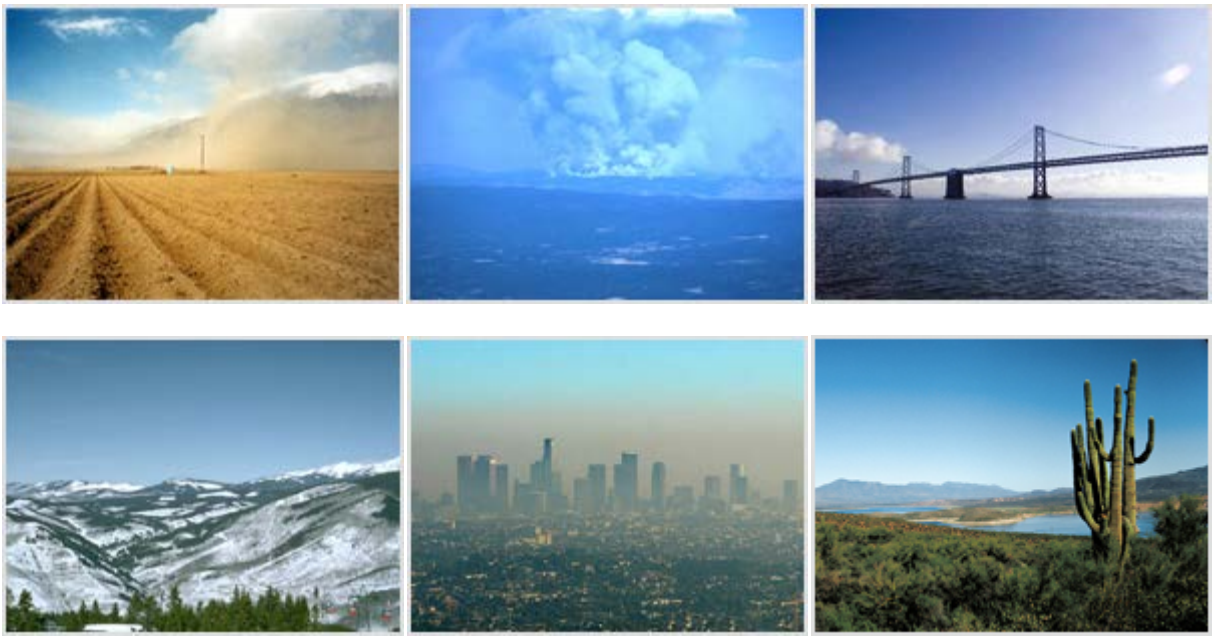

Western Regional Air Partnership (WRAP)
West-wide Jump-start Air Quality Modeling Study (WestJumpAQMS)

Draft Final Modeling Protocol

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WESTERN REGIONAL AIR PARTNERSHIP

ENVIRON

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1.0 INTRODUCTION

ENVIRON International Corporation (ENVIRON), Alpine Geophysics, LLC (Alpine) and the University of North Carolina (UNC) at Chapel Hill Institute for Environment are performing the West-wide Jump-start Air Quality Modeling Study (WestJumpAQMS) managed by the Western Governors' Association (WGA) for the Western Regional Air Partnership (WRAP). The objectives of the WestJumpAQMS are as follows:

- Initiate the next generation of regional technical analysis and support for Ozone and Particulate Matter (PM) transport and attainment demonstrations across the West.
- Further the concept developed by New Mexico Environment Department Air Quality Bureau, EPA Region 6, the Bureau of Land Management (BLM) New Mexico office, British Petroleum (BP), and the Western Regional Air Partnership (WRAP) to begin the next round of regional modeling to support western U.S. air quality planning.
- Continue work conducted at the WRAP Regional Modeling Center (RMC[1]) from 2001-2009 to provide regionally complete and consistent emissions and air quality modeling for the western U.S.
    - The RMC modeling products became the basis for many state and federal land manager air analyses in the West, including numerous NEPA studies, the Denver Ozone study, and the Four Corners Air Quality Task Force (FCAQTF) work. The regional collaboration initiated by the WRAP RMC was effective and efficient for state and regional planning and will enhance the WestJumpAQMS study through the application of WRAP-IPAMS work to compile Oil and Gas VOC and NO_X emission inventories.
- Leverage recent modeling and monitoring analyses that suggest both natural ozone impacts and international impacts are occurring in elevated rural terrain in the spring and the impacts from such events approach the level of the Ozone National Ambient Air Quality Standard (NAAQS).
- Provide a modeling platform to begin addressing the next generation of air quality issues related to Ozone, PM ($PM_{2.5}$ and PM_{10}), visibility and nitrogen and sulfur (acid) deposition.

The goals of the WestJumpAQMS include the following:

1. Incorporate all of the recent western modeling analyses into a single modeling database;
2. Perform a comprehensive model performance evaluation in an open technical forum independent of any specific project or regulatory activity (e.g., a State Implementation Plan [SIP]or action under the National Environmental Policy Act [NEPA]);
3. Perform a comprehensive source apportionment analysis to evaluate local, regional, international, and natural source impacts on elevated ozone concentrations (both rural and urban) across the West;
4. Develop a modeling platform that can be used to conduct or as a starting point for SIP analyses, regional air quality planning and NEPA (EIS) analyses in the West;
5. Allow future evaluation of local and regional control strategies that can be used to demonstrate compliance with new air quality standards; and
6. Provide a framework and recommendations for performing future analysis to address Ozone, PM, visibility, and deposition issues in the western U.S.

1 http://pah.cert.ucr.edu/aqm/308/

The WestJumpAQMS is designed to be an open regional photochemical modeling study whose databases will be available to all. WRAP has been working with its partners to develop a plan for 2011-2012 that initiates gathering of air quality data and improvements to air quality models and source apportionment work. To provide resources for this work, WRAP has acquired funding and substantial in-kind and leveraged support from western States, EPA, BLM, other Federal Land Managers, and BP.

1.1 BACKGROUND

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. In January 2010, EPA announced that they were considering lowering the 8-hour ozone NAAQS to within a range of 0.060 ppm to 0.070 ppm. In August 2011, EPA announced that the 8-hour ozone NAAQS would remain at the March 2008 0.075 ppm level. An initial implementation Memorandum was released by EPA on September 22, 2011 (McCarthy, 2011[2]) that identified 52 potential areas that would be violating the 0.075 ppm 8-hour Ozone NAAQS based on 2008-2010 observations, including many in the western U.S. EPA is finalized the designations of ozone nonattainment areas on March 30, 2012[3]. EPA has also initiated the next round of Ozone NAAQS review with the new Ozone NAAQS currently scheduled to be proposed in March 2013 and finalized in March 2014.

Figure 1-1 displays the 2008-2010 8-hour Ozone Design Values for several counties in the western U.S. along with a few more rural monitoring sites highlighted. Ozone Design Values in excess of the current (75 ppb) Ozone NAAQS generally just occur in urban areas in the western U.S., (e.g., California, Denver, Salt Lake City and Las Vegas). However, there are numerous more rural areas that are in the 70-75 ppb range. Furthermore, 2009 was a low ozone year in the western U.S. both in terms of photochemically active meteorological conditions as well as reduced emissions due to the recession.

On June 14, 2012, EPA proposed to revised the $PM_{2.5}$ NAAQS by lowering the annual $PM_{2.5}$ NAAQS from 15.0 $\mu g/m^3$ to somewhere in the 12.0 to 13.0 $\mu g/m^3$ range[4]. EPA proposes to retain the 24-hour $PM_{2.5}$ NAAQS at 35 $\mu g/m^3$ as well as setting the secondary $PM_{2.5}$ NAAQS equivalent to the primary NAAQS. But EPA is also proposes a new secondary $PM_{2.5}$ NAAQS to protect against visibility impairment in urban areas with a proposed threshold in the 28 to 30 deciview range. Figure 1-2 displays counties that are violating the current 15.0 $\mu g/m^3$ annual $PM_{2.5}$ NAAQS and the additional counties that would violate a proposed 13.0 and 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 proposed annual $PM_{2.5}$ NAAQS levels.

2 http://www.epa.gov/air/ozonepollution/pdfs/OzoneMemo9-22-11.pdf
3 http://epa.gov/oaqps001/greenbk/gnc.html
4 http://www.epa.gov/pm/actions.html#jun12

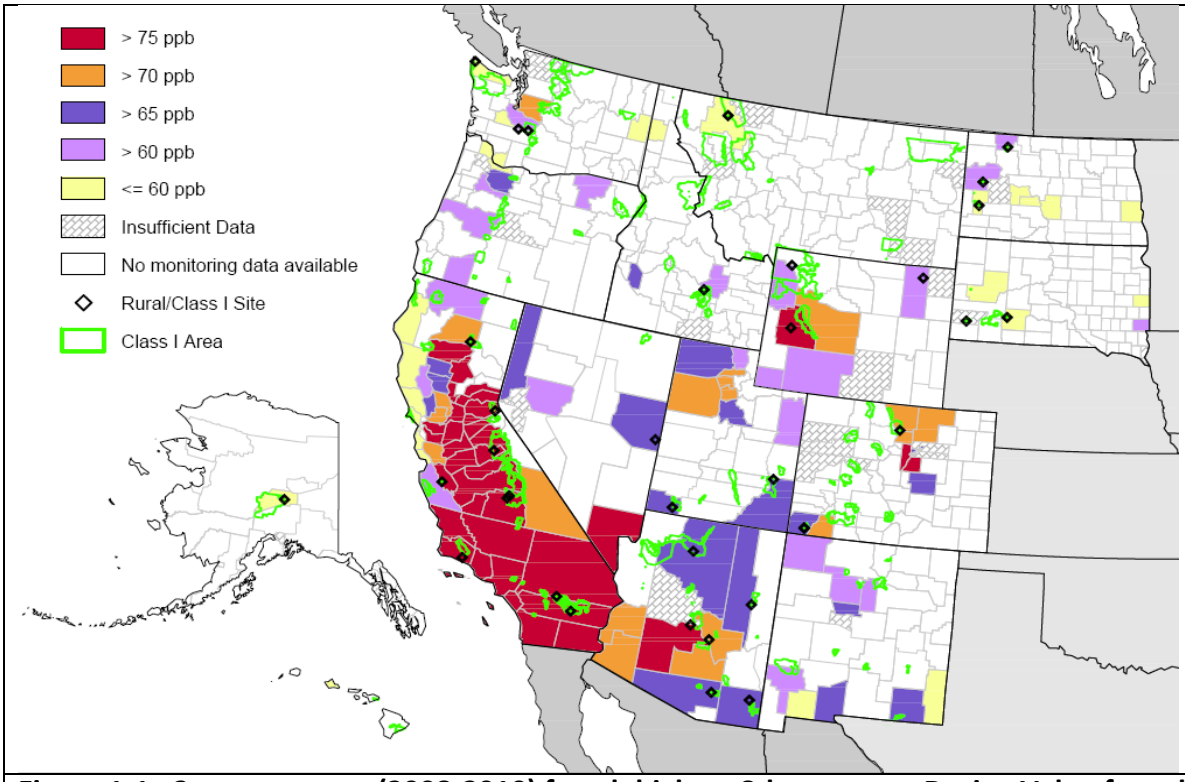


Figure 1-1. 3-year average (2008-2010) fourth highest 8-hour ozone Design Value for selected counties with color scheme indicating whether the Design Value exceeds (red) or is below the March 2008 ozone NAAQS (EPA AQS Federal Reference Method [FRM] data from the monitoring site with the highest ozone in each county).

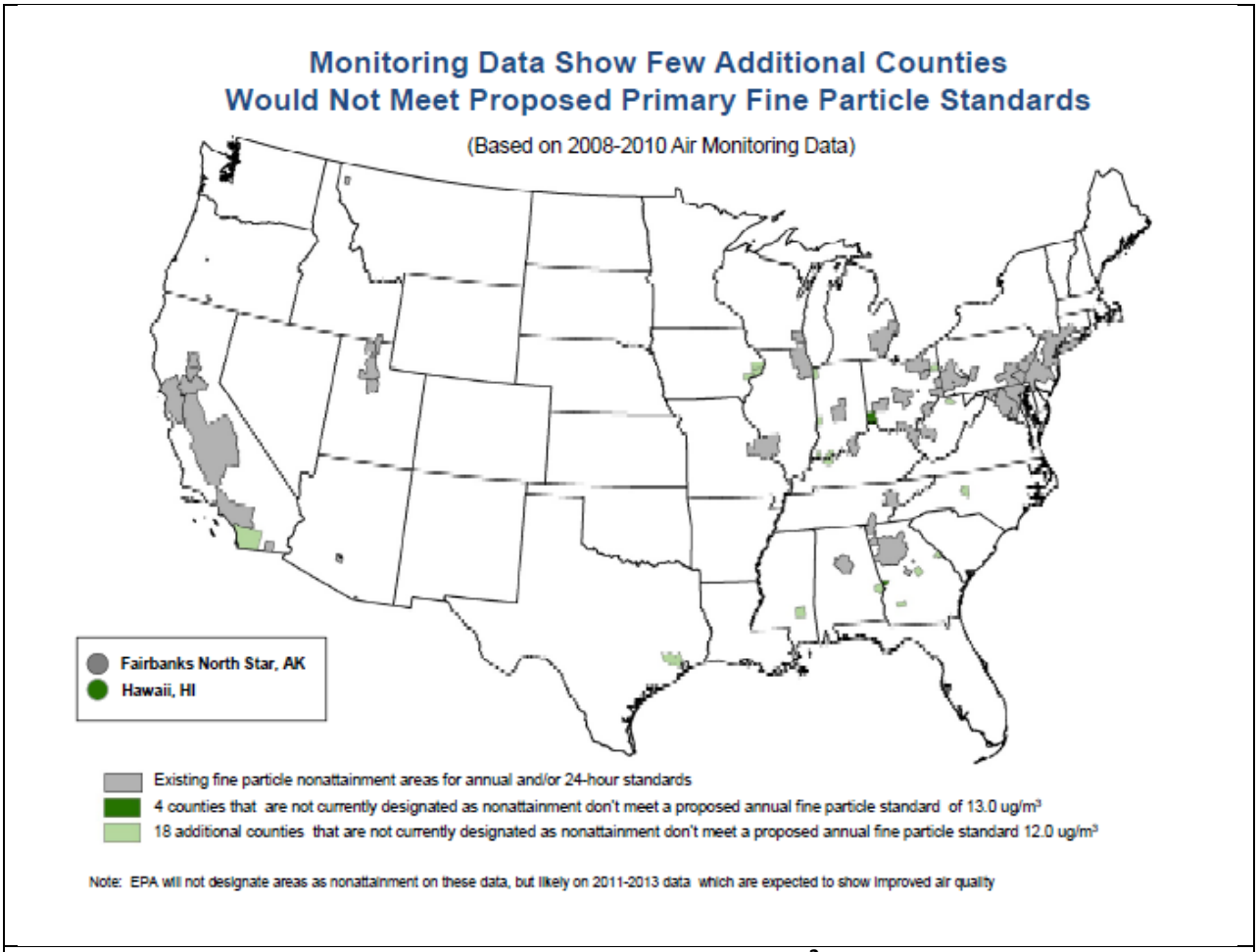


Figure 1-2. Counties that are violating the current 15.0 µg/m^3 $PM_{2.5}$ NAAQS and additional counties that would violate a proposed 13.0 µg/m^3 (dark green) and 12.0 µg/m^3 $PM_{2.5}$ NAAQS based on 2008-2010 observations (source: http://www.epa.gov/pm/actions.html#jun12).

1.2 ORGANIZATION OF THE MODELING PROTOCOL

This document represents a Modeling Protocol for the WestJumpAQMS. Although the WestJumpAQMS modeling analysis is not currently being performed to fill any particular regulatory requirement, such as a State Implementation Plan (SIP) attainment demonstration or an Environmental Impact Statement (EIS) 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. This includes following EPA's modeling guidance for ozone, $PM_{2.5}$ and visibility SIPs (EPA, 2007) that has a requirement to initiate the study with a Modeling Protocol. The Modeling Protocol serves as a roadmap for the study and is a forum for informing project participants, states, local agencies, federal agencies and stakeholders on the elements of the study. This WestJumpAQMS Modeling Protocol has the following sections:

1. Introduction: Presents a summary 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.

4. Modeling Domain Selection: Presents the modeling domains and grid structure for the modeling study.
5. WRF Meteorology: Describes how the meteorological modeling was conducted and the WRF model evaluation.
6. Emissions: Describes the source emissions and the procedures for emissions modeling and quality assurance.
7. Photochemical Modeling: Describes the procedures for conducting the photochemical grid model including the model versions, inputs and options
8. Model Performance Evaluation: Provides the procedures for conducting the model performance evaluation of the photochemical grid models.
9. Source Apportionment: The objectives, configuration and procedures for conducting the source apportionment modeling are described in this section.
10. References: References cited in the document.

