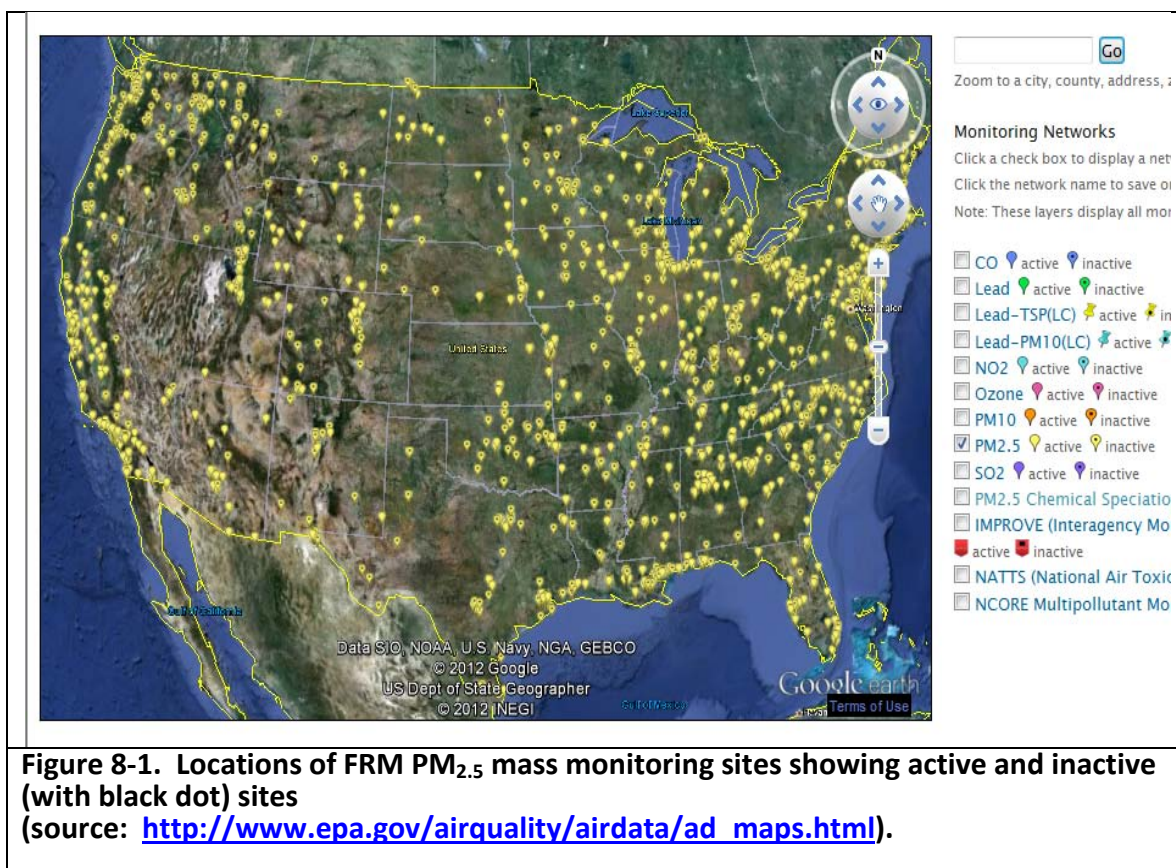
8.2 AVAILABLE AEROMETRIC DATA FOR THE MODEL EVALUATION

The following routine air quality measurement data networks operating in in 2008 will be used in the 3SAQS model performance evaluation:

> EPA AQS Surface Air Quality Data: 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[43]) database throughout the U.S. The AQS consists of many sites that tend to be mainly located in and near major cities. Thus, outside of California they will be located mainly around the larger cities including Seattle, Portland, Salt Lake City, Denver, Phoenix and Las Vegas. These data sets will be reformatted for use in the model evaluation software tools and used in the regional evaluation of the modeling system across the western U.S. There are several types of networks within AQS that measure different species. The standard hourly AQS AIRS monitoring stations typically measure hourly ozone, NO_2, NO_X and CO concentration and there are thousands of sites across the U.S. The Federal Reference Method (FRM) network measures 24-hour total $PM_{2.5}$ mass concentrations using a 1:3 day sampling frequency, with some sites operating on an everyday frequency. The Chemical Speciation Network (CSN) 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. Figures 8-1 and 8-2 show the locations of the FRM and CSN monitoring

---

[43] http://www.epa.gov/ttn/airs/airsaqs/aqsweb/

networks, respectively, the AIRS hourly network is not shown because the large number of sites makes the map unreadable.

**Figure 8-1. Locations of FRM PM$_{2.5}$ mass monitoring sites showing active and inactive (with black dot) sites
(source: http://www.epa.gov/airquality/airdata/ad_maps.html).**
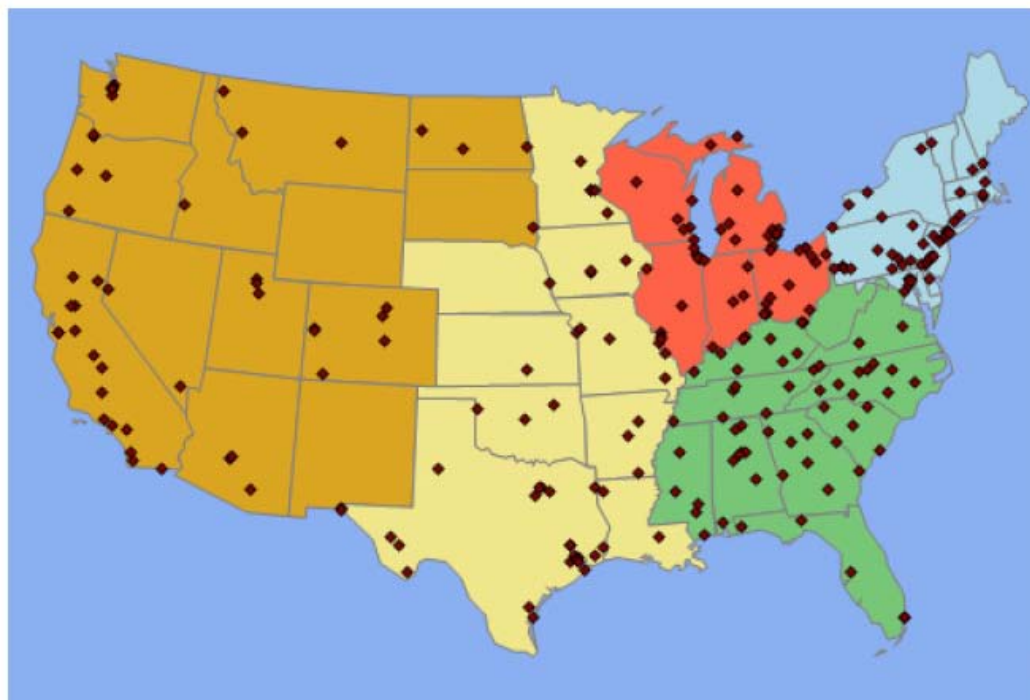
Figure 8‑2. Locations of CSN speciated PM$_{2.5}$ monitoring sites (source: http://www.epa.gov/ttn/amtic/speciepg.html).