1.3 PROJECT PARTICIPANTS

The WestJumpAQMS is being performed by the contracting team of ENVIRON International Corporation, Alpine Geophysics, LLC and University of Carolina at Chapel Hill, Center for Environmental Modeling for Policy Development under technical direction of the Western Regional Air Partnership (WRAP)/Western Governors Association (WGA). Funding for WestJumpAQMS has been provided by the State of New Mexico, EPA Region 6, New Mexico Bureau of Land Management (BLM) and the National BLM Air Program. WestJumpAQMS has had numerous conference calls discussing aspects of the study with interested parties from the WRAP States and Local Agencies, U.S. EPA, National Park Service, U.S. Forest Service, U.S. Fish and Wildlife Service, BLM and Stakeholders. The key contacts and their roles in the WestJumpAQMS modeling study are listed in Table 1-1.

Table 1-1. Key contacts in the WestJumpAQMS.

Name	Role	Organization/Contact
Tom Moore	Technical Coordinator	Western Governors' Association (WGA) Western Regional Air Partnership (WRAP) c/o CSU/CIRA 1375 Campus Delivery Fort Collins, CO 80523 (970) 491-8837 tmoore@westgov.org
Ralph Morris	Project Manager	ENVIRON International Corporation 773 San Marin Drive, Suite 2115 Novato, CA 94998 (415) 899-0708 rmorris@environcorp.com
Dennis McNally	Alpine Lead	Alpine Geophysics, LLC 7341 Poppy Way Arvada, CO 80007 (303) 421-2211 dem@alpinegeophysics.com
Zac Adelman	UNC Lead	University of North Carolina Center for Environmental Modeling for Policy Development 137 E. Franklin St., Room 665 Campus Box 6116 Chapel Hill, NC 27599-6116 (919) 966-2206 zac@unc.edu

1.4 RELATED REGIONAL MODELING STUDIES

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

1.4.1 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
- NOX SIP Call:
- Cross State Air Pollution Rule (CSAPR)
- 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)

1.4.2 2003 Denver EAC SIP Modeling

The Denver EAC SIP modeling performed 36/12/4/1.33 km photochemical modeling of the Denver Metropolitan Area (DMA) using the MM5 meteorological, EPS3 emissions and CAMx photochemical grid models and a summer 2002 period. Although the EAC SIP modeling used grid spacing as small as 1.33 km and found improved meteorological model performance at the finer grid spacing, there were little benefits in the photochemical modeling using the 1.33 km versus 4 km grid spacing. In fact ozone model performance degraded somewhat using the 1.33 km grid and the computational requirements increased substantially. Thus, the final Denver EAC SIP attainment demonstration modeling was based on the 4 km modeling results. Details on the 2003 Denver EAC SIP modeling can be found at:

http://raqc.org/sip/more/category/ozone_8-hour_standard/

1.4.3 2008 Denver Ozone SIP Modeling

As was used in the 2003 Denver EAC SIP modeling, the 2008 Denver ozone SIP modeling used the MM5 meteorological and the CAMx photochemical grid models, but SMOKE and CONCEPT were used for the 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:

http://www.colorado.gov/airquality/documents/deno308/

1.4.4 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 WestJumpAQMS and the May through August 2008 portion of the WestJumpAQMS 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. Many of the model configurations and data sources being used in the WestJumpAQMS are also being used in the Denver modeling of the 2008 episode whose details can be found in the Modeling Protocol:

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

1.4.5 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 and 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., 2005), SMOKE emissions and CMAQ and CAMx photochemical models. CMAQ was run for a 2002 base case 2018 future base-year and 2018 control scenarios to predict visibility projections in Federal Class I areas. The WRAP RMC has a website where modeling results can be obtained and 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/

1.4.6 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 several large coal-fired power plants as well (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

1.4.7 Environmental Impact Statements (EISs) and Related Modeling

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. Recently completed and ongoing BLM RMPs include the White River, Colorado River Valley, Grand Junction and Uncompahgre Field Office RMPs in Colorado. These studies used, or are using, the CAMx photochemical grid model to assess potential ozone impacts due to the cumulative oil and gas development projects in the region. Details on BLM activities in Colorado can be found at:

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

1.4.8 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.cdphe.state.co.us/ap/rmnp.html

1.5 OVERVIEW OF MODELING APPROACH

The initial procedures for the WestJumpAQMS modeling approach were documented in a draft and final Technical Scope of Work dated February 2011 and July 2011, respectively (ENVIRON, 2011a). The modeling approach was refined and described in more detail in a WestJumpAQMS Modeling Plan dated January 23, 2012 (ENVIRON, 2012a). A summary of the WestJumpAQMS emissions, meteorological and photochemical grid modeling approach is given below, with more details provided in the Chapters of this Modeling Protocol.

- The 2008 calendar year will be selected for the modeling period.
- A 36 km continental U.S. (CONUS), 12 km western U.S. (WESTUS) and several types of 4 km resolution modeling domains will be selected.
- Meteorological modeling will be conducted using the Weather Research Forecasting (WRF) modeling.
- Emissions modeling will mostly use the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system based mainly on emissions data from the Version 2.0 of the 2008 National Emissions Inventory (NEIv2.0).
- Photochemical grid modeling will be based on the Comprehensive Air-quality with extensions (CAMx) with sensitivity tests using the Community Multiscale Air Quality (CMAQ) modeling system also conducted.
- Boundary conditions (BCs) for the lateral boundaries of the 36 km CONUS domain will be based on the MOZART global chemistry model.
- Model evaluation will be conducted for ozone, particulate matter (PM) mass and speciation and ozone and PM precursor and product species as well as for visibility and deposition.
- Several types of ozone and PM source apportionment modeling will be performed to analyze the contributions of individual state's anthropogenic emissions to elevated ozone and PM concentrations.

2.0 MODEL SELECTION

This section introduces the models to be used in the WestJumpAQMS. The selection methodology presented in this chapter 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). Unlike some previous ozone modeling guidance (e.g., EPA, 1991), the EPA now recommends that models be selected for regulatory ozone 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 identifying the most appropriate candidate models that we believe are best suited to the requirements of the WestJumpAQMS, 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 WestJumpAQMS 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. 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[5] and application history.
- Publicly Available: WRF is publicly available and can be downloaded from the WRF website with no costs or restrictions[6].
- 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[7]: The non-hydrostatic version of the Advanced Research version of the Weather Research Forecast (WRF-ARW[8]) 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, 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 Models

Emissions models use base annual county-level or point source emissions data and generate the hourly gridded speciated emission inputs needed for photochemical grid models (PGMs). There are four main emissions modeling systems that have been used to generate emission inputs for PGMs:

5 http://www.wrf-model.org/wrfadmin/publications.php
6 http://wrf-model.org/users/users.php
7 http://www.wrf-model.org/index.php
8 All references to WRF in this document refer to the WRF-ARW

- Emissions Processing System (EPS3);
- Emissions Modeling System (EMS);
- Sparse Matrix Operator Kernel Emissions (SMOKE) model; and
- Consolidated Community Emissions Processing Tool (ConCEPT).

EPS was part of the Urban Airshed Model (UAM) modeling system that was delivered to EPA in 1990. Although EPS3 is still being used in some locations (e.g., Texas), it has mostly been replaced by the newer emissions models. EMS was developed in part as part of the Lake Michigan Ozone Study (LMOS) using SAS programing. As SAS is an expensive package not routinely used by the air quality modeling community and is slow, EMS is mainly not used anymore. SMOKE was developed by EPA and distributed with the CMAQ modeling system; it is the most widely used emissions modeling system in the U.S. ConCEPT is not widely used except for a ConCEPT MV module that has a unique capability to interface with Travel Demand Model (TDM) output of link-based Vehicle Miles Travelled (VMT) to produce highly resolved on-road mobile source emission inputs. The SMOKE emissions model was selected for the WestJumpAQMS for the following reasons:

- Technical: SMOKE has all the technical features needed to generate PGM emissions inputs and is more up-to-date than the other emissions models. With the exception of ConCEPT MV for on-road mobile source emissions using TDM link-based data that will not be used in WestJumpAQMS, SMOKE is technically superior to the other emissions models.
- Performance: The SMOKE model is by far the fastest running emissions model.
- Publicly Available: SMOKE is publicly available and can be downloaded from the SMOKE model website for no cost or restrictions[9].
- Demonstrated Success: The SMOKE emissions model is the most widely used emissions model in the U.S. It has been used for numerous EPA regulatory actions and ozone, $PM_{2.5}$ and visibility SIPs.

There are several other specialty emissions models that will be used in the WestJumpAQMS. EPA has developed the MOter Vehicle Emissions Simulator (MOVES) on-road mobile source emissions model and requires all states, except California, to use MOVES in future SIP modeling[10]. WRAP has recently updated the MEGAN biogenic emissions model to better simulate biogenic emissions in the western U.S. Thus, WestJumpAQMS has also adopted the MOVES and MEGAN models. Below are brief descriptions of the emissions models selected for the WestJumpAQMS.

SMOKE[11]: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is an emissions modeling system that generates hourly gridded speciated emission inputs of mobile, non-road, area, point, fire and biogenic emission sources for photochemical grid models (Coats, 1995; Houyoux et al., 2000). As with most 'emissions models', SMOKE is principally an *emission processing system* and not a true *emissions modeling system* in which emissions estimates are simulated from 'first principles'. This means that, with the exception of mobile and biogenic sources, its purpose is to provide an efficient, modern tool for converting an existing base emissions inventory data into the hourly gridded and speciated emission files required by an air quality simulation model.

9 http://www.smoke-model.org/index.cfm
10 http://www.epa.gov/otaq/models/moves/documents/420b12010.pdf
11 http://www.smoke-model.org/version2.7/

MOVES[12]**:** 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[13]: 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., 201214; Wiedinmyer, Sakulyanontvittaya and Guenther, 2007[15]). 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 recently updated the MEGAN biogenic emissions models using western U.S. data and higher resolution inputs (Sakulyanontvittaya, Yarwood and Guenther, 2012[16]).

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. One of key objectives of the WestJumpAQMS is to perform ozone and PM source apportionment modeling to examine source-receptor relationships across the western U.S. A peer-review of the source apportionment techniques in the CMAQ and CAMx models found that the CAMx source apportionment approach was both technically and operationally superior to the source apportionment algorithms in CMAQ (Arunachalam, 2009). Because of this, CAMx was selected as the main model in WestJumpAQMS, but the CMAQ model will also be applied for base case modeling.

- 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 WestJumpAQMS source apportionment modeling that is not present in CMAQ.

12 http://www.epa.gov/otaq/models/moves/index.htm
13 http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm
14 http://acd.ucar.edu/~guenther/MEGAN/MEGANv2.10_beta/MEGAN2.1_User_Guide_05-07-2012.pdf
15 http://acd.ucar.edu/~guenther/MEGAN/MEGANguideFORTRAN204.pdf
16 http://wrapair2.org/pdf/WGA_BiogEmisInv_FinalReport_March20_2012.pdf

- 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.
- Publicly Available: 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[17]: 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.). Of particular importance for the WestJumpAQMS study is the available of Ozone and Particulate Source Apportionment Technology (OSAT/PSAT) that will be used to perform source apportionment modeling across the western states.

CMAQ[18]: 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 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.

2.2 MODEL INTERACTION

Both the CAMx and CMAQ PGMs will be applied in the WestJumpAQMS project. The most current versions of these two PGMs are CAMx Version 5.4 (October 2011) and CMAQ Version 5.0.1 (July 2012). The WRF meteorological model Version 3.3 (April 2011) will be applied for the selected modeling episode and grid structure. The WRF output will be processed using the MM5CAMx and the Meteorology-Chemistry Interface Processor (MCIP) to generate meteorological inputs for the, respectively, CAMx and CMAQ models.

17 http://www.camx.com/
18 http://www.cmaq-model.org/

Day-specific hourly SO_2 and NO_X emissions for large (typically > 25 MWe) Electrical Generating Units (EGUs) will be obtained from the EPA Clean Air Markets Division's (CAMD) Continuous Emissions Monitoring (CEM) systems data. Emissions for other point sources will be based on the 2008 NEIv2.0 as described in Chapter 5. The MOVES2010a on-road mobile source emissions model will be applied to generate county-level emissions for each county in the U.S. Oil and gas emissions will be based on the latest WRAP Phase III oil and gas emissions inventory[19] for the Rocky Mountain States projected to 2008. Anthropogenic emissions for area, non-road and other source categories will be based on the 2008 NEIv2.0 as described in Chapter 5. Biogenic emissions will be generated using an enhanced version of the MEGAN biogenic emissions modeling system from a WRAP study to improve biogenic emissions modeling in the western U.S.[20] WRAP is also engaged in a study (DEASCO3) to generate improved fire emissions for the U.S.[21], which will likely be used in the WestJumpAQMS study as a sensitivity analysis. Otherwise an alternative interim fire emission inventory will be used in the initial PGM simulations based on the Fire Inventory from NCAR (FINN[22]).

With the exception of biogenic, fire, windblown dust, sea salt and lighting emissions, each major source sector will be processed separately by SMOKE to generate pre-merged PGM-ready emissions inputs. This will allow for the ease of specifying alternative source apportionment source categories in later stages of the study. Biogenic emissions will be prepared using the MEGAN model. Fire emissions will be based on the FINN processed by EPS3, which will later be replaced by the 2008 fire emissions from the DEASCO3 study. The WRAP WBD model will also be used. And sea salt and lightning emissions will be prepared using their own processors. The SMOKE processed pre-merged emissions for all source categories and the other pre-merged emissions files prepared by the other programs will be merged together to generate the PGM-ready emission inputs that include all emission sources. The SMOKE and MEGAN modeling will be performed to generate emissions in the CAMx model format and the CAMx2CMAQ processor will be used to generate CMAQ emission inputs.

19 http://www.wrapair2.org/PhaseIII.aspx
20 http://www.wrapair2.org/pdf/WGA_Task1_TechnicalAnalysisReport_ImprovedBiogenicEmissionInventories.pdf
21 http://www.wrapair2.org/pdf/JSFP_DEASCO3_TechnicalProposal_November19_2010.pdf
22 http://bai.acd.ucar.edu/Data/fire/

3.0 EPISODE SELECTION

EPA's ozone, $PM_{2.5}$ and visibility SIP modeling guidance (EPA, 2007)[23] contains recommended procedures for selecting modeling episodes, while also referencing EPA's 1-hour ozone modeling guidance for episode selection (EPA, 1991)[24.] This Chapter presents the modeling period selected for performing the WestJumpAQMS 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
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 2008 calendar year was selected for the WestJumpAQMS modeling because it satisfies more of the 8 episode selection criteria listed above than other recent years:

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

24 http://www.epa.gov/ttn/scram/guidance/guide/uamreg.pdf

1. Modeling the entire 2008 year 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[25]. 2010 included the CalNex field study[26] 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.

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 WestJumpAQMS 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.

25 http://esrl.noaa.gov/csd/groups/csd7/measurements/2008Erie/
26 http://esrl.noaa.gov/csd/projects/calnex/

4.0 DOMAIN SELECTION

This Chapter summarizes the model domain definitions for the WestJumpAQMS photochemical grid modeling (PGM), including the domain coverage, resolution, map projection, and nesting schemes for the high resolution sub-domains. It also discusses emissions, aerometric and other data available for use in model input preparation and performance testing. 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 ENVIRON and Alpine (2012).

4.1 HORIZONTAL MODELING DOMAIN

The WestJumpAQMS 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. Accordingly, a 36/12/4-km nested grid structure was selected for the WestJumpAQMS meteorological, emissions and air quality modeling. The WRF meteorological model requires use of an odd nesting ratio so the 36/12/4 km domains are using a 3:1 grid-nesting ratio. A Lambert Conformal Projection (LCP) was used for the WestJumpAQMS 36/12/4 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.
- There will be several types of 4 km domains utilized in the WestJumpAQMS study:
    - A large 4 km Inter-Mountain West Domain (IMWD) processing domain will cover all of the areas of primary interest with meteorological and emissions processing performed on the large 4 km IMWD.
    - Detailed Source Apportionment Domains (DSAD) 4 km domains will be defined so that fully linked 36/12/4 km ozone and PM source apportionment modeling can be performed to examine the upwind transport of pollutants from throughout the 36/12/4 km CONUS region into the 4 km DSAD domains, as well as downwind transport of emissions from the DSAD and other regions on downwind ozone and PM concentrations. Because the DSAD 4 km domains are run with the 36 km and 12 km domains using two-way interactive grid nesting, they cannot overlap and the boundaries need to be aligned with the 36 km parent grid cells.
    - Impact Assessment Domains (IAD) are larger 4 km domains for which stand-alone 4 km photochemical modeling databases will be developed using boundary conditions (BCs) from the 36/12 km modeling. The IADs are defined for performing air impact assessments of sources within the IAD 4 km domain on receptors within the IAD 4 km domain.

Figure 4-1 displays the 36 km CONUS, 12 km WESTUS and 4 km IMWD processing domains and the definition of their extent. The SMOKE and MEGAN emissions modeling will be conducted on the 36/12/4 km domain grid structure shown in Figure 4-1. The meteorological and emissions information will be generated on the 4 km IMWD (Figure 4-1) and then windowed out to define the meteorological and emissions photochemical grid model (PGM) inputs for the 4 km DSAD and IAD domains.

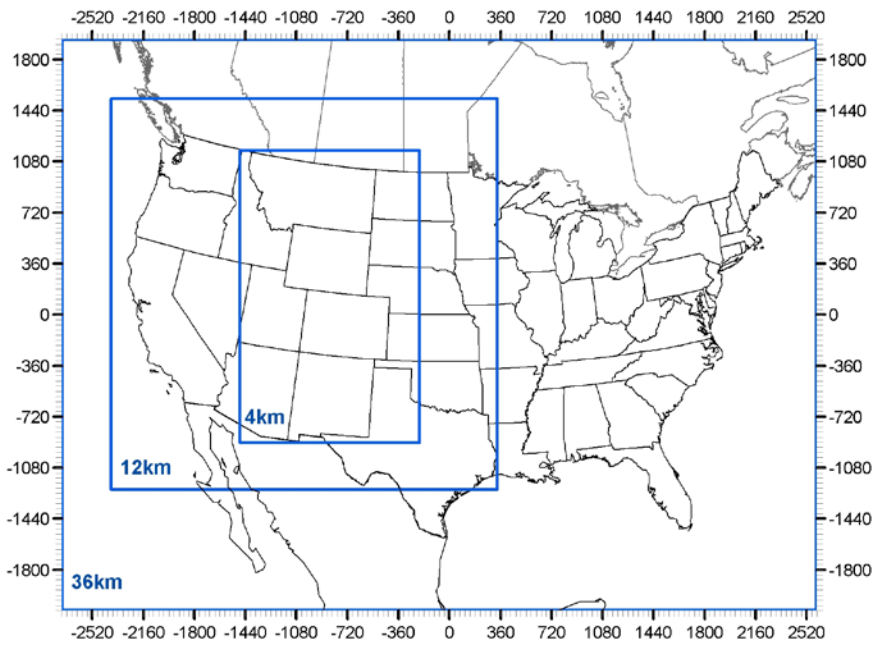


Figure 4-1. 36 km CONUS, 12 km WESTUS and 4 km IMWD processing domain used for developing PGM emission inputs.

Table 4-1. Projection parameters for the WestJumpAQMS 36/12/4 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

4.1.1 Impact Assessment Domains (IAD)

Stand-alone 4 km PGM modeling databases for the 2008 Calendar year will be developed for four Impact Assessment Domains (IADs). The IAD databases can be used to examine the potential air quality (AQ) and air quality related values (AQRVs) impacts of proposed new sources within the IAD on nearby (typically within 300 km) areas that will also reside in the IAD, as is typically done in an EIS or RMP. Figure 4-2 displays the relationship between the 4 km IMWD processing domain and the four proposed 4 km IADs. Also shown in Figure 4-2 are the oil and gas (O&G) development basins and the locations of existing O&G development wells in 2006. Close ups of the four IADs are shown in Figures 4-3 through 4-6. The four IADs are defined using the same Lambert Conformal map projection as discussed previously (Table 4-1).

- The San Juan, NM IAD includes the North and South San Juan Basins and nearby Class I areas in the Four Corners region (Figure 4-3) and can be used to assess the AQ/AQRV impacts due to O&G developments in the San Juan Basin.
    - 173 x 191 4 km resolution with SW and NE corners of (-1336, -724) and (-644, 40).
- The CO-UT IAD domains covers the Uinta, Piceance and D-J Basins domain is depicted in Figure 4-4 and can be used to assess the AQ/AQRV impacts due to developments in the Uinta, Piceance and Denver-Julesburg Basins.
    - 245 x 191 4 km resolution with SW and NE corners of (-1336, -328) and (-356, 436).
- The Wyoming IAD includes the Southwest Wyoming, Wind River, Big Horn and Powder River Basins and nearby Class I areas (Figure 4-5).
    - 218 x 164 4 km resolution with SW and NE corners of (-1228, 68) and (-356, 724).
- The MT-ND IAD includes the Williston and North-Central Montana Basin and is shown in Figure 4-6.
    - 272 x 155 4 km resolution with SW and NE corners of (-1300, 536) and (-212, 1156).

The definitions of these four proposed IADs will be updated after discussions with BLM representatives to assure that they meet their needs before the stand-alone 4 km photochemical grid modeling databases are developed. In particular we will discuss the IAD 4 km domain definitions with the BLM State Office air specialists in New Mexico, Colorado, Utah, Wyoming and Montana/Dakotas.

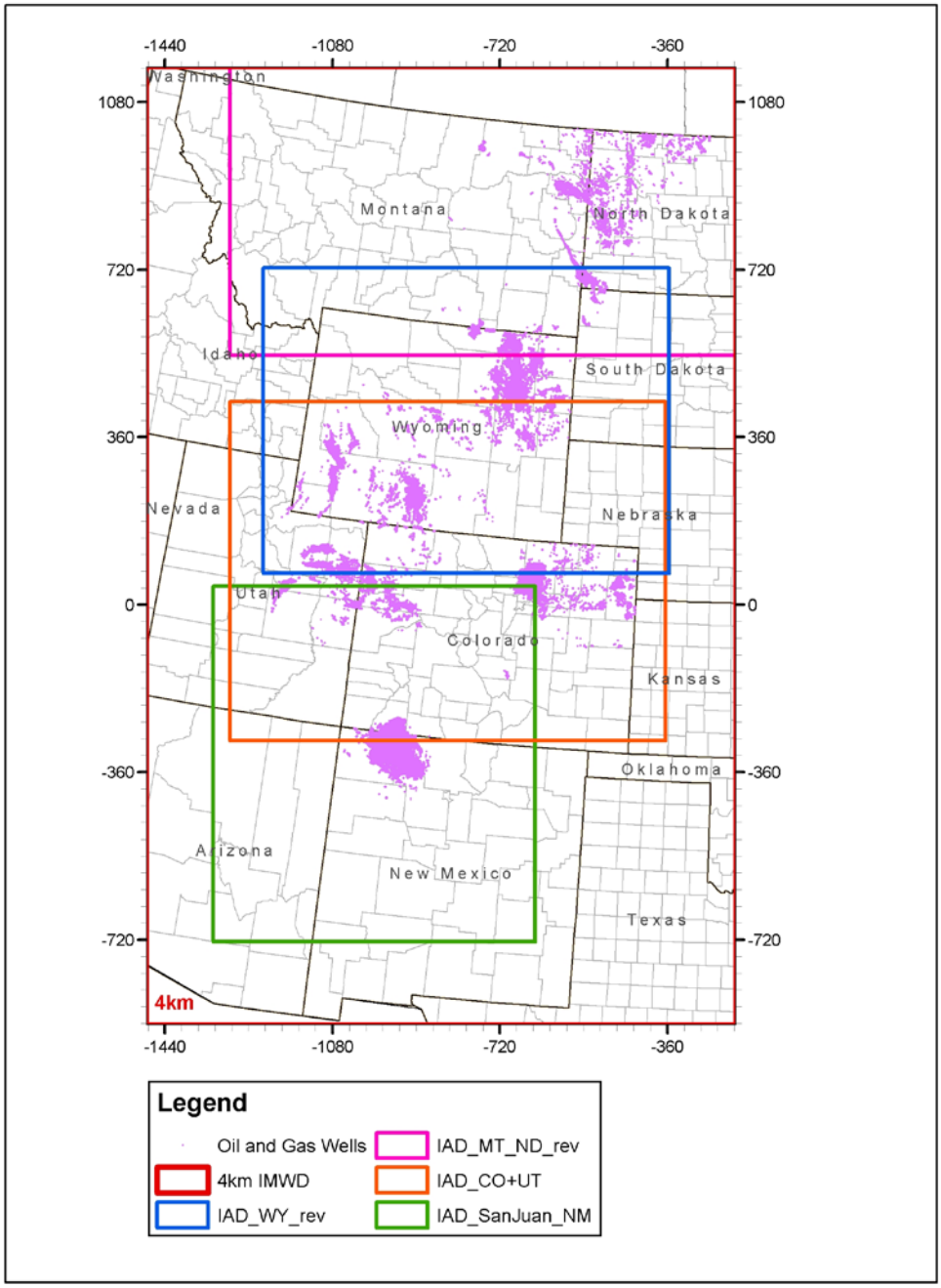


Figure 4-2. 4 km IMWD processing domain and proposed four 4 km Impact Assessment Domains (IAD) for which stand-alone 4 km photochemical modeling databases will be developed for 2008.

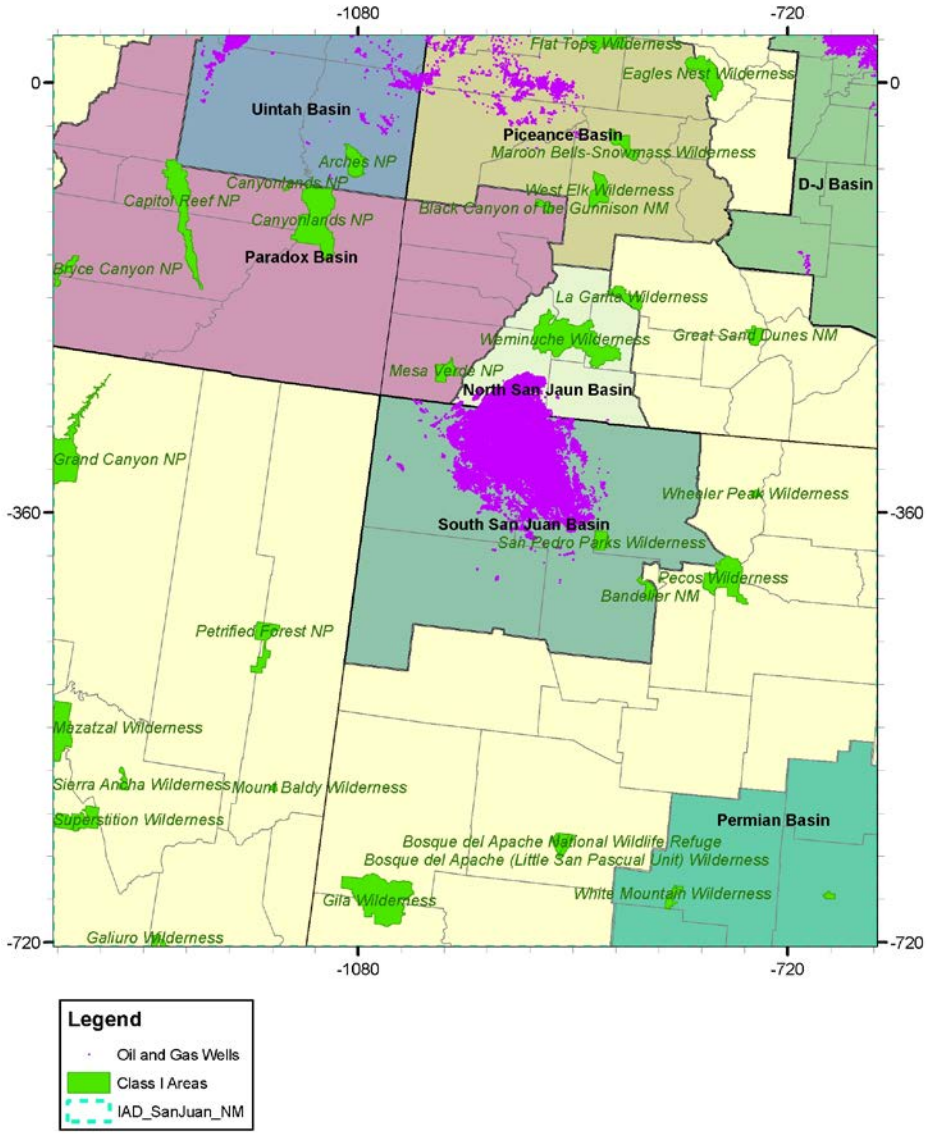


Figure 4-3. Proposed Four Corners 4 km IAD domain that includes the North and South San Juan Basins.

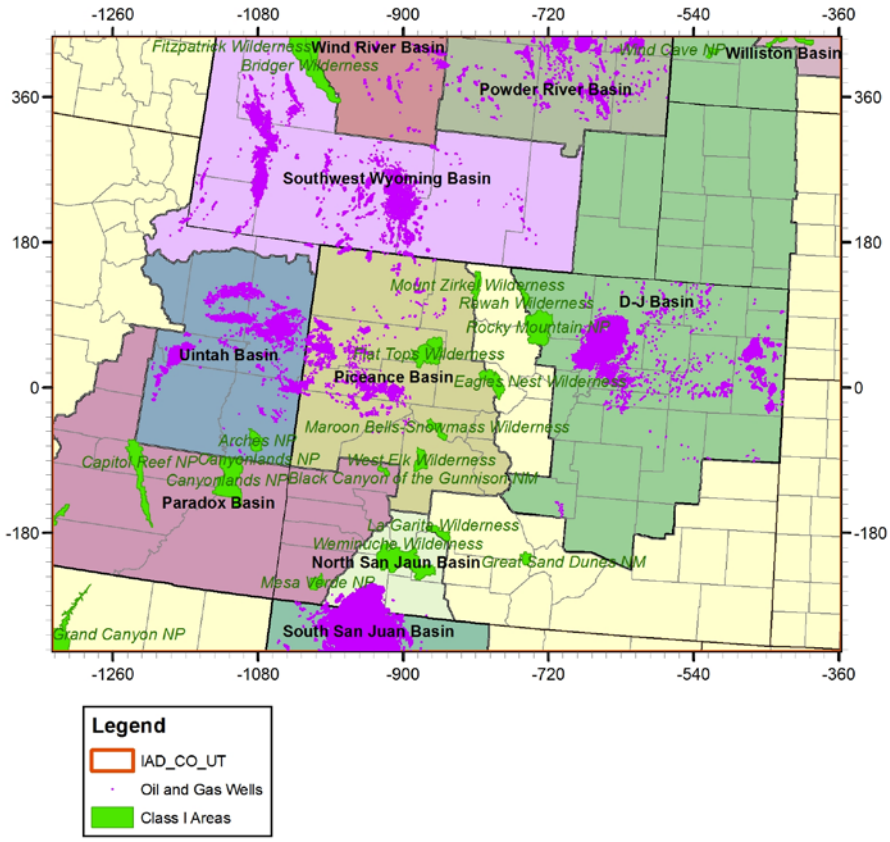


Figure 4-4. Proposed Utah-Colorado 4 km IAD domain that includes the Uinta, Piceance and Denver-Julesburg Basins.