IMPROVE Monitoring Network: The Interagency Monitoring of Protected Visual Environments (IMPROVE[44]) 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 can be more urban-oriented. Figure 8-3 shows the locations of the approximately 150 IMPROVE and IMPROVE protocol sites across the U.S.
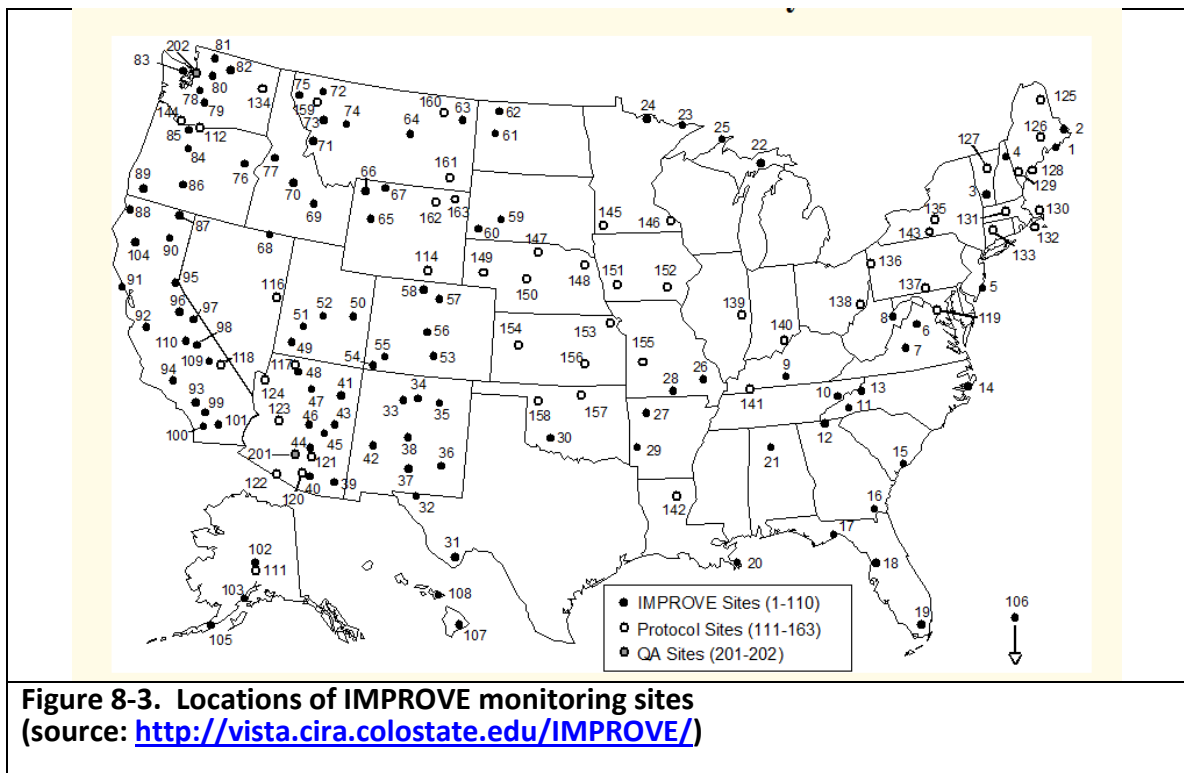
Figure 8-3. Locations of IMPROVE monitoring sites (source: http://vista.cira.colostate.edu/IMPROVE/)

---

[44] http://vista.cira.colostate.edu/IMPROVE/

CASTNet Monitoring Network: The Clean Air Status and Trends Network (CASTNet[45]) 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). Figure 8-4 displays the locations of the ~80 CASTNet sites across the U.S.

Figure 8-4. Locations of CASTNet monitoring sites
(source: http://epa.gov/castnet/javaweb/index.html).
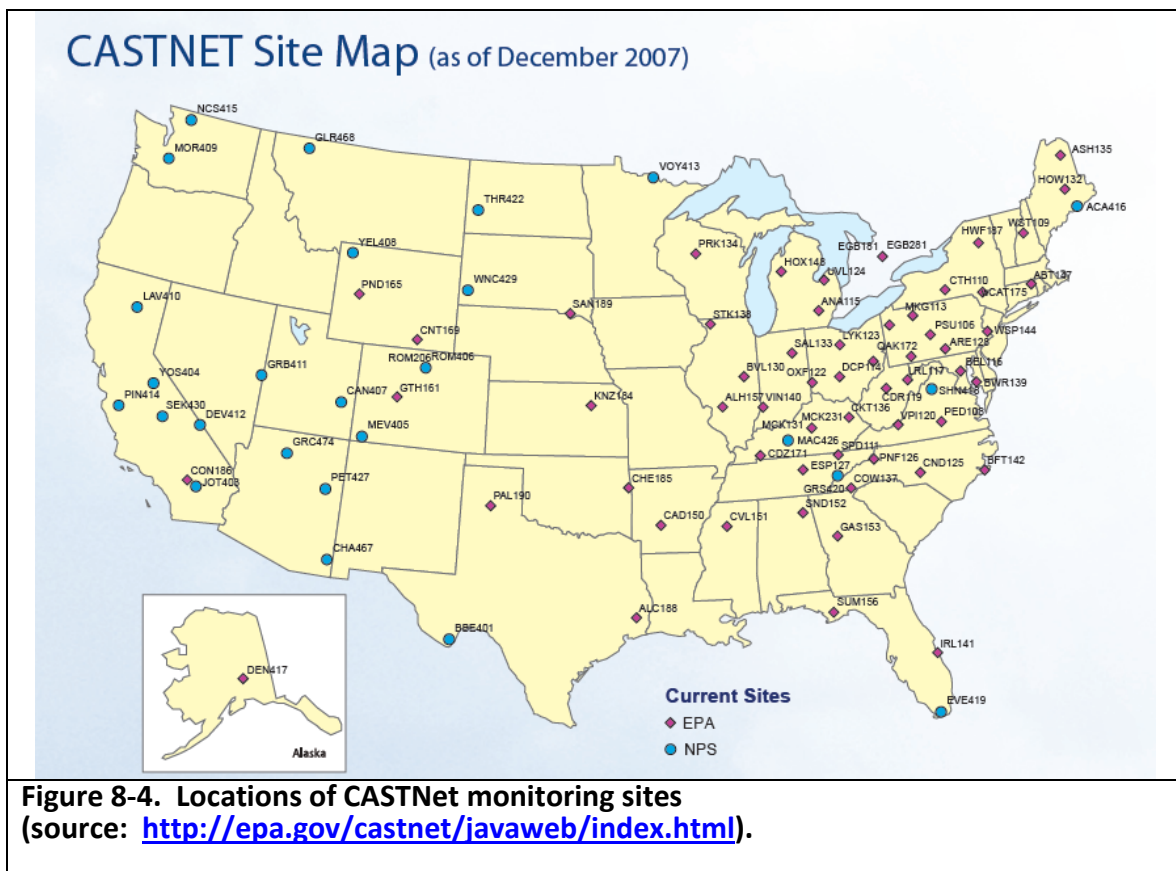
NADP Network: The National Acid Deposition Program (NADP[46]) collects weekly samples of SO_4, NO_3 and NH_4 in precipitation (wet deposition) in their National Trends Network (NTN) at over a 100 sites across the U.S. that are mainly located in rural areas away from big cities and major point sources. Seven NADP sites also collect daily wet deposition measurements (AIRMON) when precipitation occurs. Over 20 of the NADP sites also collect weekly mercury (MDN) samples. Figure 8-5 shows the locations of the NADP NTN, AIRMoN and MDN monitoring sites. Note that observed sulfate and nitrate dry deposition can be estimated at CASTNet sites using concentrations and a micro-meteorological model that produces a deposition velocity. But these are not true observations, but model estimates of the observations.

Figure 8-5. Locations of NADP monitoring sites (source: http://nadp.sws.uiuc.edu/).
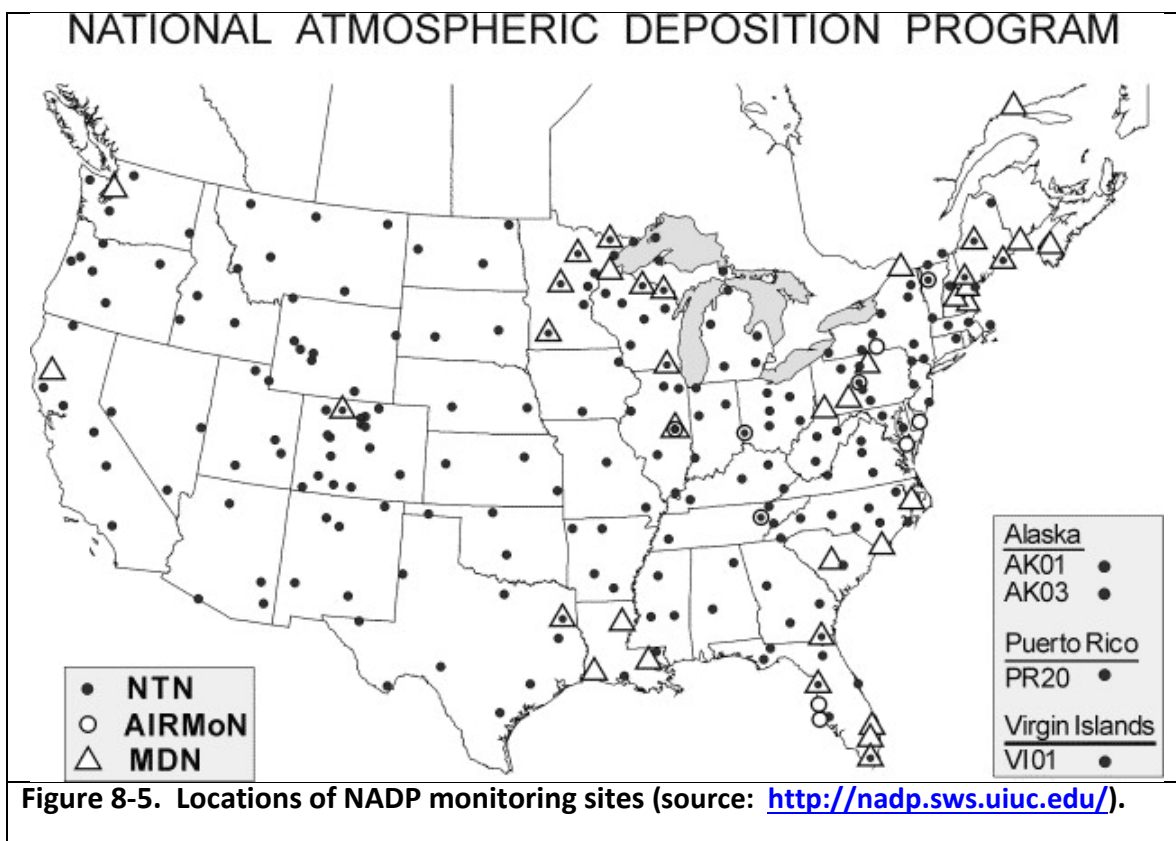
Ozonesonde Network: The NOAA Earth Systems Research Laboratory (ESRL) operates several ozonesonde sites[47] throughout the world that measure the vertical structure of ozone concentrations throughout the troposphere and into the lower stratosphere. Ozonesonde monitoring sites within the 3SAQS modeling domain include: (1) Trinidad Head on the coast in northern California; (2) Boulder, Colorado; and (3) at the University of Alabama at Huntsville.