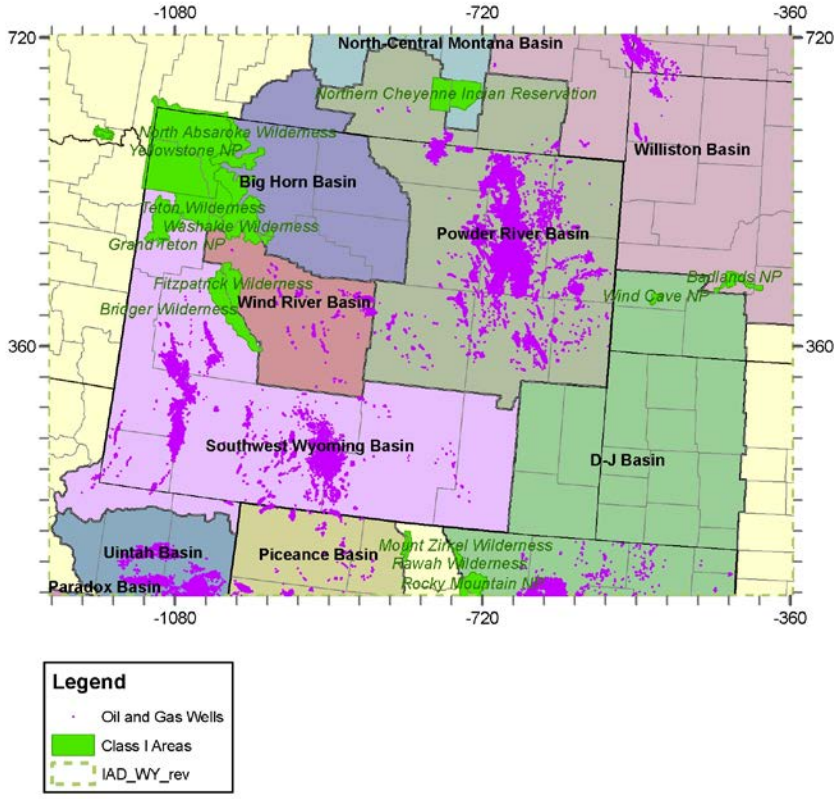


Figure 4-5. Proposed Wyoming 4 km IAD domain that includes the Southwest Wyoming and Powder River Basins.

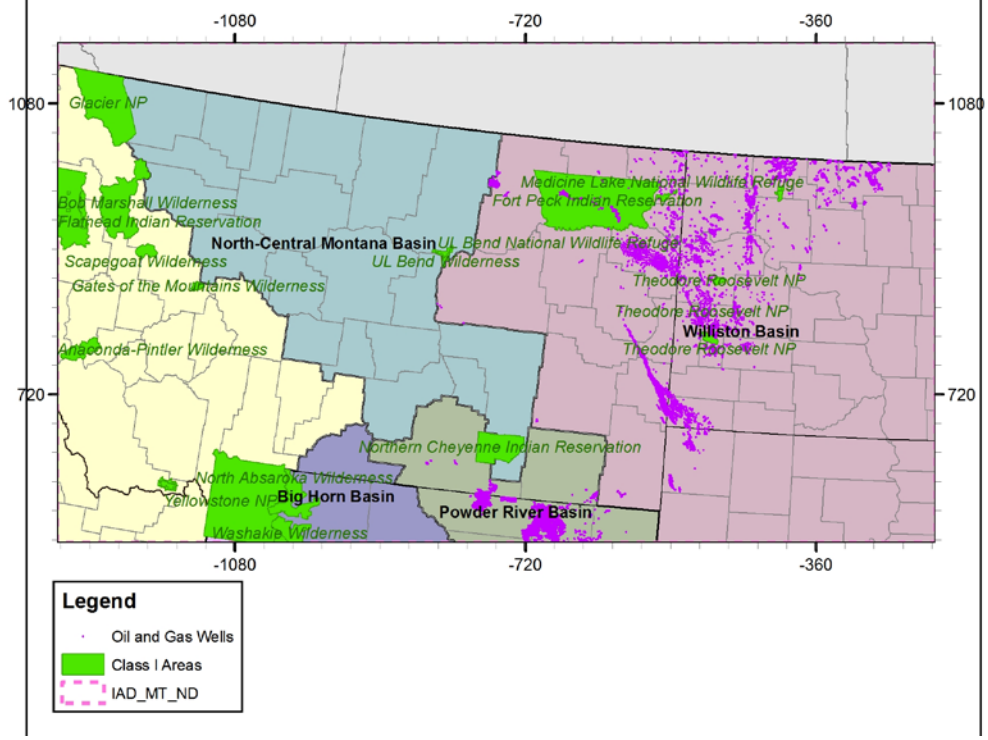


Figure 4-6. Proposed Montana-North Dakota 4 km IAD domain that includes the Williston basin.

4.1.2 Detailed Source Apportionment Domains (DSAD)

The DSAD 4 km domains are designed to nest within the 12 km WESTUS domain and be used with two-way grid nesting to assess transport into and out of the DSAD domains. Consequently, they must be compliant with the CAMx two-way grid nesting rules (e.g., 4 km domain boundaries must align with the parent 36 km CONUS domain grid cells and they cannot overlap). The DSAD domains were defined to include all of the major oil and gas development areas in the Rocky Mountain region. Figure 4-7 displays the six proposed 4 km DSADs and their relationship with the 4 km IMWD processing domain with Figures 4-8 through 4-13 displaying each individual DSAD. Below we give the extent and origin of each of the proposed DSAD domains that use the same Lambert Conformal projection discussed earlier (Table 4-1). Note that the proposed DSAD domain definitions are undergoing review and refinement, in particular we are looking into whether the boundaries for different DSAD domains can be defined along the same edges so that no area is lost between the DSAD domains.

- Southeast New Mexico (NM_SE) DSAD (Figure 4-8).
  - 137 x 83 4 km resolution with SW and NE corners of (-1084, -904) and (-536, -572).
- Four Corners DSAD (Figure 4-9).
  - 101 x 92 4 km resolution with SW and NE corners of (-1192, -508) and (-788, -140).
- Uinta-Piceance Basins DSAD (Figure 4-10).
  - 119 x 110 4 km resolution with SW and NE corners of (-1264, -112) and (-788, 328).

- D-J Basin/Denver DSAD (Figure 4-11).
  - 92 x 110 4 km resolution with SW and NE corners of (-760, -112) and (-392, 328).
- Powder River Basin DSAD (Figure 4-12).
  - 173 x 92 4 km resolution with SW and NE corners of (-1192, 356) and (-500, 724).
- Montana-North Dakota DSAD (Figure 4-13).
  - 182 x 83 4 km resolution with SW and NE corners of (-940, 752) and (-212, 1084).

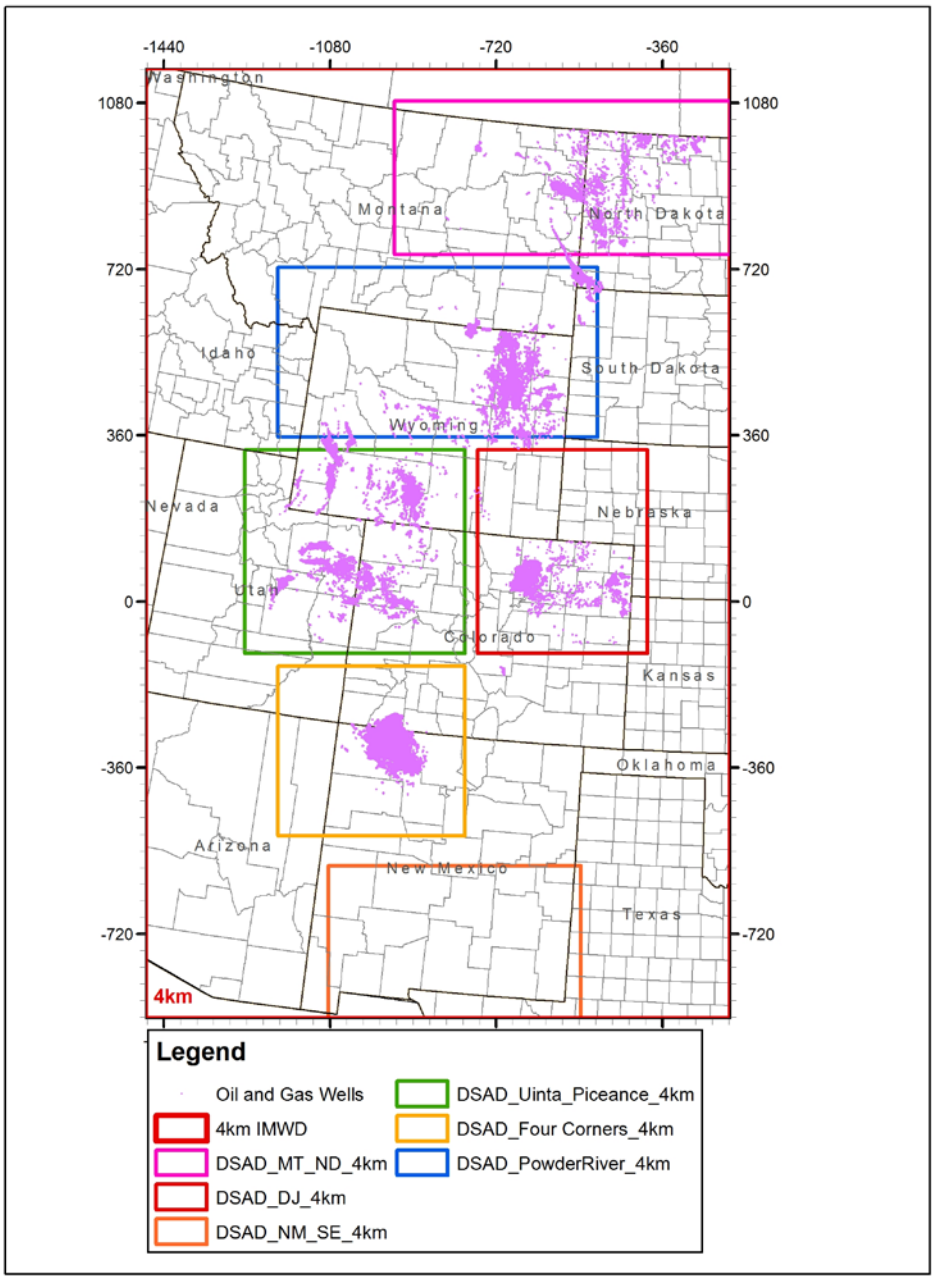


Figure 4-7. Relationship between the six proposed 4 km DSAD domains and the 4 km IMWD processing domain.

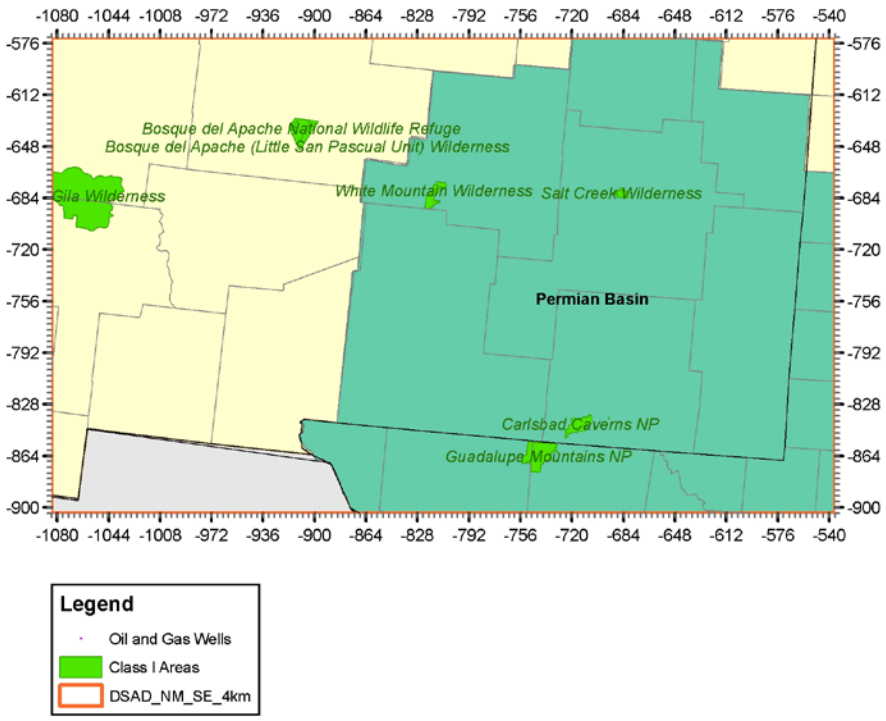


Figure 4-8. Proposed Southeastern New Mexico 4 km DSAD domain that includes the northern portion of the Permian Basin.

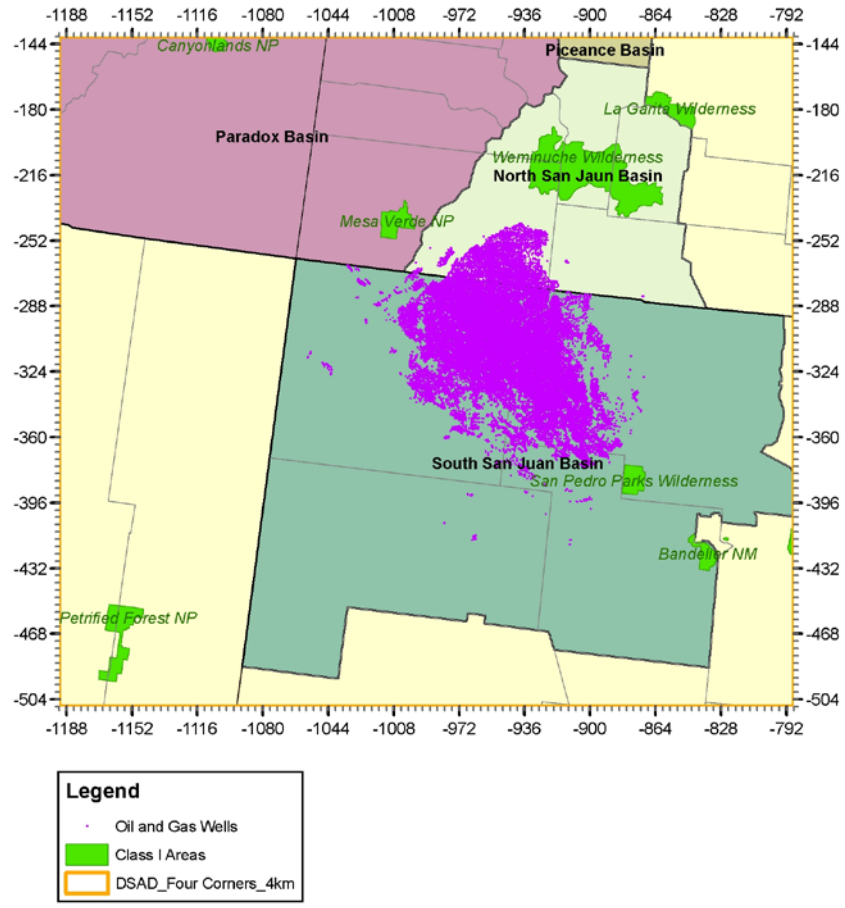


Figure 4-9. Proposed Four Corners 4 km DSAD domain that includes the North and South San Juan Basins.

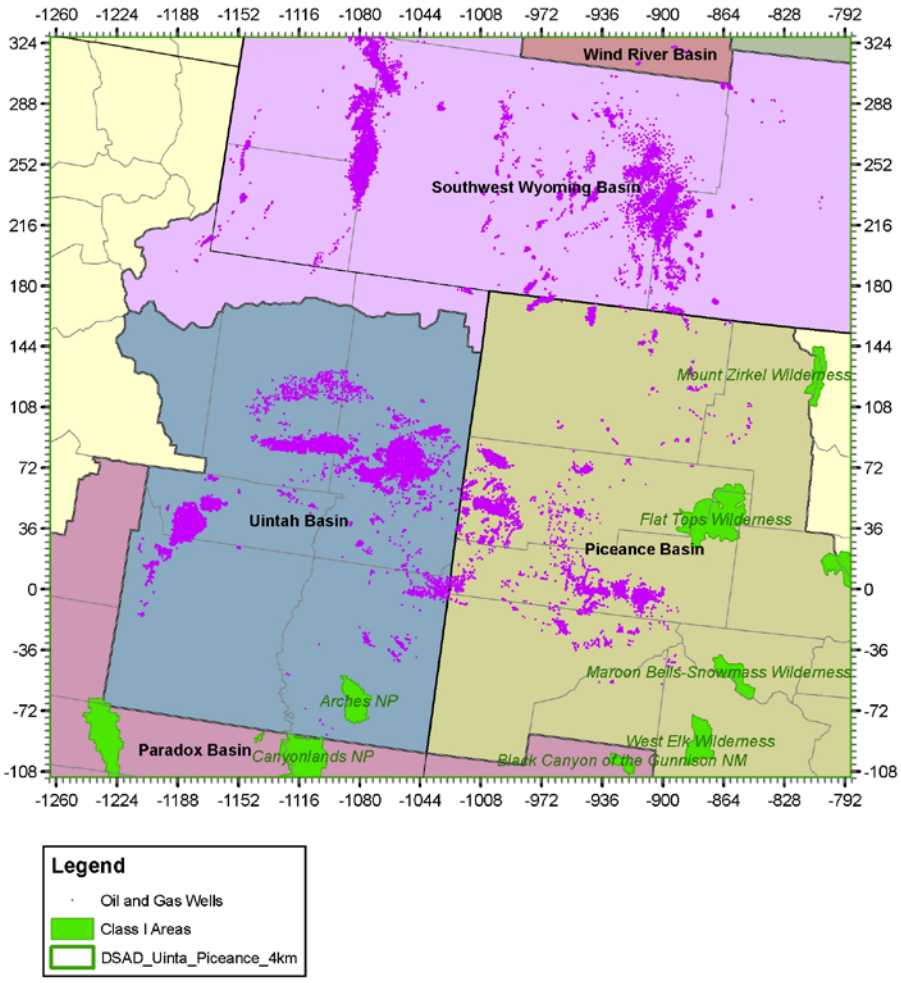


Figure 4-10. Proposed Utah-Colorado 4 km DSAD domain including the Uinta and Piceance Basins.

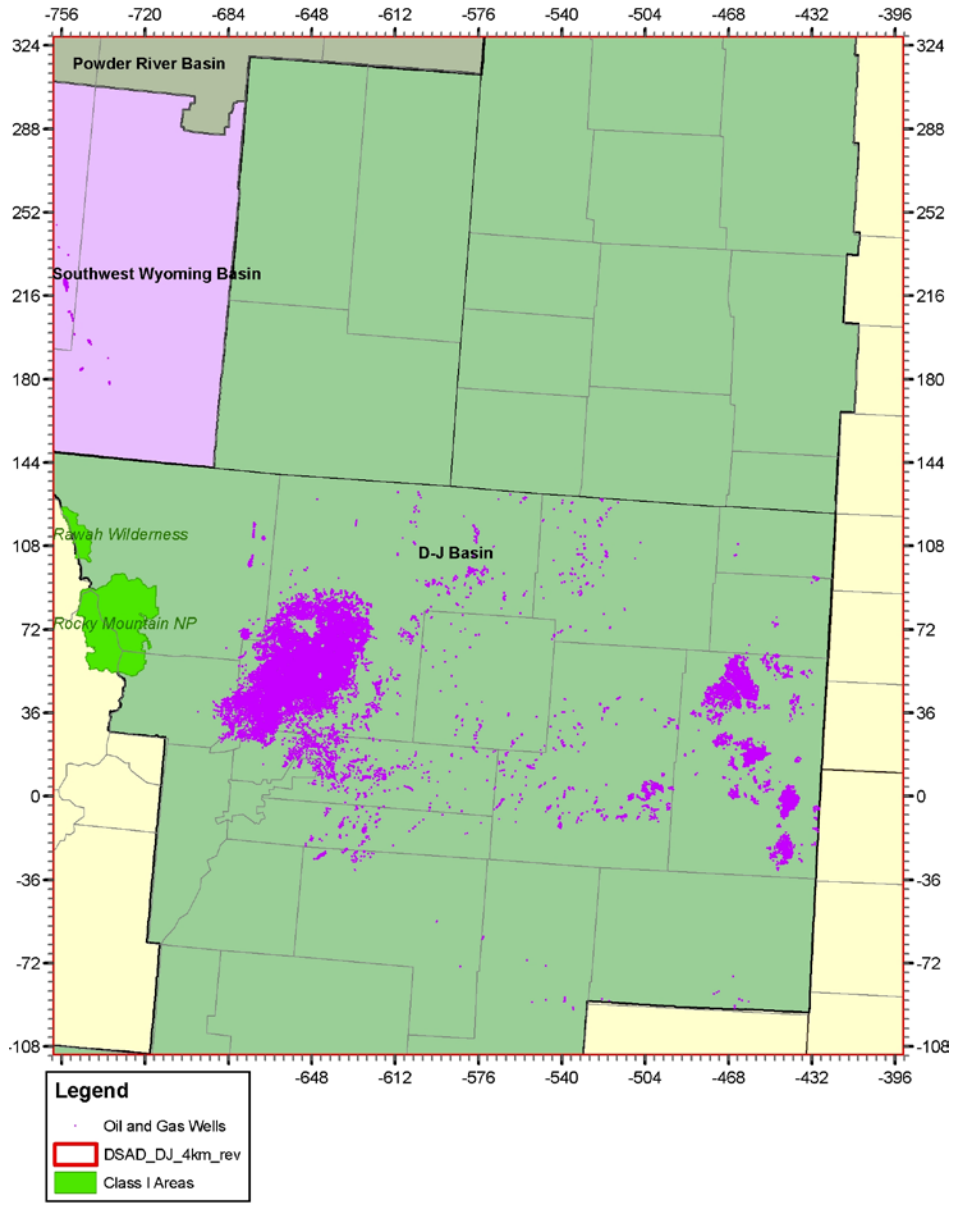


Figure 4-11. Proposed Denver-Julesburg Basin 4 km DSAD domain.

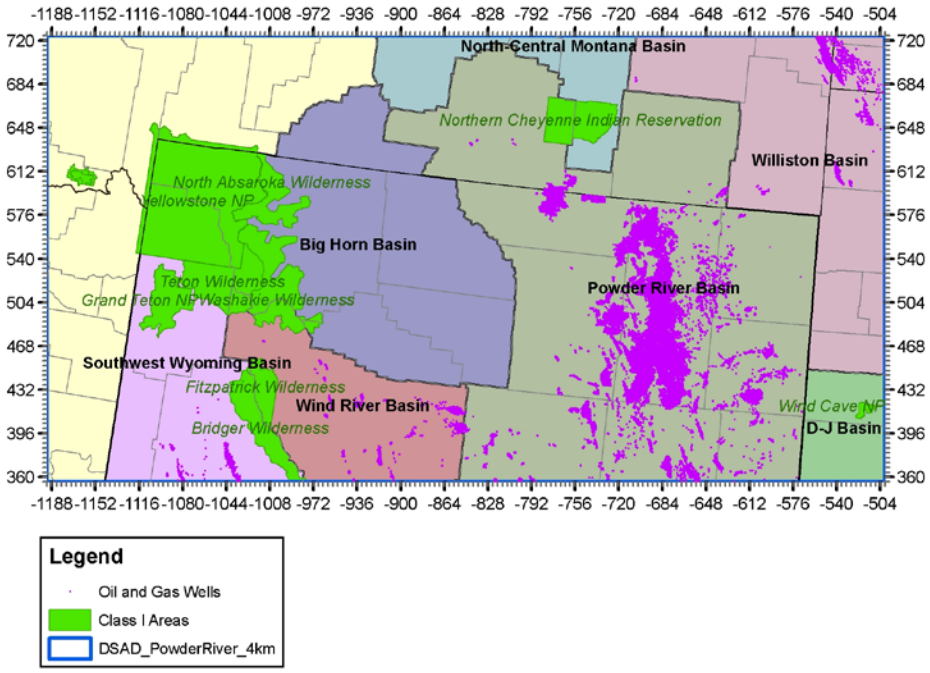


Figure 4-12. Proposed Wyoming 4 km DSAD domain.

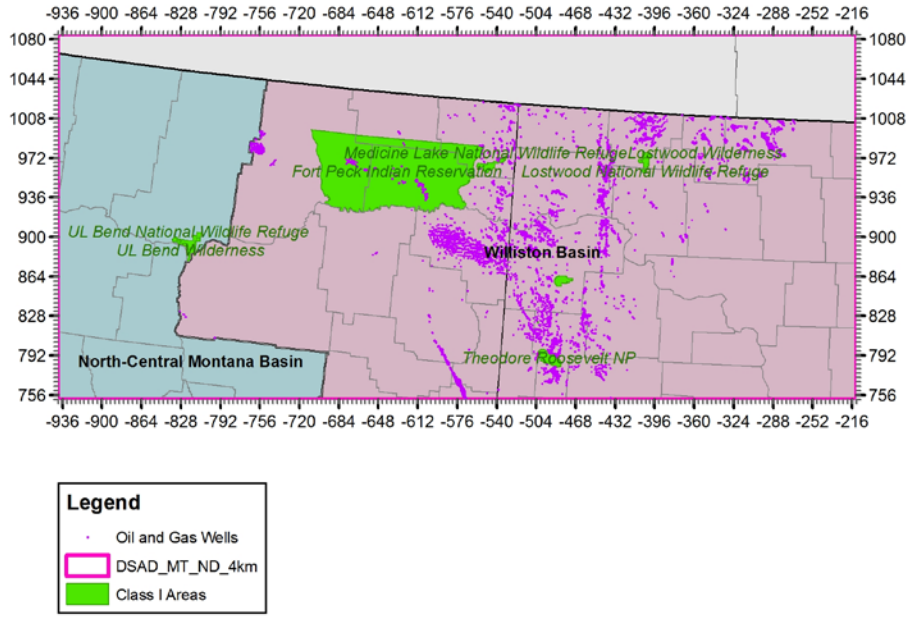


Figure 4-13. Proposed Montana-North Dakota 4 km DSAD domain.

4.2 VERTICAL DOMAIN STRUCTURE

The CAMx/CMAQ 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, 2012[27]). 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/CMAQ simulations whereby multiple WRF layers are combined into one CAMx layer to reduce the air quality model computational time. Table 4-2 displays the approach for collapsing the WRF 36 vertical layers to 25 vertical layers in CAMx and CMAQ. 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 4-2 is collapsing two WRF layers into one CAMx/CMAQ layer for the lowest four layers in CAMx/CMAQ. In the past, the lowest layers of MM5/WRF were mapped directly into CAMx/CMAQ 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.

The Denver ozone SIP planning modeling of the May-August 2008 period used the same vertical layer structure as being used in WestJumpAQMS. 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. Based on this analysis we feel the layer collapsing scheme for CAMx/CMAQ modeling in Table 4-2 is justified.

27 http://www.wrapair2.org/pdf/WestJumpAQMS_2008_Annual_WRF_Final_Report_February29_2012.pdf

Table 4-2. 37 Vertical layer definition for WRF simulations (left most columns), and approach for reducing to 25 vertical layers for CAMx/CMAQ by collapsing multiple WRF layers (right columns).

WRF Meteorological Model					CAMx/CMAQ Air Quality Model		
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. 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

WestJumpAQMS 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/CMAQ meteorological inputs for the 36 km CONUS, 12 km WESTUS and 4 km IMWD processing domains as well as all of the IAD and DSAD 4 km domains depicted in Figures 4-1 through 4-14 in Chapter 4. The WRF modeling domain was defined to be slightly larger than the CAMx/CMAQ PGM modeling domains to eliminate the occurrence of boundary artifacts in the meteorological fields used as input to CAMx/CMAQ. 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 WestJumpAQMS 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^{o}, -97^{o} with true latitudes of 33^{o} and 45^{o}. The 12 km has 256 x 253 grid cells with offsets from the 36 km grid of 15 columns and 26 rows. The 4 km domain was defined to be slightly bigger than the 4 km IMWD processing domain discussed in Chapter 4 and shown in Figure 4-1. The three 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)[28]. 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. The 4 km IMWD was based on the 30 sec. (~900 m) 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.

28 http://dss.ucar.edu/

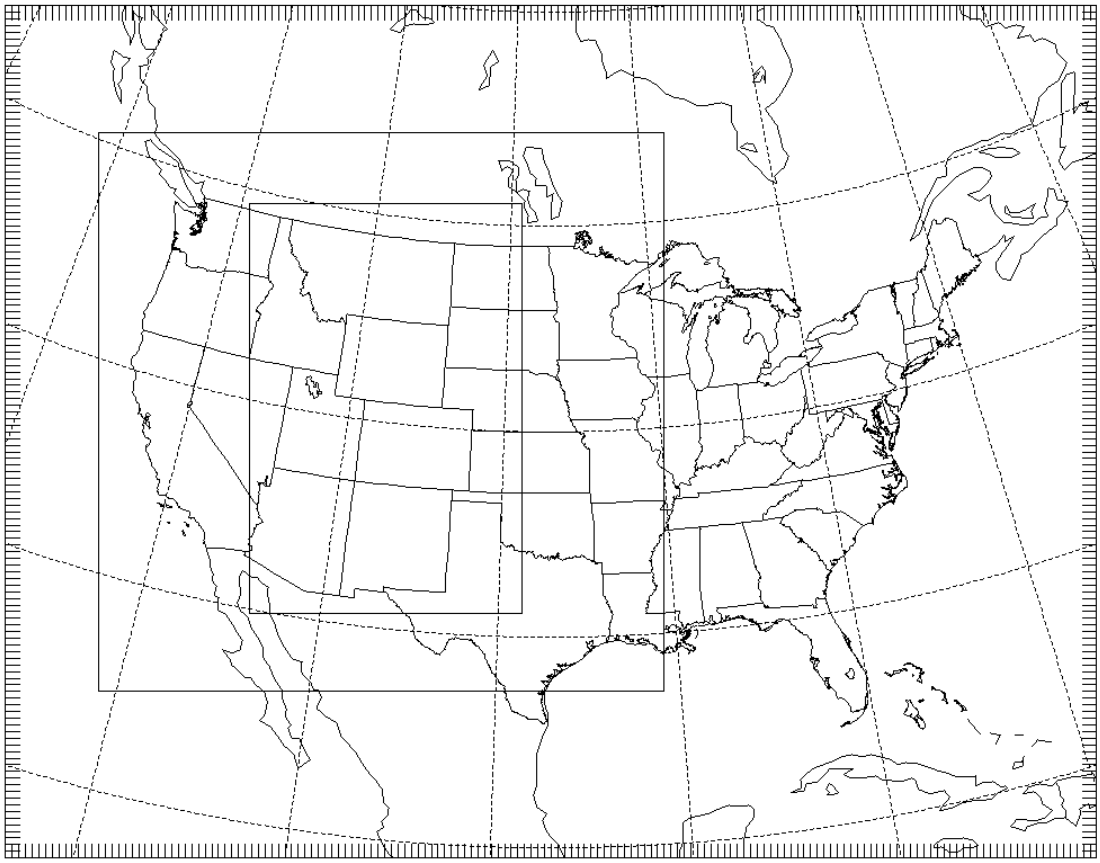


Figure 5-1. WRF 36/12/4 km grid structure for the WestJumpAQMS meteorological modeling.

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)[29] observation archive. The MADIS archive includes the National Climatic Data Center (NCDC)[30] observations and the National Data Buoy Center (NDBC) Coastal-Marine Automated Network C-MAN[31] 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)

29 Meteorological Assimilation Data Ingest System. http://madis.noaa.gov/
30 National Climatic Data Center. http://lwf.ncdc.noaa.gov/oa/ncdc.html
31 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 (NOAH, 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[32]). 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.

32 http://wrapair2.org/pdf/WestJumpAQMS_2008_Annual_WRF_Final_Report_February29_2012.pdf

6.0 EMISSIONS

Emissions modeling will be performed for the 36 km CONUS, 12 km WESTUS and 4 km IMWD processing domains. Separate streams of emissions modeling will be conducted for each major source category to assist in the quality assurance and quality control (QA/QC) process and for ease of performing source apportionment modeling in later stages of the study. Emissions Technical Memorandums have been or are in the process of being prepared for each major source category. These memorandums describe the source of the emissions, and how they will be processed for inputs to the photochemical grid models. The thirteen emissions Technical Memorandums are as follows:

1. Point Sources including Electricity Generating Units (EGUs) and Non-EGUs;
2. Area plus Non-Road Mobile Sources;
3. On-Road Mobile Sources that will be based on MOVES;
4. Oil and Gas Sources (5 installments covering different locations);
5. Fires Emissions including wildfire, prescribed burns and agricultural burning;
6. Fugitive Dust Sources;
7. Off-Shore Shipping Sources;
8. Ammonia Emissions;
9. Biogenic Emissions;
10. Eastern USA Emissions;
11. Mexico/Canada;
12. Sea Salt and Lightening Emissions; and
13. Emissions Modeling Parameters including spatial surrogates, temporal adjustment parameters and chemical (VOC and PM) speciation profiles.