---

[46] http://nadp.sws.uiuc.edu/NADP/
[47] http://www.esrl.noaa.gov/gmd/ozwv/ozsondes/index.html

There may be other special study air quality or related monitoring sites that were operating during 2008 (e.g., CalNex). However, since the 3SAQS is performing a regional air quality assessment of the western U.S., the focus of the model performance evaluation will be on the regional networks described above.

8.3 MODEL PERFORMANCE STATISTICS, GOALS AND CRITERIA

For over two decades, ozone model performance has been compared against EPA's 1991 ozone modeling guidance performance goals as follows (EPA, 1991):

- Unpaired Peak Accuracy (UPA)   ≤ ±20%

- Mean Normalized Bias (MNB)   ≤ ±15%

- Mean Normalized Gross Error (MNGE)   ≤ 35%

In EPA's 1991 ozone modeling guidance, these performance metrics were for hourly ozone concentrations. The UPA compared the daily maximum 1-hour predicted and observed ozone concentration that was matched by day, but not necessarily by location and by hour of the day. Since a photochemical grid model predicts ozone concentrations everywhere and the observed ozone is limited to a monitoring network, it would be fortuitous that the actual highest hourly ozone concentration in a region occurred at a monitoring site, so one would expect a perfect model to have an overestimation tendency for the UPA performance metric.

The MNB/MNGE uses hourly predicted and observed ozone concentrations paired by time and location and is defined as the difference between the predicted and the observed hourly ozone divided by the observed hourly ozone concentrations averaged over all predicted/observed pairs (see Table 8-2) within a given region and for a given time period (e.g., by day, month or modeling period). The MNGE is defined similarly only it uses the absolute value of the difference between the predicted and observed hourly ozone concentrations so is an unsigned metric. As the MNB/MNGE performance metrics divide by the observed hourly ozone concentration, the metric is calculated just using the predicted and observed hourly ozone pairs for which the observed hourly ozone concentration is above a threshold concentration. In the 1991 EPA modeling guidance an observed hourly ozone threshold concentrations of 60 ppb is suggested. Since 1991 these ozone performance goals have been extended to 8-hour ozone concentrations and from urban to more rural areas. Given the large reductions in ozone over the last two decades and the lower ozone concentrations associated with the 8-hour ozone time averaging and rural locations, the observed ozone threshold for 8-hour ozone concentrations has been reduced, with a 40 ppb threshold frequently used. And in rural areas with lower ozone values a lower observed ozone threshold has also been used.

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 8-1 (Boylan, 2004; Morris et al., 2009a,b). However, unlike the 1991 ozone model performance goals that use the MNB and MNGE performance metrics, for PM species the Fractional Bias (FB) and Fractional Error (FE) are utilized with no observed concentration threshold screening. The FB/FE differ from the MNB/MNGE in that the difference in the predicted and observed concentrations are divide by the average of the predicted and observed values, rather than just the observed value as in the MNB/MNGE. This results in the FB being bounded by -200% to

+200% and the FE being bounded by 0% to +200%. There are additional statistical performance metrics that evaluate correlation, scatter as well as bias and error and a full suite of model performance metrics will be calculated for all species as given in Table 8-2.

Table 8-1. 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
≤±15%	≤35%	PM model performance Criteria, considered average PM performance. Exceeding this level of performance for PM species with significant mass may be cause for concern.

It should be pointed out that these model performance goals and criteria are not used to assign passing or failing grades to model performance, but rather to help interpret the model performance and intercompare across locations, species, time periods and model applications. As noted in EPA's current modeling guidance "By definition, models are simplistic approximations of complex phenomena" (EPA, 2007, pg. 98). The model inputs to the air quality models vary hourly, but tend to represent average conditions that do not account for unusual or extreme conditions. For example, an accident or large event could cause significant increases in congestion and motor vehicle emissions that are not accounted for in the average emissions inputs used in the model. This is seen in PM modeling at some monitoring sites that fail to capture the high PM concentrations on July 4 due to fireworks and other activities associated with this holiday (traffic and BBQ) that increase PM emissions.

More recently, 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, Baker and Phillips, 2012). Although these recommendations are not official EPA guidance, they are useful for consideration in the 3SAQS model performance evaluation:

- 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.

  o Given this recommendation the MNB/MNGE will just be calculated for ozone using an appropriate observed ozone cut-off concentration (e.g., 60 or 40 ppb).

- 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).

- $PM_{2.5}$ should also be evaluated separately for each major component species (e.g., SO4, NO3, NH4, EC, OA and OPM2.5).

- Evaluation should be performed for subsets of the data including, high observed concentrations (e.g., ozone > 60 ppb), by subregions and by season or month.

- Evaluation should include more than just ozone and $PM_{2.5}$, such as SO_2, NO_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 will incorporate the recommendations of Simon, Baker and Philips (2012) into the 3SAQS model performance evaluation. The 3SAQS evaluation products will include qualitative and quantitative evaluation for the following model output species:

- Maximum daily 1-hour and maximum daily 8-hour average (MDA8) ozone, including MDA8 with a 60 ppb threshold

- Carbon monoxide, nitrogen dioxide, NOx, volatile organic compounds (VOCs), ammonia

- Total PM2.5, elemental carbon, organic carbon, sulfate, nitrate, ammonium, and visibility metrics

- Total sulfur and total nitrogen wet and dry deposition

Table 8-2. Definition of model performance evaluation statistical measures used to evaluate the CTMs.

Statistical Measure	Mathematical Expression	Notes
Accuracy of paired peak (Ap)	$$\dfrac{P - O_{peak}}{O_{peak}}$$	Comparison of the peak observed value (O_{peak}) with the predicted value at same time and location
Coefficient of determination (r2)	$$\dfrac{\left[\sum\limits_{i=1}^{N}(P_i - \overline{P})(O_i - \overline{O})\right]^2}{\sum\limits_{i=1}^{N}(P_i - \overline{P})^2 \sum\limits_{i=1}^{N}(O_i - \overline{O})^2}$$	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)	$$\dfrac{\sum\limits_{i=1}^{N}\left|P_i - O_i\right|}{\sum\limits_{i=1}^{N}O_i}$$	Reported as %
Root Mean Square Error (RMSE)	$$\left[\dfrac{1}{N}\sum\limits_{i=1}^{N}\left(P_i - O_i\right)^2\right]^{\frac{1}{2}}$$	Reported as %
Fractional Gross Error (FE)	$$\dfrac{2}{N}\sum\limits_{i=1}^{N}\left|\dfrac{P_i - O_i}{P_i + O_i}\right|$$	Reported as % and bounded by 0% to 200%
Mean Absolute Gross Error (MAGE)	$$\dfrac{1}{N}\sum\limits_{i=1}^{N}\left|P_i - O_i\right|$$	Reported as concentration (e.g., µg/m^3)
Mean Normalized Gross Error (MNGE)	$$\dfrac{1}{N}\sum\limits_{i=1}^{N}\dfrac{\left|P_i - O_i\right|}{O_i}$$	Reported as %
Mean Bias (MB)	$$\dfrac{1}{N}\sum\limits_{i=1}^{N}\left(P_i - O_i\right)$$	Reported as concentration (e.g., µg/m^3)
Mean Normalized Bias (MNB)	$$\dfrac{1}{N}\sum\limits_{i=1}^{N}\dfrac{\left(P_i - O_i\right)}{O_i}$$	Reported as %
Mean Fractionalized Bias (Fractional Bias, FB)	$$\dfrac{2}{N}\sum\limits_{i=1}^{N}\left(\dfrac{P_i - O_i}{P_i + O_i}\right)$$	Reported as %, bounded by -2005 to +200%
Normalized Mean Bias (NMB)	$$\dfrac{\sum\limits_{i=1}^{N}(P_i - O_i)}{\sum\limits_{i=1}^{N}O_i}$$	Reported as %
Bias Factor (BF)	$$\dfrac{1}{N}\sum\limits_{i=1}^{N}\left(\dfrac{P_i}{O_i}\right)$$	Reported as BF:1 or 1: BF or in fractional notation (BF/1 or 1/BF).