6.1 EMISSION DATA SOURCES

Version 2.0 of the 2008 National Emissions Inventory (NEIv2.0[33]) will be the basis for most of the emissions modeling. Table 6-1 summarizes the emission models and sources of emissions that is based primarily on the 2008 NEIv2.0 with the following enhancements:

- Major (≥25 MWe) Electrical Generating Units (EGUs) point source SO_2 and NO_X emissions will use Continuous Emissions Monitor (CEM) measurement data that are available online from the EPA Clean Air Markets Division (CAMD[34]). These data are hour-specific for SO_2, NO_x and heat input. The

33 http://www.epa.gov/ttnchie1/net/2008inventory.html
34 http://www.epa.gov/airmarkets/

temporal variability of other pollutant emissions (e.g., PM) for the CEM sources will be simulated using the hourly CEM heat input data to allocate the annual emissions from the NEIv2.0 to each hour of the year. Emissions, locations and stack parameters for point sources without CEM devices will be based on the 2008 NEIv2.0.

- The WRAP-IPAMS Phase III 2006 oil and gas emission inventories will be projected to 2008 for all Phase III basins that are currently available. In addition, new oil and gas emissions inventory will be developed for the Permian Basin in southeastern New Mexico/northwestern Texas.
- On-road mobile source emissions will be based on the MOVES2010a[35] model with county-specific weekday and weekend day VMT and monthly meteorology for the 2008 baseline modeling year.
- The NEIv2.0 ammonia emissions based on the Carnegie Mellon University ammonia model will be reviewed and updated as better data are available.
- The WRAP windblown dust (WBD) model [36] will be used to generate WBD emissions using day-specific hourly meteorology.
- Sea salt and lightning emissions will be generated.
- Emissions from fires (wildfires, prescribed burns and agricultural burning) will initially be based on the Fire Inventory from NCAR (FINN[37]). When available, the WestJumpAQMS will use the 2008 fire emissions inventory developed in the Joint Fire Sciences Program (JFSP) Deterministic and Empirical Assessment of Smoke's Contribution to Ozone (DEASCO3[38]) study.
- Biogenic emissions will be generated using an enhanced version of the Model of Emissions of Gases and Aerosols in Nature (MEGAN[39]) that is being updated by WRAP.
- Mexico emissions will use 2008 projections from the 1999 Mexico national emissions inventory.
- The Environment Canada 2006 emissions inventory based on the National Pollutant Release Inventory (NPRI) will be used for Canada.
- New spatial surrogates for the emissions will be developed using the latest 2010 Census data that are now available and will include population and housing statistics for 2010 and interpolations for the years between 2000 and 2010.

35 http://www.epa.gov/otaq/models/moves/index.htm
36 http://www.wrapair.org/forums/dejf/fderosion.html
37 http://bai.acd.ucar.edu/Data/fire/
38 https://www.firescience.gov/projects/11-1-6-6/proposal/11-1-6-6_11-1-6_attachment_1_primary.pdf
39 http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm

Table 6-1. Summary of sources of emissions and emission models to be used in generating PGM emissions inputs for the WestJumpAQMS study.

Emissions Component	Configuration	Details
Model Code	SMOKE Version 3.1	http://www.smoke-model.org/index.cfm
Oil and Gas Emissions	Update WRAP Phase III 2006 to 2008	Also add 2008 Permian Basin O&G Emissions http://www.wrapair2.org/pdf/Memo_4a_OG_Jun06_2012_Final.pdf http://www.wrapair2.org/pdf/Memo_4b_OG_June07_2012_Final.pdf
Area Source Emissions	2008 NEI Version 2.0	Western state updates, then SMOKE processing of http://www.epa.gov/ttn/chief/net/2008inventory.html
On-Road Mobile Sources	MOVES2010a	County specific emissions run for monthly weekday and weekend days.
Point Sources	2008 CEM and Non-CEM Sources	Use 2008 day-specific hourly measured CEM for SO2 and NOX emissions for CEM sources, 2008 NEIv2.0 for other pollutants and non-CEM sources
Off-Road Mobile Sources	2008 NEIv2.0	Based on EPA NONROAD model http://www.epa.gov/oms/nonrdmdl.htm
Wind Blown Dust Emissions	WRAP Wind Blown Dust (WBD)	WRAP WBD Model with 2008 WRF meteorology
Ammonia Emissions	NEIv2.0	Based on CMU Ammonia Model. Review and update spatial allocation if appropriate.
Biogenic Sources	MEGAN	Enhanced version of MEGAN Version 2.1 from WRAP Biogenics study http://www.wrapair2.org/pdf/WGA_BiogEmisInv_FinalReport_March20_2012.pdf
Fires	FINN placeholder and then 2008 DEASCO3	Fire Inventory from NCAR (FINN) used as placeholder until 2008 DEASCO3 fire inventory is available: http://www.wrapair2.org/pdf/JSFP_DEASCO3_TechnicalProposal_November19_2010.pdf
Temporal Adjustments	Seasonal, day, hour	Based on latest collected information
Chemical Speciation	CB6 Chemical Speciation	Updated rate constants, kinetics and reactions in CB6. Use CB05 in CMAQ since CB6 not supported by CMAQ. http://www.cmascenter.org/conference/2010/abstracts/emery_updates_carbon_2010.pdf
Gridding	Spatial Surrogates based on landuse	Develop new spatial surrogates using 2010 census data and other data
Growth and Controls	TBD	Future attainment year(s) to be determined
Quality Assurance	QA Tools in SMOKE; PAVE, VERDI plots; Summary reports	Follow WRAP emissions QA/QC plan.

6.2 ON-ROAD MOBILE SOURCES

Mobile sources describe a wide variety of vehicles, engines, and equipment that under their own power can move from one location to another on paved and un-paved roads. There is a distinction between on-road sources and those sources that are non-road. On-road sources include vehicles used for the transportation of passengers or freight. Non-road sources distinguish between commercial-military marine vessels/railroad (on-rail)/aircraft and all other non-road categories (e.g., construction equipment, recreational equipment, agricultural equipment, etc.).

On-road mobile sources include light-duty vehicles, light-duty trucks, heavy-duty vehicles, buses and motorcycles used for transportation of goods and passengers on established roadways. On-road vehicles may be fueled with gasoline, diesel fuel, or alternative fuels such as alcohol or natural gas.

6.2.1 MOVES

The MOtor Vehicle Emissions Simulator (MOVES[40]) is EPA's current tool to construct on-road mobile source emissions estimates for national, state, and county level inventories of criteria air pollutants, greenhouse gas emissions, and some mobile source air toxics from highway vehicles (EPA, 2012a). In addition, MOVES can make projections for energy consumption (total, petroleum-based, and fossil-based). EPA requires that all new regulatory modeling studies use the MOVES model for mobile source emissions (EPA, 2012c).

The WestJumpAQMS on-road mobile source emission modeling was conducted using MOVES2010a. In April 2012, EPA released MOVES2010b after WestJumpAQMS completed its MOVES modeling. According to EPA's documentation, the primary difference between MOVES2010b and MOVES2010a is related to performance issues (e.g., computing run time) and the emission estimates produced by the two versions of MOVES are nearly identical[41]. EPA's technical guidance for State Implementation Plans (SIPs) and transportation conformity notes that studies that started with MOVES2010a do not have to switch to the new MOVES2010b (EPA, 2012b[42]). Given the near identical emissions, EPA's MOVES modeling guidance and the significant effort WestJumpAQMS has invested in its MOVES modeling to date, rerunning with MOVES2010b is not necessary.

MOVES2010a can be configured to estimates emissions directly (i.e., emissions inventory mode) or estimates emissions factors (i.e., emissions factor mode). There are three main approaches for using MOVES to generate hourly gridded speciated emission inputs needed for photochemical grid models (e.g., CAMx and CMAQ):

- Run MOVES in emissions inventory mode using county-specific representative hourly temperature, vehicle miles traveled (VMT) and other inputs (e.g., fleet mix and fuel type) to generate hourly county-level on-road mobile source emissions. The Sparse Matrix Operator Kernel Emissions (SMOKE) emissions modeling system is then used to grid and speciate the hourly county-level MOVES emissions.
- Use the SMOKE-MOVES tool that accesses a MOVES emission factor lookup table using gridded hourly meteorological data and representative VMT, fleet mix, fuel type, etc. for the grid cell to generate gridded hourly on-road emission estimates that are then speciated into the appropriate chemical species. The MOVES lookup table is generated by running MOVES multiple times in emissions factor mode for different temperatures, fuel types, etc.

40 http://www.epa.gov/otaq/models/moves/index.htm
41 http://www.epa.gov/otaq/models/moves/documents/420f12014.pdf
42 http://www.epa.gov/otaq/models/moves/documents/420b12028.pdf

- Use CONCEPT-MOVES that combines link-based VMT data from a Transportation Demand Model (TDM) with hourly meteorological data and a MOVES emissions factor lookup table to generate hourly gridded speciated on-road mobile source emissions.

For the WestJumpAQMS project, MOVES2010a was run in the emissions inventory mode to estimate hourly emissions at the county level for a representative weekend day and weekday for each month of 2008. CONCEPT-MOVES is limited to locations with TDM data and SMOKE-MOVES would require more resources than available for the study. A modified version of MET4MOVES was run to prepare representative average meteorology for 2008 by month, hour, and county that is suitable for use by MOVES2010a. These new hourly estimates of temperature and relative humidity, based on the WestJumpAQMS 2008 WRF run (ENVIRON and Alpine, 2012), replace the current default meteorology that exists in the MOVES2010a (movesdb20100830.zonemonthhour database). MOVES2010a was run using the existing MOVES2010a default data sets, with the replacement meteorology, to estimate emissions (tons per hour) for all PM and OZONE pollutants by county/month/weekend day-weekday/hour by appropriate SCC and MOVES2010a process (e.g., extended idle, running exhaust, etc.). The resulting emissions estimates were converted to SMOKE-ready area source, hourly data sets suitable for processing by SMOKE/SMKINVEN. A modified version of SMKINVEN is used to process the hour-specific emissions estimates.

6.2.2 SMOKE Modeling of MOVES Estimates

The MOVES estimated county-level on-road mobile source emissions estimates were spatially allocated to the 36/12/4 km modeling domains using the SMOKE emissions model and recent mobile source spatial surrogates developed using the 2010 census and other data. This includes new spatial surrogate categories specific to new source categories in MOVES (e.g., heavy duty truck idling at rest stops). As MOVES2010a estimates hourly on-road mobile source emissions estimates by county by month for a representative weekend day and weekday, there is no need to temporally allocate the emissions using SMOKE. However, in order for SMOKE to properly utilize these hourly emissions estimates, a modified version of SMOKE is required. The MOVES hourly gridded mobile source emissions were chemically speciated to the CB6 chemical mechanism using CB6 chemical speciation profiles based on the SPECIATE4.3 database.

6.3 AREA AND NON-ROAD MOBILE SOURCES

The 2008 NEIv2.0 area and non-road emissions will be processed using the SMOKE emissions model and new 2010 census spatial surrogates and default temporal and CB6 speciation adjustments. Several source categories within the area and non-road category will be removed from the NEIv2.0 so that they can be replaced or updated and separately processed so that more thorough QA/QC could be performed. The source categories that were extracted from the NEIv2.0 area and non-road sources were as follows:

- Oil and gas (O&G) exploration and production sources will be removed from the NEIv2.0. For locations covered by the WRAP Phase III O&G Basins, they will be replaced by the WRAP Phase III 2006 emissions projected to 2008. New 2008 O&G emissions will be developed for the Permian Basin in southeastern New Mexico/northwestern Texas. The 2008 NEIv2.0 O&G emissions will be used for the remainder of the U.S. locations.
- Ammonia emissions due to livestock and fertilizer sources will be removed from the NEIv2.0 and processed separately.
- Aircraft, locomotive and marine (alm) sources will also be processed separate as their own source group in the emissions modeling. The marine sources do not include large ocean going (Class 3) vessels that will be processed under the off-shore shipping category.

- Fire emissions were also removed from the NEIv2.0 and initially replaced by the Fire INventory from NCAR (FINN) fire emissions that will ultimate be replaced by the 2008 fire emissions developed as part of the DEASCO3 study.
- Fugitive dust emissions were also removed from the NEIv2.0 for separate processing.

6.3.1 Area Sources

The NEI Area (or Non-Point) data category contains emission estimates for sources which individually are too small in magnitude or too numerous to inventory as individual point sources, and which can often be estimated more accurately as a single aggregate source for a County or Tribal area. Area source (non-point) emissions are emissions sources that are summed over a geographic region, rather than specifically located. Examples of area sources include small industrial, residential, consumer product, and agricultural emissions. For emissions modeling purposes, these types of emissions are defined by state and county (or tribal) identifiers, and SCC codes. After extracting the area source categories from the NEIv2.0 as indicated above, the remaining area sources in the NEIv2.0 will be processed by SMOKE as their own source category.

6.3.2 Non-Road Sources

The NEI Non-Road data categories contain mobile sources which are estimated for version 2.0 of the 2008 NEI using the EPA NONROAD[43] model, run within the National Mobile Inventory Model (NMIM[44]). The non-road emissions have been compiled as both annual total emissions, and average day emissions by month. In order to take the best advantage of the monthly and seasonal variability of the non-road emissions sources, we will use the monthly options for SMOKE modeling inputs.

Note that emissions data for aircraft, locomotives, and commercial marine vessels are not included in the NEI non-road data category starting with the 2008 NEI. These three non-road mobile source categories are handled as special cases, with separate input processing streams. Aircraft engine emissions occurring during Landing and Takeoff Operations (LTO) and the Ground Support Equipment (GSE) and Auxiliary Power Units (APU) associated with the aircraft are now included in the point data category at individual airports in the 2008 NEI. Emissions from locomotives that occur at rail yards are also included in the point data category. In-flight aircraft emissions, locomotive emissions outside of the rail yards, and commercial marine vessel emissions (both underway and port emissions) are included in the Non-Point data category.

6.4 2008 OIL AND GAS EMISSIONS

For Basins covered by the WRAP-IPAMS Phase III 2006 oil and gas (O&G) emissions, the WRAP Phase III O&G emissions will be projected to 2008. New 2008 O&G emissions will be developed for the Permian Basin in southeastern New Mexico/northwestern Texas. For all other Basins the 2008 O&G emissions from the NEIv2.0 will be used.

6.4.1 2008 Phase III O&G Emissions Update

The WRAP Phase III 2006 baseline O&G inventories will be projected to 2008 for the following basins:

- Denver-Julesburg Basin (CO)
- Piceance Basin (CO)
- Uinta Basin (UT)

43 http://www.epa.gov/otaq/nonrdmdl.htm
44 http://www.epa.gov/otaq/nmim.htm

- North San Juan Basin (CO)
- South San Juan Basin (NM)
- Wind River Basin (WY)
- Powder River Basin (WY)
- Greater Green River Basin (WY)
- Williston Basin – Pending (MT and ND)

Prior to developing the 2008 inventory updates for the basins completed as part of Phase III or the Permian Basin, analysis will be conducted using a commercial database to obtain production-related statistics. The analysis will utilize the Enerdeq database published by IHS Global, also referred to as the "PI Dwight's" database. This database was used to develop the Phase III inventories and it contains production statistics that are of significantly higher quality than the primary data in individual state O&G Commission databases.

Processing of the IHS data for the 2008 projections will follow the same methodology as used in the Phase III study[45]. Summaries of production statistics will be extracted from the IHS database, including well count by well type and location, spud count, production of gas by well type and well location, production of liquid petroleum (oil or condensate) by well type and well location, and production of water by well type and well location. All data will be summarized at the county and basin level, for tribal and non-tribal land separately as applicable to each basin. As no new survey work is anticipated in this study, the IHS database analysis will not include an analysis of company-specific production statistics as done in the development of the Phase III 206 O&G emission inventories. The resulting production statistics data will be summarized at the county, tribal and basin levels for all basins including the Permian Basin.