8.4 SUBREGIONAL EVALUATION OF MODEL PERFORMANCE

The evaluation of the CAMx 36/12 km base case simulations will focus on a monthly, quarterly and annual model performance at monitors in Colorado, Utah, and Wyoming. We will also examine a few high ozone episodes for more detailed analysis and determine how well the model performs on ozone exceedance days and locations.

8.5 EXAMPLE MODEL PERFORMANCE DISPLAYS

Below are several examples of model performance displays that will be considered in the 3SAQS model performance evaluation. We find these visual comparisons of modeled and observed data provide a much better venue for conveying the model performance than tabular summaries of statistical performance metrics.

8.5.1 Model Evaluation Tools

There are several model performance evaluation tools that may be used in the model evaluation, including the following:

- UCR Analysis Tool: The UCR Analysis Tool was developed by the WRAP Regional Modeling Center (RMC) and is a quick and accurate model performance tool that operates under the Linux operating system to generate performance statistics, scatterplots and time series plots for a selected time period. Although the model performance displays are flat pictures (i.e., cannot be changed, such as modifying the scale), many different displays can be generated quickly that can be examine using slide shows to obtain a lot of information on model performance down to the individual site and individual day.

- PAVE and VERDI: The Package for Analysis and Visualization (PAVE[48]) and Visualization Environment for Rich Data Interpretation (VERDI[49]) are visualization tools specifically designed to visualize photochemical grid model output. They can run on both a Linux and Windows environment, so, like the UCR Analysis Tool, can be used while the photochemical grid model is running or has recently been completed. Both tools are primarily used for spatial maps where modeled tile plots can be displayed with superimposed observations. VERDI can also generate scatter and time series plots. Although VERDI has replaced PAVE, which is no longer supported, because the modeling community has scripts already set up for PAVE, PAVE is easier to use and VERDI does not have some of the functionality of PAVE, PAVE is still a useful and viable model evaluation tool.

- Excel: The Microsoft Excel spreadsheet software tool is used extensively to generate various model performance displays (e.g., scatter, time series and soccer plots) under Windows. Like SURFER, the modeling results and observations must be processed to get them into Excel. But once the data are in Excel, the user has lots of control over the displays.

- AMET: The Atmospheric Model Evaluation Tool (AMET[50]) was developed by EPA and consists of MySQL and r code with various scripts for generating the usual model evaluation graphics. It is more difficult to set up than the UCR, PAVE and VERDI tools but can generate useful model evaluation graphics and statistics.

---

[48] http://www.cmascenter.org/index.cfm?model=pave
[49] http://www.verdi-tool.org/
[50] http://www.epa.gov/AMD/ModelEvaluation/performance.html

In the following sections we present examples of model performance evaluation graphics using the above tools like we will use in the 3SAQS model performance evaluation. Because there is some redundancy in the some of the displays generated by the different evaluation tools, not all tools will be applied to generate all of the different types of displays.

8.5.2 Scatter Plots

Figure 8-6 displays example scatter plots using the UCR Analysis Tool, VERDI, Excel and AMET. The UCR Analysis Tool scatterplot (Figure 8-6, top left) can contrast the performance of two base case model runs in one scatterplot and also plots the 1:1 line of perfect agreement for reference. In this example the UCR tool scatterplot is comparing total $PM_{2.5}$ mass model performance across 30 Federal Reference Method (FRM) monitoring sites using a 4 km (blue) and 12 km (red) CAMx model simulation. The UCR Analysis Tool scatterplot also provides performance statistics (in this example FB, FE and R^2) and linear regression data fit between the predictions and observations. The example VERDI scatterplot (Figure 8-6, top right) was taken off the VERDI website and plots annual oxidized nitrogen wet vs. dry deposition. We are less familiar with this capability so are unsure whether performance measures can also be plotted at the same time. An example Excel scatterplot is given in the bottom left panel of Figure 8-6 and was taken from the 2008 Denver ozone SIP. This example plots observed daily maximum 8-hour ozone concentrations versus predicted ones near the monitor and includes not only the 1:1 line of perfect agreement, but two plotted lines that indicate when the predicted and observed values are within ±20% of each other; in the past EPA had a performance goal that the predicted daily maximum 8-hour ozone concentration near a monitor be within ±20% of the observed value most of the time. The final example scatterplot in the lower right panel of Figure 8-6 was generated using AMET and shows CMAQ monthly average sulfate performance for August 2006. The AMET scatterplot can also display statistical performance measures and in this case uses separate symbols for SO_4 measured by different monitoring networks; this feature can be important as different monitoring networks may use different measurement technology that have different biases, which is not an issue in this case for sulfate but does allow for a separate assessment of performance at the more rural IMPROVE versus more urban STN networks.

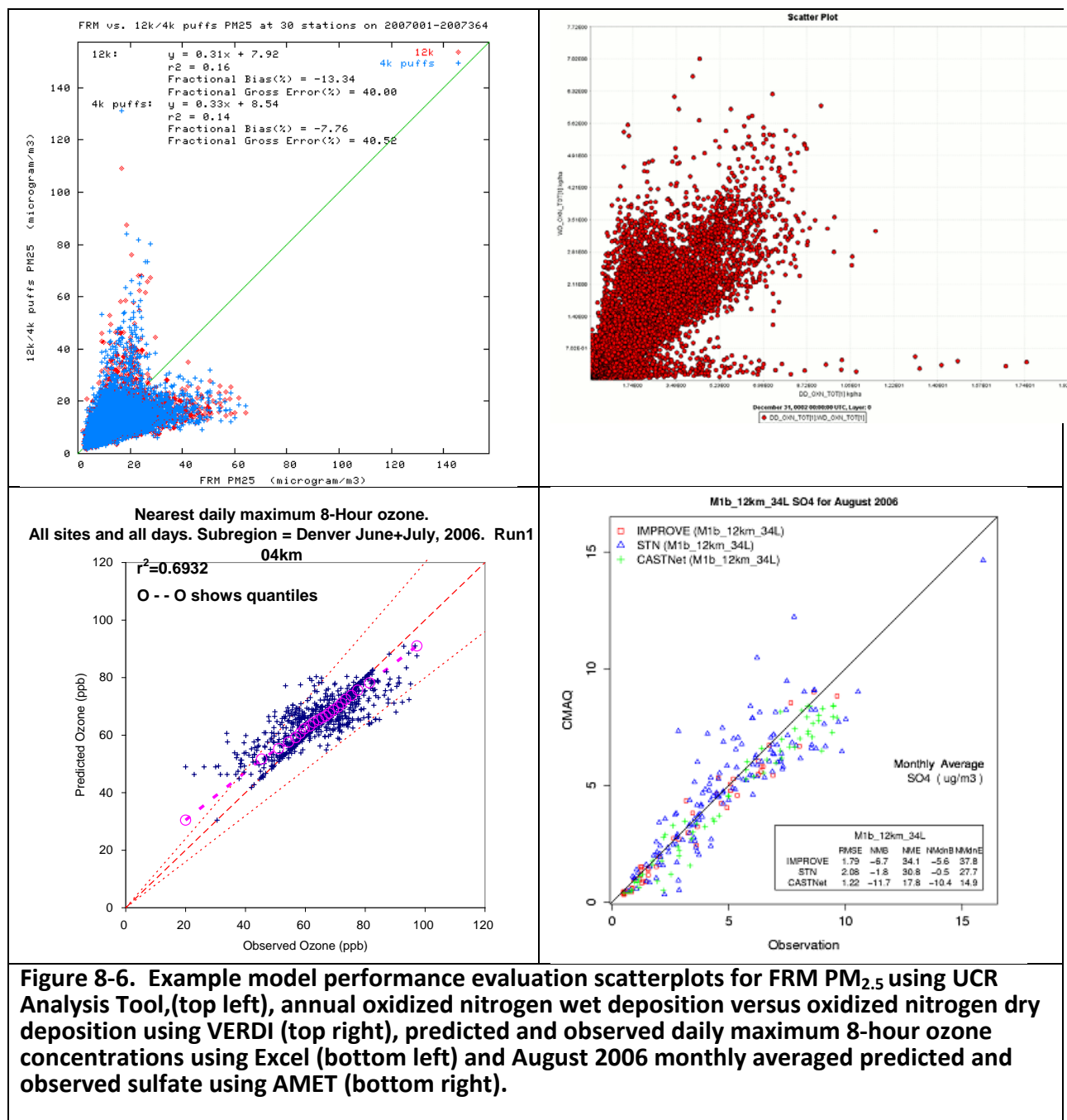Figure 8-6. Example model performance evaluation scatterplots for FRM PM$_{2.5}$ using UCR Analysis Tool,(top left), annual oxidized nitrogen wet deposition versus oxidized nitrogen dry deposition using VERDI (top right), predicted and observed daily maximum 8-hour ozone concentrations using Excel (bottom left) and August 2006 monthly averaged predicted and observed sulfate using AMET (bottom right).