The 2008 production statistics from the IHS database will be used to project the Phase III baseline 2006 O&G inventories. The projections will be developed as scaling factors that represented the ratio of the value of a specific activity parameter in 2008 to the value in 2006. The scaling factors will be developed at the county and tribal levels for all basins. Scaling factors will then be matched to all source categories considered as part of the Phase III inventories, using the same cross-referencing analysis conducted as part of the midterm (2012) projections in the Phase III study.

Where specific scaling factors are estimated to be less than one (1), indicating a reduction in an activity parameter from 2006 to 2008, all emissions factors and activity data will be assumed to be identical in 2008 as in 2006 and no further analysis will be needed for those source categories matched to the activity parameter. In this case, the 2008 emissions for will be developed assuming application of the scaling factor directly. Where scaling factors are estimated to be greater than one (1), it is assumed that some growth in activity has occurred in the 2006-2008 time period. A simplified controls analysis, will be conducted specific to each basin and utilizing the control measures identified as part of the midterm projections work for the Phase III project. The controls analysis will only consider broad control factors, rather than detailed analyses as conducted in the Phase III midterm projections. Where no significant impact of controls from federal or state regulations are anticipated in the 2006-2008 time period, no control fraction for the specific source category will be assumed.

For Colorado Basins, the permitted O&G 2008 emissions will be based on the APEN database rather than projected from the WRAP Phase III 2006 O&G emissions. In addition, the Colorado Department of Health and Development (CDPHE) has found that not all condensate Flash VOC emissions that were assumed to be

45 http://www.wrapair2.org/PhaseIII.aspx

controlled 95% by flares make it to the flare and are instead vented to the atmosphere. Thus, CDPHE has introduced the concept of a Capture Efficiency (CE) for condensate flare control that assumes only 75% of the condensate Flash VOC emissions are actually controlled by the flare and the other 25% is released to the atmosphere. The WRAP Phase III 2006 unpermitted condensate tank O&G emissions are either projected to 2008 (D-J Basin) or the 2008 APEN condensate tank emissions are reduced (Piceance Basin) in order for the total 2008 condensate production in the inventory to match the 2008 IHS database production statistics.

6.4.2 2008 Emission Inventory for the Permian Basin

A study prepared by Applied EnviroSolutions, Inc. (AES) on 2007 O&G emissions in the New Mexico portion of the Permian Basin along with 2008 O&G emissions from the Texas Commission on Environmental Quality (TCEQ) will be used to develop a comprehensive inventory of the Permian Basin. The AES study was commissioned for the Bureau of Land Management (BLM) Carlsbad Field Office (CFO), and used a methodology developed by ENVIRON for the Central Regional Air Planning Association (CENRAP)[46]. The preparation of the 2008 inventory for the Permian Basin will expand on the AES study, including both additional emissions estimates in the Permian Basin. The steps in developing the Permian Basin inventory are described below.

For the New Mexico portion of the Permian Basin, additional O&G area source categories may need to be added to the inventory that are not included in the AES study. The AES study only examined emissions from wellhead/lateral compression, heaters, and flaring. Given the prevalence of both O&G production in the Permian Basin, additional emissions of ozone precursors (nitrogen oxides and volatile organic compounds) are expected from tanks, fugitive emissions, pneumatic devices, dehydrators, drilling, blowdown and completion venting, well workovers, and other source categories. To estimate emissions from these categories, we will rely on previous source category emissions estimates from other Phase III basins, and will attempt to gather input data from other basin inventories matched as closely as possible to the production type in the Permian Basin. Where applicable, the adjacent inventory for the South San Juan Basin will serve as the primary reference for these additional O&G area source category emission estimates. For the missing source categories in the Permian Basin, we will use the total inventories by source category from other Phase III basins scaled by the appropriate activity parameters to generate unit-level emissions factors for each source category. These will then be scaled by the 2008 production data in the Permian Basin by county and tribal land to generate new emissions estimates for the missing source categories. Where appropriate, scaling will also account for variations in the volatile fraction of produced gas in the Permian Basin relative to the other Phase III basins. The same scaling will be applied for tank source categories (oil, condensate and water tanks), but it should be noted that the volatile fraction of the liquid to scale the emissions will be used rather than rerun the E&P TANK model, as it is not expected that sufficient data will be available to rerun the model. For those area sources for which emissions were estimated by AES, the AES emissions will be scaled from 2007 to 2008 using scaling factors developed from the production statistics. No control analysis will be used for these projections. Emissions data from permitted point sources of oil and gas in the New Mexico portion of the Permian Basin (primarily gas processing plants and compressor stations) have been gathered by AES as part of the study and will be used directly. The previously estimated area source emissions, the newly estimated area source emissions and the point source emissions will be aggregated into a single inventory for the New Mexico portion of the Permian Basin. The inventory will be formatted similarly to other Phase III basins.

For the Texas portion of the Permian Basin, we will use the area source inventory as described above for the New Mexico portion of the basin along with data from the TCEQ, and expand this to the counties in Texas

46 http://www.cenrap.org/html/presentations.php

that lie within the boundaries of the basin if appropriate. The emissions estimates from the New Mexico portion of the Basin will be scaled by the appropriate production statistic to generate unit-level emissions factors, and these will be applied to the production data for the Texas counties. For the permitted sources in Texas, we will conduct outreach to the Texas Commission on Environmental Quality (TCEQ) and request a database of permitted oil and gas sources. The permitted sources emission data will be aggregated with the area source estimates to generate an inventory of the Permian Basin in Texas. It will be similarly formatted in the Phase III format, and combined with the New Mexico portion of the basin for a comprehensive Permian Basin inventory.

6.4.3 2008 O&G Emissions for the Remainder of the U.S.

The WRAP Phase III Basins and Permian Basin O&G emissions described above covers most of an area including northwestern TX, NM, CO, UT, WY, MT and ND. For areas within these states not covered by the WRAP Phase III and Permian Basins, and O&G emissions outside of this region, the O&G emissions from the 2008 NEIv2.0 will be used.

6.5 FIRE EMISSIONS

For the initial WestJumpAQMS photochemical modeling, emissions from fires will be based on the Fire Inventory from NCAR (FINN[47]). When available, the fire emissions will be based on the comprehensive 2008 fire emissions inventory being developed in the DEASCO3[48] project sponsored by the Joint Fire Science Program (JFSP). The WestJumpAQMS emissions Technical Memorandum Number 5[49] on fire emissions compared the 2008 FINN fire emissions and the 2008 BlueSky/SMARTFIRE fire emissions in the NEIv2.0 and selected the FINN for the interim 2008 fire emissions until the DEASCO3 study emissions are ready because: (1) FINN is more complete spatially (e.g., includes Canada); (2) FINN has more complete species; (3) BlueSky/SMARTFIRE may overstate fire emissions; and (4) FINN fires are better documented. As described in Technical Memorandum No. 5, the FINN emissions will be processed to generate the hourly gridded emissions using the CB6 chemical species and the WRAP plume rise methodology.

6.6 AMMONIA EMISSIONS

Ammonia emissions for livestock and due to fertilizer will be based on the 2008 NEIv2.0 that used the CMU ammonia model[50]. The updated spatial surrogates for locations of Concentrated Animal Feeding Operations (CAFOs) developed as part of the NPS ROMANS study will be used. The WestJumpAQMS project team is currently reviewing the documentation on ammonia emissions and the CMU ammonia model application as they prepare emissions Technical Memorandum Number 8 on ammonia emissions.

6.7 OCEAN GOING VESSELS

Large ships, such as container ships, tankers, bulk carriers and cruise ships, are significant contributors to air pollution in many of our nation's cities and ports. There are two types of diesel engines used on large ships: main propulsion and auxiliary engines. The main propulsion engines on most large ships are "Category 3" marine diesel engines, which can stand over three stories tall and run the length of two school buses. Auxiliary engines on large ships typically range in size from small portable generators to locomotive-size engines.

47 http://bai.acd.ucar.edu/Data/fire/data/README_FINNv1_04192011.pdf
48 http://www.wrapair2.org/pdf/JSFP_DEASCO3_TechnicalProposal_November19_2010.pdf
49 http://www.wrapair2.org/pdf/Memo_5_Fires_Apr27_2012_Final.pdf
50 http://www.cmu.edu/ammonia/

The 2008 off-shore shipping emissions inventory were based on the 2008 NEIv2.0. These emissions are developed and carried as point sources, rather than the area-level files generally used for off-road mobiles sources, including marine emissions sources. Using the point source format allows for: (1) detailed location information for the emissions, rather than use of generalized spatial allocation profiles; and (2) processing of the emissions as elevated sources, rather than distributing all of Class 3 marine emissions into the lowest level of the model. Emissions from large marine vessels are buoyant and emitted out of tall stacks several stories high so would not be injected in the lowest layer of the model, which is approximately 24 m thick for the WestJumpAQMS modeling. Thus, it is important to treat them as point sources.

Details on the Off-Shore Shipping emissions are provided in a report "Documentation for the Commercial Marine Vessel Component of the National Emissions Inventory – Methodology" prepared by Eastern Research Group (ERG, 2010[51]) dated March 30, 2010. The WestJumpAQMS emissions Technical Memorandum Number 7[52] describes the off-shore shipping emissions and how they will be processed for input into the photochemical grid models.

It should be noted that the Off Shore Shipping emissions category discussed in this section includes just the Class 3 Commercial Marine source. Smaller vessels (Class 1 and 2) are included with the Non-Road Mobile Source discussed in Section 6.3.2. The latest 2008 emissions inventory for ocean going vessels used in the WestJumpAQMS are similar to what was used for the Emissions Control Area (ECA) analysis[53].

6.8 BIOGENIC EMISSIONS

WRAP performed a Western Biogenic Emissions Update Study that enhanced the MEGAN biogenic emissions model to better simulate biogenic emissions in the western U.S. The WestJumpAQMS project will use the new enhanced version of MEGAN along with the 2008 WRF 36/12/4 km data to generate hourly gridded speciated biogenic emission inputs. Details on the WRAP Biogenic Emissions Update Study can be found in the study's final report (Sakulyanontvittaya, Yarwood and Guenther, 2012[54]) with a summary provided in the WestJumpAQMS emissions Technical Memorandum Number 9[55] on biogenic emissions.

6.9 SPATIAL ALLOCATION

New spatial allocation surrogates will be developed at 4 km resolution for the CONUS domain using the latest 2010 CENSUS and other new data. The 4 km surrogate distributions will be used directly for disaggregating the county-level emissions to the 4 km grid cells in the IMWD as well as collapsed to 36 and 12 km resolution for spatial allocation to the 36 km CONUS and 12 km WESTUS domains. Table 6-2 summarizes the spatial surrogates to be used for spatial allocation in the WestJumpAQMS SMOKE emissions modeling. More details are provided in the WestJumpAQMS emissions Technical Memorandum Number 13 on SMOKE modeling parameters.

51 http://www.epa.gov/ttn/chief/net/nei08_alm_popup.html
52 http://www.wrapair2.org/pdf/OffshoreShippingEmissionsMemo_7WestJumpAQMS_Jan23_2012.pdf
53 http://www.epa.gov/otaq/oceanvessels.htm
54 http://www.wrapair2.org/pdf/WGA_BiogEmisInv_FinalReport_March20_2012.pdf
55 http://www.wrapair2.org/pdf/Memo_9_Biogenics_May9_2012_Final.pdf

Table 6-2. Spatial surrogate distributions to be used in the SMOKE emissions modeling spatial allocations.

Shapefile	Description	Type	Year	Source
cty_pophu2k_revised	U.S. County Boundaries	Polygon	2005	U.S. Census Bureau
pophu_bg2010	Population/ Housing	Polygon	2010	U.S. Census Bureau
rd_ps_tiger2010	Roadways	Line	2010	U.S. Census Bureau
waterway_ntad2011	Waterways	Line	2010	U.S. Bureau of Transport Statistics
rail_tiger2010	Railways	Line	2010	U.S. Census Bureau
exits**	Highway Exits	Point	2010	ESRI
mjrrds**	Major Roads	Line	2010	ESRI
transterm**	Transportation Terminals	Point	2010	ESRI
fema_bsf_2002bnd	Building footprints	Polygon	2010	FEMA
heating_fuels_acs0510_c2010	Home heating fuels	Polygon	2010	U.S. Census Bureau

6.10 TEMPORAL ALLOCATION

Temporal profiles are available from the U.S. EPA for a wide range of emissions sources. While the majority of the temporal profiles available from the EPA represent nationally averaged emissions sources, state-specific monthly profiles exist for prescribed fires, wildfires, livestock, and some mobile sources. For most sources we will base the WestJumpAQMS emissions modeling gtemporal allocations on the U.S. EPA temporal profiles distributed with the 2008 NEIv2.0[56] (filename: amptpro_2008aa_us_can_revised_06oct2011_v0.txt). Several source categories use episode emissions that already have hourly emissions so will not use the temporal allocation profiles. These emissions categories include: large point sources with measured hourly CEM emissions; on-road mobile sources that use the MOVES monthly weekday/weekend day hourly emissions; biogenic emissions from MEGAN; and fire emissions.

As part of the WestJumpAQMS modeling process we will evaluate the quality and appropriateness of the EPA default temporal profiles. While it is unlikely that new profiles will be added, there is a possibility of changing the assignments of existing profiles to inventory sources through updates to the temporal cross-reference file. The EPA default cross walk file between SCC codes and temporal allocations is available on the NEIv2.0 website[57].

6.11 CHEMICAL SPECIATION

The U.S. EPA develops speciation profiles from information stored in the SPECIATE database[58]. The current SPECIATE database (version 4.3) is the official repository of volatile organic compound (VOC) and particulate matter (PM) emissions source profiles for different categories of emissions sources. SPECIATE contains 5,592 profiles of chemical mass fractions from source testing conducted by EPA, state agencies, or published in the

56 http://www.epa.gov/ttnchie1/net/2008inventory.html
57 ftp://ftp.epa.gov/EmisInventory/2008v2/doc/scc_eissector_xwalk_2008neiv2.xlsx
58 http://www.epa.gov/ttnchie1/software/speciate/

literature since the 1970's. Of the current profiles in SPECIATE, 3,570 are for PM sources, 1,775 are for VOC sources, and 247 are for other gases, such as mercury. The most recent update to the SPECIATE database occurred with the release of version 4.3 in September 2011. S PECIATE 4.3 include 405 new profiles obtained from a combination of recommendations for EPA Office of Transportation and Air Quality, EPA and state-sponsored studies of various industrial processes, and literature reviews conducted by the SPECIATE workgroup.

Part of the speciation process for VOCs includes converting inventory reactive organic gases (ROG) to total organic gases (TOG). This step is required because inventoried VOC excludes methane in the mass of total VOC while the speciation profiles include methane. Before the speciation profiles can be applied to the inventory, the inventory VOC must be scaled up to account for the missing methane mass. SCC-specific ROG-to-TOG conversion factors are included with the speciation profiles to prepare the inventories for speciation.

The WestJumpAQMS CAMx photochemical modeling will be using the very latest Carbon Bond version 6 (CB6) chemical mechanism (Yarwood et al., 2010[59]). Thus, the SMOKE emissions modeling will be performed using new CB6 speciation profiles, based on the SPECIATE V4.3 database, and ROG-to-TOG conversion factors recently developed by ENVIRON. ENVIRON developed an interface to the SPECIATE database called the Speciation Tool. The WRAP Phase III Basin-specific CB05 VOC speciation profiles will be used for O&G VOC emissions in those Basins. Since CB6 is backwards compatible with CB05 this will not cause any problems.

6.12 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 and to facilitate source apportionment modeling at later stages of the WestJumpAQMS. 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 WestJumpAQMS 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)

59 http://www.cmascenter.org/conference/2010/abstracts/emery_updates_carbon_2010.pdf

Table 6-3. Emissions processing categories and temporal allocation approach.