8.5.3 Time Series Plots

Time series of predicted and observed concentrations are a staple of any model performance evaluation as it allows the user to directly assess how the model is reproducing the time evolution of the observations at different sites. Figure 8-7 displays an example predicted and observed time series comparison for 24-hour average PM$_{2.5}$ concentrations for a FRM monitoring site in Pennsylvania and the first quarter of 2007 for a CAMx 4 km and 12 km simulation using the UCR Analysis Tool. The UCR Analysis Tool also displays the FB and FE statistical performance metric, which in this case achieves the PM Performance Goal. The right panel in Figure 8-7 displays time series of CAMx predicted and observed hourly ozone concentrations for July 8-11, 2008 for two sites in the Denver area that was generated using Excel. The observed ozone values are the symbols and the predicted value at the monitoring site is the line. The shaded area represents the maximum and minimum predicted value in a 5 x 5 array of grid cells centered on the monitoring site; this allows an assessment of whether the monitor is in a location of steep modeled concentration gradients.
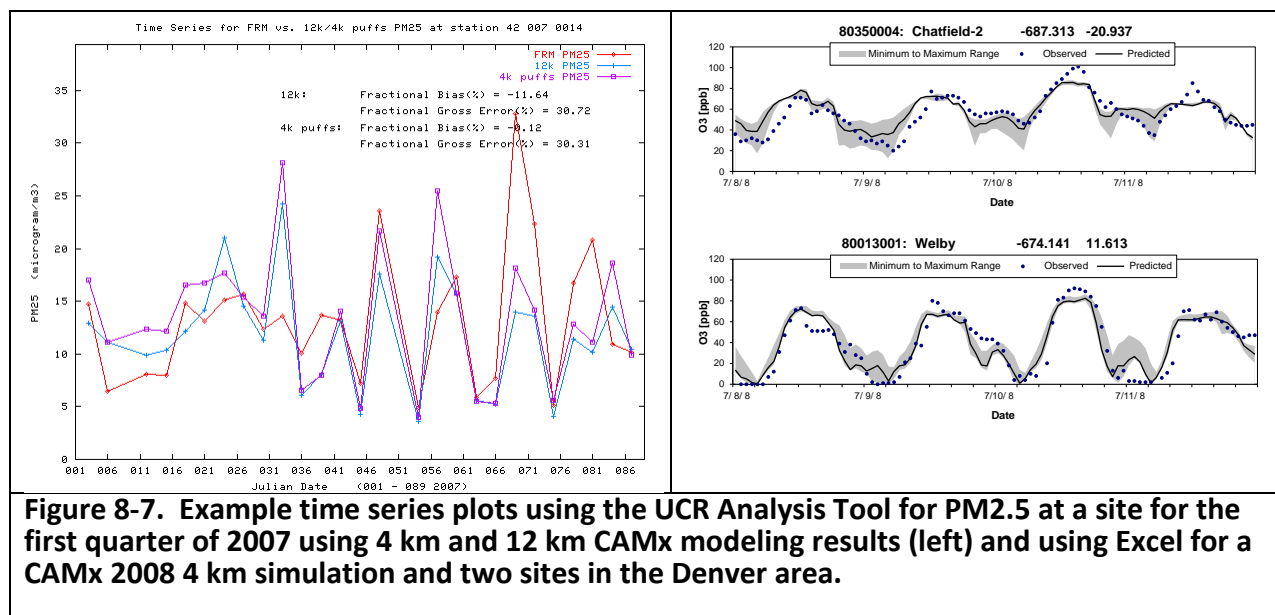
Figure 8-7. Example time series plots using the UCR Analysis Tool for PM2.5 at a site for the first quarter of 2007 using 4 km and 12 km CAMx modeling results (left) and using Excel for a CAMx 2008 4 km simulation and two sites in the Denver area.

8.5.4 Bar Charts of Model Performance Statistics

Figure 8-8 displays daily ozone model performance statistics for the Denver area and July 2008 (bars) and compares them with EPA's 1991 ozone performance goals that was prepared using a CAMx post-processor that interfaces with Excel. In a single plot one can assess how often the model achieves performance goals and whether it tends to have an overall under- or over-prediction bias.

Figure 8-8. Example of hourly ozone model performance statistics comparing the UPA, MNB and MNGE statistics with EPA's 1991 ozone performance goals (red lines).
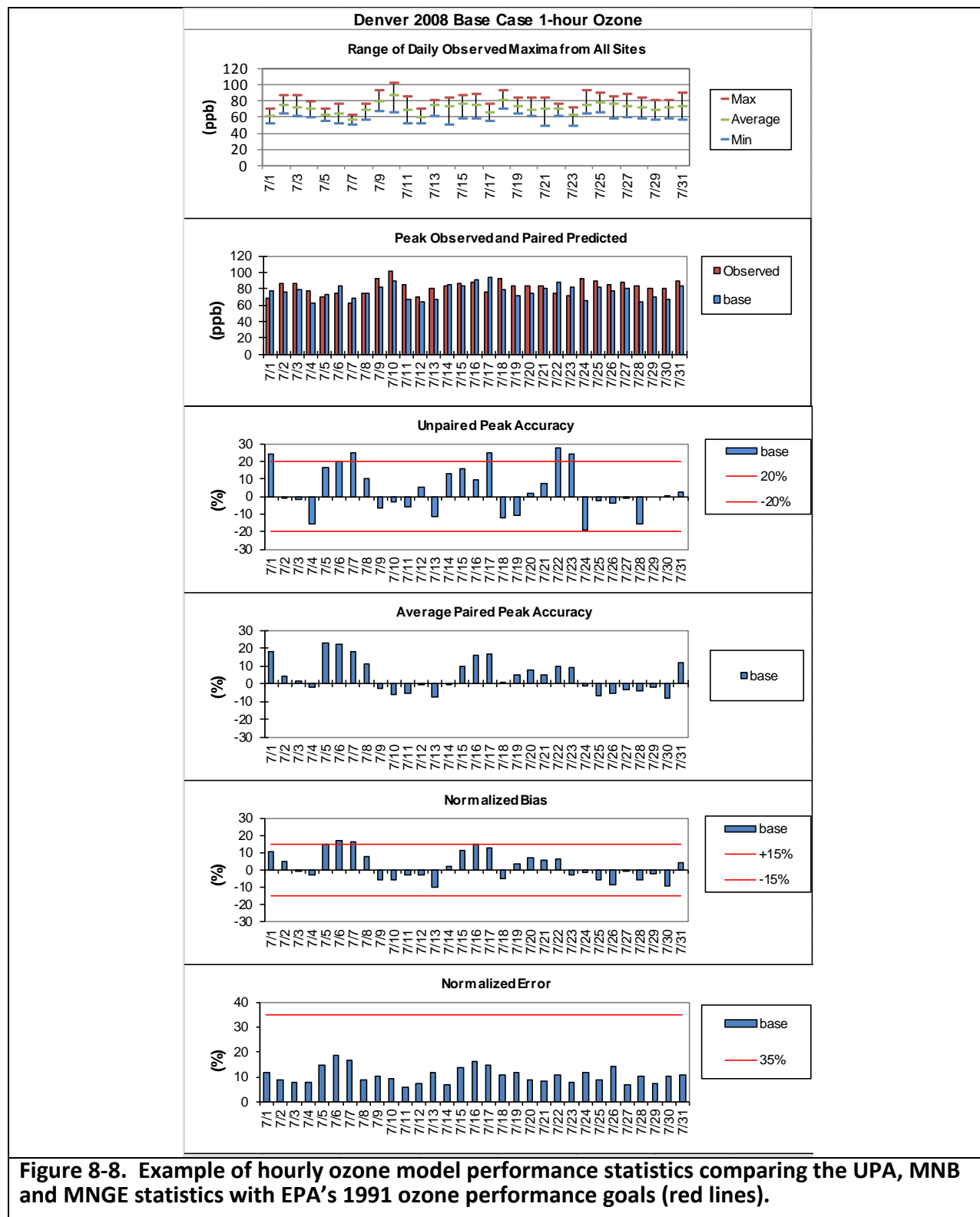
8.5.5 SoccerPlots Comparing Model Performance Statistics with Performance Goals

Soccer plots compare model performance statistical metrics against model performance goals and criteria. For example, Figure 8-9 displays two example soccerplots of FRM PM$_{2.5}$ model performance for a 2007 CAMx 4 km Midwest application and the VISTAS/ASIP 2002 12 km CMAQ application for Georgia. In these soccerplots, the fractional bias (FB) and fractional error (FE) are on the x-axis and y-axis, respectively, and the symbols represent the monthly average model performance. The boxed areas represent the PM Performance Goals and Criteria (Table 8-1). When the monthly average FE/FB symbol falls within the inner box (i.e., scores a goal) the PM Performance Goals is achieved, whereas if it falls within the outer box then the PM Performance Criteria is achieved. The seasonal trends in model performance can quickly be gaged by these soccer plots. For example, in both the 2007 CAMx (Figure 8-9, left) and 2002 CMAQ (Figure 8-9, right) applications the models exhibit a summer PM$_{2.5}$ underestimation bias that fails to achieve the PM Performance Goal, but does achieve the PM Performance Criteria.

Figure 8-9. Example soccerplots comparing monthly PM$_{2.5}$ fractional bias and error versus the PM Performance Goals and Criteria (Table 8-1) for a 2007 Midwest CAMx application (left) and the VISTAS/ASIP 2002 CMAQ application for Georgia (right).
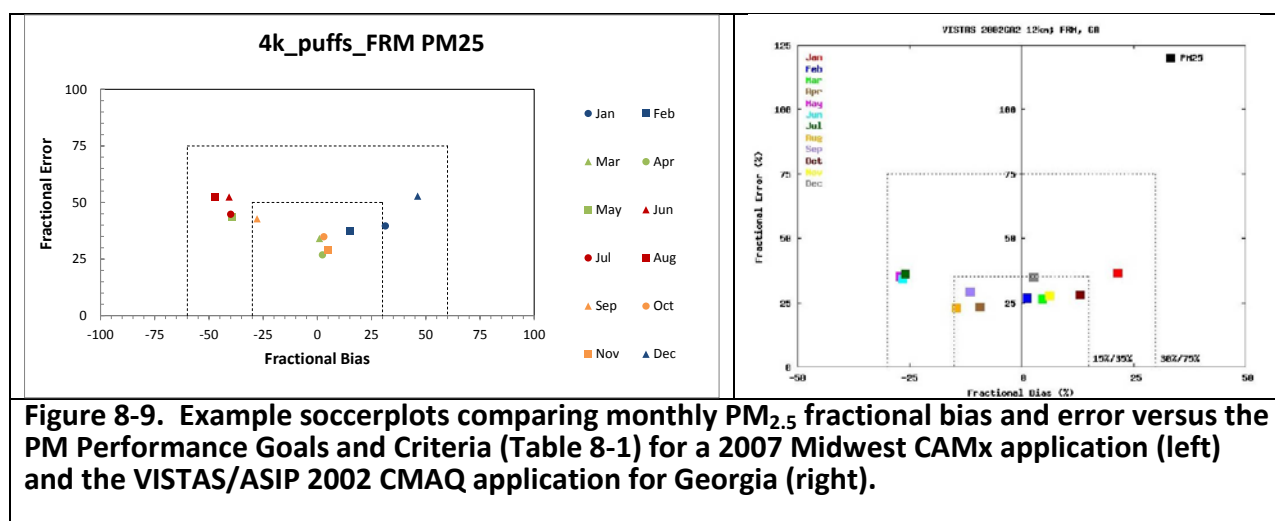
8.5.6 Spatial Plots of Model Performance

Examples of spatial displays of modeling results are presented in Figure 8-10. The top left panel of Figure 8-10 is from the VISTAS/ASIP 2002 CMAQ modeling (Morris et al., 2009a) and compares the predicted 24-hour average PM$_{2.5}$ concentrations on September 5, 2002 (the tile plot) with superimposed observations (the diamond symbols) using the same color scale that was generated using PAVE. When the observed symbols are the same color as the background spatial distribution of the model predictions then the predictions and observations agree with each other. The top right panel of Figure 8-10 shows an example tile plot of ozone model predictions from the VERDI website; VERDI can also do superimposed observations but since our scripts are set up for PAVE we have not migrated to VERDI yet. The bottom left panel of Figure 8-10 is a spatial map of predicted daily maximum 8-hour ozone concentrations with superimposed observations on July 10, 2008 that was generated by SURFER for the Denver area. However, unlike the PAVE plot, the observations are plotted as their concentration values as numbers rather than as colored symbols. These kinds of displays are useful in understanding spatial offsets in the modeling results. The lower right panel of Figure 8-10 displays the spatial distribution of the VISTAS CMAQ 2002 nitrogen wet deposition by spatially interpolating the Mean Normalized Bias (MNB) statistics from the NADP monitoring sites.
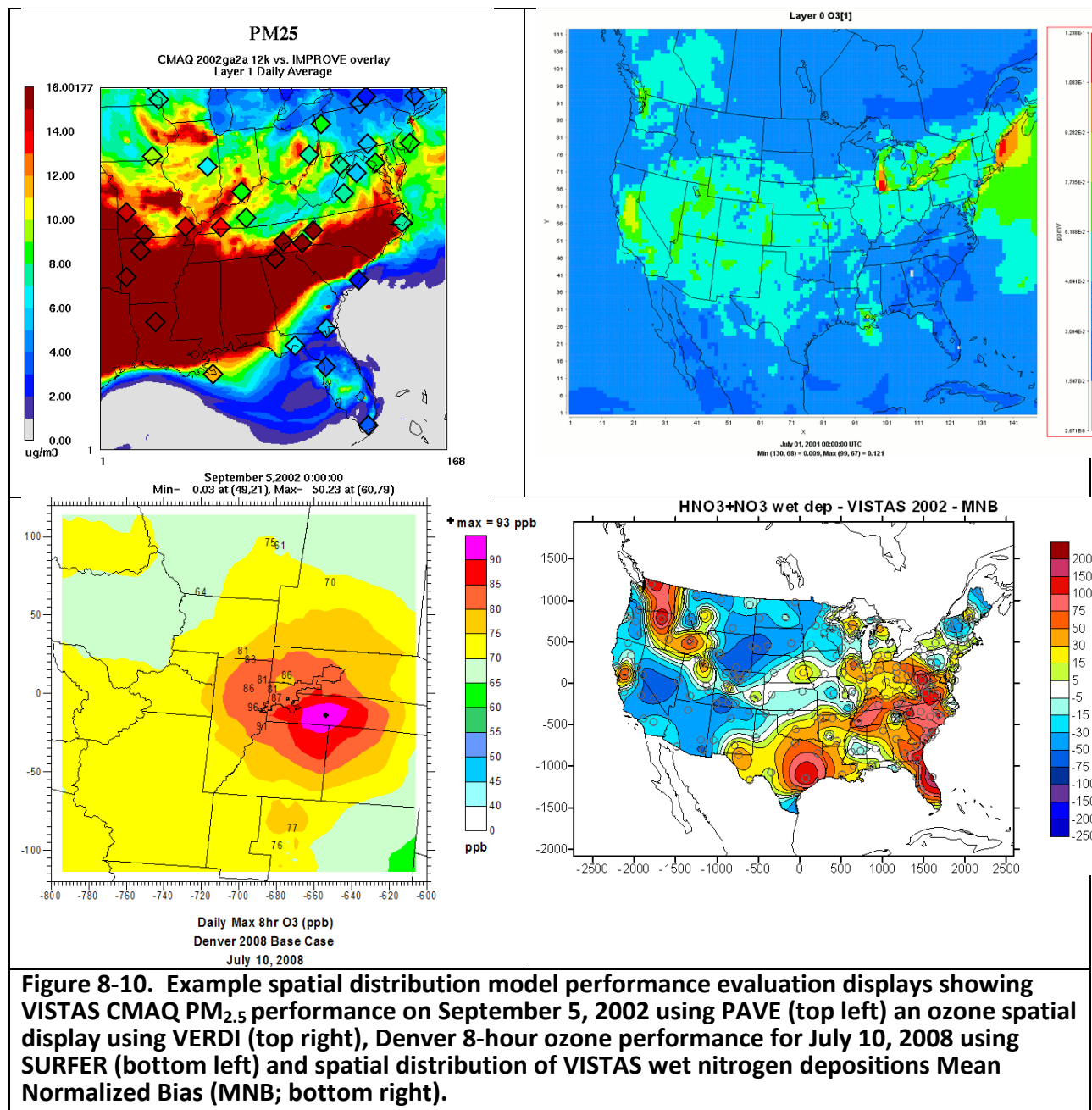
Figure 8-10. Example spatial distribution model performance evaluation displays showing VISTAS CMAQ PM$_{2.5}$ performance on September 5, 2002 using PAVE (top left) an ozone spatial display using VERDI (top right), Denver 8-hour ozone performance for July 10, 2008 using SURFER (bottom left) and spatial distribution of VISTAS wet nitrogen depositions Mean Normalized Bias (MNB; bottom right).

8.6 SUMMARY OF MODEL PERFORMANCE

A model performance of the CAMx 36/12 2008 base case simulations will be conducted for ozone, ozone precursors, methane, PM$_{2.5}$ and speciated PM$_{2.5}$ concentrations and wet sulfur and nitrogen depositions over the three state region. This will be followed by subregional evaluation of the 12 and 4 km modeling results focusing on subdomains in the western U.S. potentially including the IAD and DSAD subdomains and by state. Dry deposition will be evaluated as appropriate (note that dry deposition "measurements" are obtained through application of a surface layer model) and we will keep track of the nitrogen species components in the modeled wet and dry deposition.

9.0 WEBSITE AND REPORTING

Because of the sheer volume of information that will be generated as part of the meteorological and emissions modeling, and in the model performance evaluation, the results will be made available on a project website with summary reports and PowerPoint presentations also generated. We will post data and reports as work is completed. Note that WESTAR is also managing the 3-state data warehouse that will also be distributing related information.

9.1 INTERACTIVE WEBSITE

As modeling steps and results are completed from the 3SAQS project, they will be made available on an interactive website that will allow users to drill down in the model evaluation or source apportionment results to obtain more detailed analysis down to individual monitoring sites. This will allow users to assess Ozone/PM contributions at specific monitoring sites, as well as how well the model performed at the same monitoring site.

In addition to the contributions to ozone and $PM_{2.5}$ Design Values, raw modeling results of daily contributions as well as contributions to visibility impairment and deposition at Class I areas (IMPROVE monitoring sites) will be generated. Quality assurance displays will also be made available.

The website will include an interactive source apportionment visualization tool to allow users to customize their graphics.

As the 3SAQS project website is being developed, preliminary reports and results are available on the UNC website:

http://www.ie.unc.edu/cempd/projects/data_viewer/index.cfm?project=3SAQS

10.2 REPORTS

Summary reports and PowerPoint presentations will be prepared at the end of each major task. An important component of the reporting summaries will be examples of where more information can be obtained on the website. The following reports have been or will be prepared under the 3SAQS:

- Technical Scope of Work

- Modeling Plan

- 3SDW Design Document

- 2008 Modeling Protocol (this document)

- 2008 Base Case and Model Performance Evaluation Report

- Final Report

10.0 ACRONYMS

ACHD	Allegheny County Health Department
ACM	Asymmetric Convective Mixing
AES	Applied Envirosolutions
AMET	Atmospheric Model Evaluation Tool
APCA	Anthropogenic Precursor Culpability Assessment
APU	Auxiliary Power Units
AQ	Air Quality
AQRV	Air Quality Related Value
AQS	Air Quality System
BC	Boundary Condition
BEIS	Biogenic Emissions Information System
BLM	Bureau of Land Management
CAFOS	Concentrated Animal Feeding Operations
CAMD	Clean Air Markets Division
CAMx	Comprehensive Air-quality Model with extensions
CASTNet	Clean Air Status and Trends Network
CAVR	Clean Air Visibility Rule
CB05	Carbon Bond mechanism version 5
CB05	Carbon Bond mechanism version 6
CD-C	Continental Divide-Creston
CDPHE	Colorado Department of Health and Environment
CEM	Continuous Emissions Monitor
CENRAP	Central Regional Air Planning Association
CMAQ	Community Multiscale Air Quality modeling system
CMU	Carnegie Mellon University
ConCEPT	Consolidated Community Emissions Processing Tool
CONUS	Continental United States
CPC	Center for Prediction of Climate
CSAPR	Cross State Air Pollution Rule
CSN	Chemical Speciation Network
DDM	Decoupled Direct Method
DEASCO3	Deterministic and Empirical Assessment of Smoke's Contribution to Ozone
DMA	Denver Metropolitan Area
DSAD	Detailed Source Apportionment Domain
EAC	Early Action Compact
ECA	Emissions Control Area
EGU	Electrical Generating Units
EIS	Environmental Impact Statement
EM	Emissions Model
EMS	Emissions Modeling System
EPA	Environmental Protection Agency
EPS	Emissions Processing System
ERG	Eastern Research Group
ESRL	Earth Systems Research Laboratory

FB	Fractional Bias
FCAQTF	Four Corners Air Quality Task Force
FE	Fractional Error
FINN	Fire INventory from NCAR
FLM	Federal Land Manager
FRM	Federal Reference Method
FWS	Fish and Wildlife Service
GCM	Global Chemistry Model
GEOS-Chem	Goddard Earth Observing System (GEOS) global chemistry model
GSE	Ground Support Equipment
HDDM	Higher order Decoupled Direct Method
IAD	Impact Assessment Domain
IMPROVE	Interagency Monitoring of Protected Visual Environments
IMWD	Inter-Mountains West Processing Domain
IPAMS	Independent Petroleum Association of the Mountain States
JSFP	Joint Science Fire Program
LCP	Lambert Conformal Projection
LTO	Landing and Takeoff Operations
LSM	Lane Surface Model
MADIS	Meteorological Assimilation Data Ingest System
MATS	Mercury and Air Toxics Standards
MATS	Modeled Attainment Test Software
MCIP	Meteorology-Chemistry Interface Processor
MEGAN	Model of Emissions of Gases and Aerosols in Nature
MM	Meteorological Model
MM5	Version 5 of the Mesoscale Model
MNGE	Mean Normalized Gross Error
MNB	Mean Normalized Bias
MOVES	Motor Vehicle Emissions Simulator
MOZART	Model for OZone And Related chemical Tracers
NAAQS	National Ambient Air Quality Standard
NADP	National Acid Deposition Program
NCAR	National Center for Atmospheric Research
NCDC	National Climatic Data Center
NDBC	National Data Buoy Center
NEI	National Emissions Inventory
NEPA	National Environmental Policy Act
NMB	Normalized Mean Bias
NME	Normalized Mean Error
NMIM	National Mobile Inventory Model
NOAA	National Oceanic and Atmospheric Administration
NPRI	National Pollutant Release Inventory
NPS	National Park Service
NSPS	New Source Performance Standard
O&G	Oil and Gas
OA	Organic Aerosol
OSAT	Ozone Source Apportionment Technology

PA	Process Analysis
PAVE	Package for Analysis and Visualization
PBL	Planetary Boundary Layer
PGM	Photochemical Grid Model
PiG	Plume-in-Grid
PM	Particulate Matter
PPM	Piecewise Parabolic Method
PSAT	Particulate Source Apportionment Technology
QA	Quality Assurance
QC	Quality Control
RAQC	Regional Air Quality Council
RMC	Regional Modeling Center
RMNP	Rocky Mountain National Park
RMP	Resource Management Plan
ROMANS	Rocky Mountain Atmospheric Nitrogen and Sulfur Study
SCC	Source Classification Code
SIP	State Implementation Plan
SMOKE	Sparse Matrix Kernel Emissions modeling system
SOA	Secondary Organic Aerosol
TCEQ	Texas Commission on Environmental Quality
UAM	Urban Airshed Model
UCR	University of California at Riverside
UNC	University of North Carolina
UPA	Unpaired Peak Accuracy
USFS	United States Forest Service
VERDI	Visualization Environment for Rich Data Interpretation
VISTAS	Visibility Improvements for States and Tribal Associations in the Southeast
VMT	Vehicle Miles Traveled
WBD	Wind Blown Dust model
WEA	Western Energy Alliance
West-CARMMS	Western Colorado Air Resource Management Modeling Study
WESTAR	Western States Air Resources Council
WESTUS	Western United States
WRAP	Western Regional Air Partnership
WGA	Western Governors' Association
WRF	Weather Research Forecasting model

11.0 REFERENCES

Adelman, Z. 2004: Quality Assurance Protocol – WRAP RMC Emissions Modeling with SMOKE, Prepared for the WRAP Modeling Forum by the WRAP Regional Modeling Center, Riverside, CA

BLM. 2012. Environmental Impact Statement Continental Divide-Creston Natural Gas Development Project, Draft. Air Quality Technical Support Document (AQTSD), Appendix E: Diagnostic Sensitivity Test Modeling Results to Achieve Final Base Case Model Configuration for the Continental Divide-Creston O&G EIS. Bureau of Land Management, Wyoming High Desert District, Rawlins Field Office. November. (http://www.blm.gov/wy/st/en/info/NEPA/documents/rfo/cd_creston.html).

Boylan, J.W., M.T. Odman, J.G. Wilkinson, A.G. Russell, K.G. Doty, W.B. Norris, and R.T. McNider. 2003. Development of a comprehensive multiscale "one-atmosphere" modeling system: Application to the Southern Appalachian Mountains. *Atmos. Environ.*, **36** (23), 3721-3734.

Boylan, J.W. 2004. Calculating Statistics: Concentration Related Performance Goals. EPA PM Model Performance Workshop, Chapel Hill, NC. February 11.

Coats, C.J., 1995. Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System, MCNC Environmental Programs, Research Triangle Park, NC.

Colella, P., and P.R. Woodward. 1984. The Piecewise Parabolic Method (PPM) for Gas-dynamical Simulations. *J. Comp. Phys.*, **54**, 174-201.

Emery, C.A., E. Tai, E., R. E. Morris, G. Yarwood. 2009a. Reducing Vertical Transport Over Complex Terrain in CMAQ and CAMx; AWMA Guideline on Air Quality Models Conference, Raleigh, NC, October 26-30, 2009.

Emery, C.A., E. Tai, R.E. Morris, G. Yarwood. 2009b. Reducing Vertical Transport Over Complex Terrain in Photochemical Grid Models; 8th Annual CMAS Conference, Chapel Hill, NC, October 19-21, 2009.ENVIRON. 2011a. User's Guide – Comprehensive Air Quality Model with Extensions – Version 5.40. ENVIRON International Corporation, Novato, California. September. (www.camx.com).

ENVIRON. 2011a. User's Guide – Comprehensive Air Quality Model with Extensions – Version 5.40. ENVIRON International Corporation, Novato, California http://www.camx.com. September.

ENVIRON. 2011b. Western Regional Air Partnership (WRAP) West-wide Jump-start Air Quality Modeling Study (WestJumpAQMS) Scope of Work. ENVIRON International Corporation, Novato, California. June 20. (http://www.wrapair2.org/pdf/WestJumpAQMS_SoW_July20_2011revision.pdf).

ENVIRON. 2012a. Western Regional Air Partnership (WRAP) West-wide Jump-start Air Quality Modeling Study (WestJumpAQMS) Modeling Plan. ENVIRON International Corporation,

Novato, California. January 23.
(http://www.wrapair2.org/pdf/WestJumpAQMS_Modeling_Plan_Final_Jan23_2012.pdf).

ENVIRON and Alpine. 2012b. Western Regional Air Partnership (WRAP) West-wide Jump-start
Air Quality Modeling Study (WestJumpAQMS) – WRF Application/Evaluation. ENVIRON
International Corporation, Novato, California. Alpine Geophysics, LLC. University of
North Carolina. February 29.
(http://www.wrapair2.org/pdf/WestJumpAQMS_2008_Annual_WRF_Final_Report_February29_2012.pdf).

ENVIRON. 2012c. Improved biogenic emission inventories across the West – Final Report.
ENVIRON International Corporation, Novato, California. March 19.
(http://www.wrapair2.org/pdf/WGA_BiogEmisInv_FinalReport_March20_2012.pdf)

EPA. 1991. Guideline on the Regulatory Application of the Urban Airshed Model. U.S.
Environmental Protection Agency, Office of Air Quality Planning and Standards,
technical Support Division, Source Receptor Analysis Branch, Research Triangle Park,
North Carolina. July. (http://www.epa.gov/ttn/scram/guidance/guide/uamreg.pdf).

EPA. 2007. Guidance on the Use of Models and Other Analyses for Demonstrating Attainment
of Air Quality Goals for Ozone, PM2.5 and Regional Haze. U.S. Environmental Protection
Agency, Research Triangle Park, NC. EPA-454/B-07-002. April.
(http://www.epa.gov/ttn/scram/guidance/guide/final-03-pm-rh-guidance.pdf).

EPA. 2012. Technical Support Document – Preparation of Emission Inventories for the Version
5.0, 2007 Emissions Modeling Platform. U.S. Environmental Protection Agency, Research
Triangle Park, NC. December 14.
(http://epa.gov/ttn/chief/emch/2007v5/2007v5_2020base_EmisMod_TSD_13dec2012.pdf)

Hertel O., R. Berkowics, J. Christensen and O. Hov. 1993. Test of two numerical schemes for
use in atmospheric transport-chemistry models. *Atmos. Environ.*, **27**, 2591-2611.

Houyoux, M. R., C. J. Coats Jr., A. Eyth, and S. Lo, Emissions modeling for SMRAQ: A seasonal
and regional example using SMOKE, paper presented at Computing in Environmental
Resource Management, Air and Waste Manage. Assoc., Research Triangle Park, N. C., Dec.
2-4, 1996.

Houyoux, M.R., Vukovich, J.M., Coats Jr., C.J., Wheeler, N.J.M., Kasibhatla, P.S., 2000. Emission
inventory development and processing for the Seasonal Model for Regional Air Quality
(SMRAQ) project. Journal of Geophysical Research 105(D7), 9079-9090.

Simon, H., K. Baker and S. Phillips. 2012. Compilations and Interpretation of Photochemical
Model Performance Statistics Published between 2006 and 2012. *Atmos. Env.* 61 (2012)
124-139. December.
(http://www.sciencedirect.com/science/article/pii/S135223101200684X).

Skamarock, W. C. 2004. Evaluating Mesoscale NWP Models Using Kinetic Energy Spectra. *Mon.
Wea. Rev.*, Volume 132, pp. 3019-3032. December.
(http://www.mmm.ucar.edu/individual/skamarock/spectra_mwr_2004.pdf).

Skamarock, W. C., J. B. Klemp, J. Dudhia, D. O. Gill, D. M. Barker, W. Wang and J. G. Powers. 2005. A Description of the Advanced Research WRF Version 2. National Center for Atmospheric Research (NCAR), Boulder, CO. June. (http://www.mmm.ucar.edu/wrf/users/docs/arw_v2.pdf)

Skamarock, W. C. 2006. Positive-Definite and Monotonic Limiters for Unrestricted-Time-Step Transport Schemes. *Mon. Wea. Rev.*, Volume 134, pp. 2241-2242. June. (http://www.mmm.ucar.edu/individual/skamarock/advect3d_mwr.pdf).

Tonnesen, G., Z. Wang, M. Omary, C-J. Chien, Y. Wang, R. Morris, S. Kemball-Cook, Y. Jia, S. Lau, B. Koo, Z. Adelman, A. Holland and J. Wallace. 2006. Final Report for the Western Regional Air Partnership (WRAP) 2002 Visibility Model Performance Evaluation. WRAP Regional Modeling Center (RMC). February. http://pah.cert.ucr.edu/aqm/308/reports/final/2002_MPE_report_main_body_FINAL.pdf

Wiedinmyer, C., T. Sakulyanontvittaya and A. Guenther. 2007. MEGAN FORTRAN code V2.04 User Guide. NCAR, Boulder, CO. October 29. (http://acd.ucar.edu/~guenther/MEGAN/MEGANguideFORTRAN204.pdf).

Yarwood, G., J. Jung, G. Z. Whitten, G. Heo, J. Mellberg and M. Estes. 2010. Updates to the Carbon Bond Mechanism for Version 6 (CB05). 2010 CMAS Conference, Chapel Hill, NC. October. (http://www.cmascenter.org/conference/2010/abstracts/emery_updates_carbon_2010.pdf)

Yarwood, G., S. Rao, M. Yocke and G. Whitten. 2005. Updates to the Carbon Bond Mechanism: CB05. ENVIRON International Corporation, Novato, California. Prepared for Deborah Luecken, U.S. Environmental Protection Agency, RTP, NC. December 8. (http://www.camx.com/publ/pdfs/cb05_final_report_120805.aspx).