No.	Emissions Processing Category (Abbr)	Inventory Source	Temporal	Processing Comments
1	Nonpoint/Area (nonpt)	NEI08v2	mwdss_mon	Remove oil & gas, agricultural NH3, and dust,; includes commercial marine and rail
2	Livestock NH3 (lv)	NEI08v2	mwdss_mon	Do not apply met-based temporal profiles; separate out for possible sensitivity later
3	Fertilizer NH3 (ft)	NEI08v2	mwdss_mon	Group with lv as a full agricultural NH3 sector (ag)
4	Fugitive and Road Dust (fd)	NEI08v2	mwdss_mon	Includes paved and unpaved road dust; apply transport factors but not met factors
5	Residential Wood Combustion (rwc)	NEI08v2	mwdss_mon	Do not apply met-based temporal profiles; separate out for possible sensitivity later
6	Area Oil & Gas (og)	IPAMS	mwdss_mon	Basin specific speciation profiles and spatial surrogates
7	Nonroad mobile (nr)	NEI08v2	mwdss_mon	Includes NMIM commercial marine and rail
8	MOVES RPD (rpd)	MOVES2010a	hourly met	Representative weekday and weekends for each year; process as hourly area sources
9	MOVES RPP (rpp)	MOVES2010a	hourly met	Representative weekday and weekends for each year; process as hourly area sources
10	MOVES RPV (rpv)	MOVES2010a	hourly met	Representative weekday and weekends for each year; process as hourly area sources
11	CEM Point (ptcem)	NEI08v2/CAMD	daily	Anomalies removed from 2008 CAMD data
12	Non-CEM Point (ptncem)	NEI08v2	mwdss_mon	Removed oil & gas sources and transferred to ptog sector; includes point aircraft and ports
13	Point Oil & Gas (ptog)	IPAMS	mwdss_mon	Combination of WRAP Phase III inventory and NEI08v2 for areas not covered by WRAP EI
14	Point Fires (ptfire)		daily	
15	Commercial Marine (ptseca)	NEI08v2	aveday_mon	
16	Lightning NOx (lnox)		hourly met	Gridded hourly NO emissions tied to WRF convective rainfall
17	Sea salt (ss)		hourly met	Surf zone and open ocean PM emissions
18	Windblown Dust (wbd)	WRAP WBD Model	hourly met	
19	MEGAN Biogenic (bg)	MEGAN2.1	hourly met	Use new versions of MEGAN V2.10 updated by WRAP for the western U.S.
20	Mexico Area (mexar)	Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2008
21	Mexico Point (mexpt)	Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2008
22	Mexico Mobile (mexmb)	Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2008
23	Canada Area (canar)	Canada NPRI	mwdss_mon	Environment Canada 2006 Inventory
24	Canada Point (canpt)	Canada NPRI	mwdss_mon	Environment Canada 2006 Inventory
25	Canada Mobile (canmb)	Canada NPRI	mwdss_mon	Environment Canada 2006 Inventory

Separate Quality Assurance (QA) and Quality Control (QC) will be performed for each stream of emissions processing and in each step. SMOKE includes advanced quality assurance features that include error logs when emissions are dropped or added. The QA/QC procedures developed under the WRAP RMC will be used (Adelman, 2004) that includes visual displays that such as:

- Spatial plots of the hourly emissions for each major species (e.g., NOX, VOC, some speciated VOC, SO2, NH3, PM and CO);
- Vertical average emissions plots for major species and each of the grids;
- Diurnal plots of total emissions by major species and by state; and
- Summary tables of emissions for major species for each grid and by major source category.
- This QA information will be examined against the original point and area source data and summarized in an overall QA/QC assessment.

Scripts to perform the emissions merging of the appropriate biogenic, on-road, non-road, area, low-level, fire, and point emission files will be written to generate the CAMx-ready two-dimensional day-specific hourly speciated gridded emission inputs. The point source and, as available elevated fire, emissions would be processed into the day-specific hourly speciated emissions in the CAMx-ready point source format.

The resultant CAMx model-ready emissions will be subjected to a final QA using spatial maps, vertical plots and diurnal plots to assure that: (1) the emissions were merged properly; (2) CAMx inputs contain the same total emissions; and (3) to provide additional QA/QC information. Emission inputs for the CMAQ model will be generated by processing the CAMx-ready emissions using the CAMx2CMAQ processor.

6.13 REPORTING

As discussed at the beginning of this section, 13 emissions Technical Memorandums have been, or are in the process of being, prepared that discuss the emissions source data, assumptions and processing procedures for each major source category. These Technical Memorandums provide documentation of the emissions by each source category.

After performing the emissions modeling, summary reports on the emissions will be generated and distributed to project participants. Details on the emissions and all of the QA/QC graphics and summaries will be uploaded to the project website so that they are available to all participants. Chapter 8 discusses the project website in more detail.

7.0 PHOTOCHEMICAL MODELING

The WestJumpAQMS project will conduct photochemical modeling using both the CAMx and CMAQ photochemical grid models (PGMs). Applying both PGMs will provide insight into the capabilities of photochemical modeling for the western U.S. and what features are important. Because a major objective of the study is to address western U.S. ozone and particulate matter (PM) source-receptor relationships using ozone and PM source apportionment techniques, CAMx will be the primary model due to its more advanced ozone and PM source apportionment tools (Arunachalam, 2009) and ability to perform two-way grid nesting. However, CMAQ will also be run for the 2008 base case scenario and evaluated against ambient air quality measurements; we have found that running both models has provided unique and valuable insight into model performance. For example, in VISTAS where CMAQ was the lead model the CAMx base case modeling and model performance evaluation identified deficiencies in the CMAQ secondary organic aerosol (SOA) that was subsequently enhanced resulting in improved CMAQ organic aerosol (OA) model performance.

Three types of PGM model simulations will be conducted:

- 2008 base case modeling that is used in the model performance evaluation.
- Ozone source apportionment modeling to characterize ozone source receptor relationships across the western states including the contributions of upwind emissions to elevated ozone concentrations in the western U.S. as well as estimating the impact of emissions in the western U.S. on downwind elevated ozone concentrations.
- Particulate Matter (PM) source apportionment to characterize $PM_{2.5}$, visibility and sulfur and nitrogen deposition source-receptor relationships in the western U.S.

The WestJumpAQMS photochemical modeling will also form a framework for future air quality modeling in the western U.S. This potentially includes the development of State implementation Plans (SIPs) and air quality modeling to support the development of Environmental Impact Statements (EISs) and Resource Management Plans (RMPs) to address requirements of the National Environmental Policy Act (NEPA). This Chapter describes the model configurations for the CAMx and CMAQ 2008 base case simulations, whereas Chapter 8 describes the model performance evaluation procedures and Chapter 9 describes the ozone and PM source apportionment modeling methodologies.

7.1 CAMX AND CMAQ SCIENCE AND INPUT CONFIGURATIONS

Table 7-1 summarizes the CAMx and CMAQ science configurations and options to be used for the 2008 base case simulations. The latest version of CAMx, which is currently Version 5.4 (released October 2011), will be used. CAMx V5.4 includes several recent updates that will be used in the WestJumpAQMS such as the new CB6 chemical mechanism. The model will be configured to predict both ozone and PM species. The current version of CMAQ is Version 5.0.1 that was released in July 2012.

Many common parameterizations will be selected for both CAMx and CMAQ. Both models 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 and CMAQ will use the analogous vertical mixing approach. The CB6 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. However, CMAQ V5.0.1 does not support CB6 so will use the CB05 chemical mechanism. Additional CAMx and CMAQ inputs will be as follows:

Meteorological Inputs: The WRF-derived meteorological fields will be processed to generate CAMx and CMAQ meteorological inputs using the, respectively, WRFCAMx and MCIP processors, 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[60] global chemistry model. Considerations were also given to generating the 2008 36 km CONUS domain BCs using output from the GEOS-Chem[61] or AM3[62] 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/CMAQ LCP coordinate system and vertical layer structure and to map the MOZART chemical species to the CB6 and CB05 chemical mechanisms being used by CAMx and CMAQ, respectively.

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[63]). 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[64] 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 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. Photolysis rates for the CMAQ model will be base in the JPROC[65] processor. CMAQ will also be operated using the in-line photolysis rates option so that photolysis rates can be adjusted based on the current modeled concentrations.

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 and, when used, 4 km nested domains for the last two days of 2007 before the start of the 2008 calendar year (January 1, 2008).

Although for the most part CMAQ will be configured in a similar manner as CAMx, since CMAQ does not support two-way grid nesting, CB6 chemistry or Plume-in-Grid it would be operated using one-way grid nesting and no Plume-in-Grid. Many CMAQ inputs (e.g., ICBCs and emissions) will be generated using the corresponding CAMx inputs and the CAMx2CMAQ processor.

60 http://www.acd.ucar.edu/wrf-chem/mozart.shtml
61 http://acmg.seas.harvard.edu/geos/
62 http://www.gfdl.noaa.gov/atmospheric-model
63 http://ozoneaq.gsfc.nasa.gov/
64 http://cprm.acd.ucar.edu/Models/TUV/
65 http://www.ie.unc.edu/cempd/products/cmaq/op_guidance_4.6/html/ch02s02s03.html

Table 7-1. CAMx (Version 5.4) and CMAQ (Version 5.0.1) model configurations for WestJumpAQMS.

Science Options	Configuration	Details
Model Codes	CAMx V5.4 – October 2011 Release CMAQ V5.0.1 – July 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	36/12/4 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
4 km grid	Several DSAD 4-km domains	Also set up 4 km IADs as a one-way nest
Vertical Grid Mesh	25 vertical layers, defined by WRF	Layer 1 thickness ~24- m. Model top at ~19-km above MSL
Grid Interaction	36/12/4 km two-way nesting for CAMx	One-way grid nesting for CMAQ
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	CMAQ has no subgrid-scale Plume-in-Grid module
Chemistry		
Gas Phase Chemistry	CB6 in CAMx	CB05 in CMAQ V5.0.1
Meteorological Processor	WRFCAMx and MCIP 4.1	Compatible with CAMx V5.4 and CMAQ V5.0.1
Horizontal Diffusion	Spatially varying	K-theory with Kh grid size dependence
Vertical Diffusion	CMAQ-like in WRF2CAMx	ACM2 for CMAQ V5.0.1
Diffusivity Lower Limit	Kz_min = 0.1 to 1.0 m^2/s or 2.0 m^2/s	Possible sensitivity tests for Kz_min
Deposition Schemes		
Dry Deposition	Zhang dry deposition scheme (CAMx) M3Dry Pleim dry deposition (CMAQ)	Zhang 2003
Wet Deposition	CAMx and CMAQ-specific formulation	rain/snow/graupel/virga
Numerics		
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) -- Fast Solver	EBI implemented in both CAMx and CMAQ
Vertical Advection Scheme	Implicit scheme w/ vertical velocity update (CAMx) New vertical velocity scheme (CMAQ)	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	PPM in both CAMx and CMAQ
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 and CMAQ models 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 and CMAQ 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 and CMAQ performance evaluations 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 and use of higher (4 km) model resolution. 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 WestJumpAQMS 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[66]) 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

66 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.

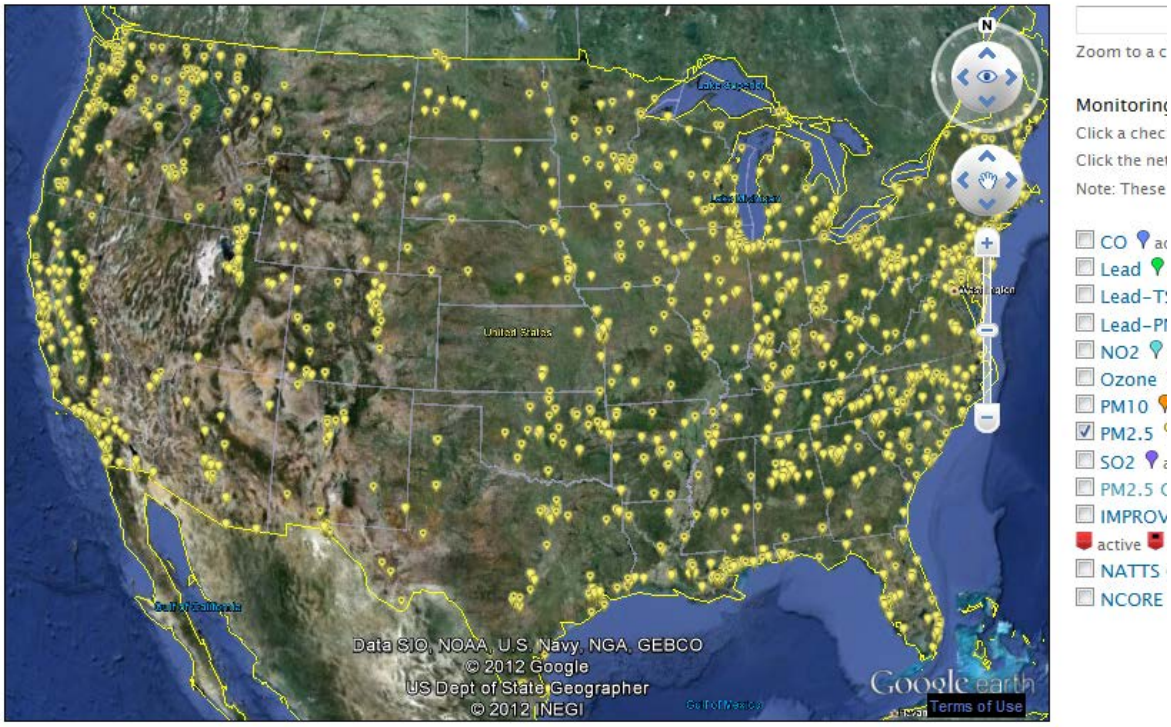


Figure 8-1. Locations of FRM $PM_{2.5}$ mass monitoring sites showing active and inactive (with black dot) sites (source: http://www.epa.gov/airquality/airdata/ad_maps.html).

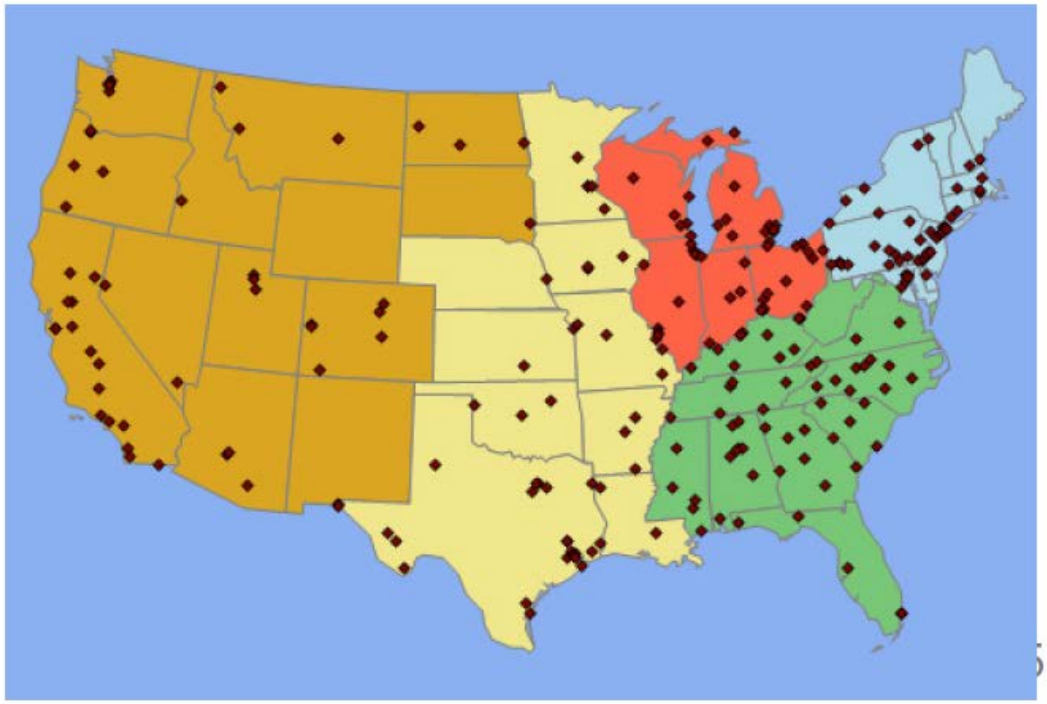


Figure 8-2. Locations of CSN speciated $PM_{2.5}$ monitoring sites (source: http://www.epa.gov/ttn/amtic/speciepg.html).

IMPROVE Monitoring Network: The Interagency Monitoring of Protected Visual Environments (IMPROVE[67]) 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.

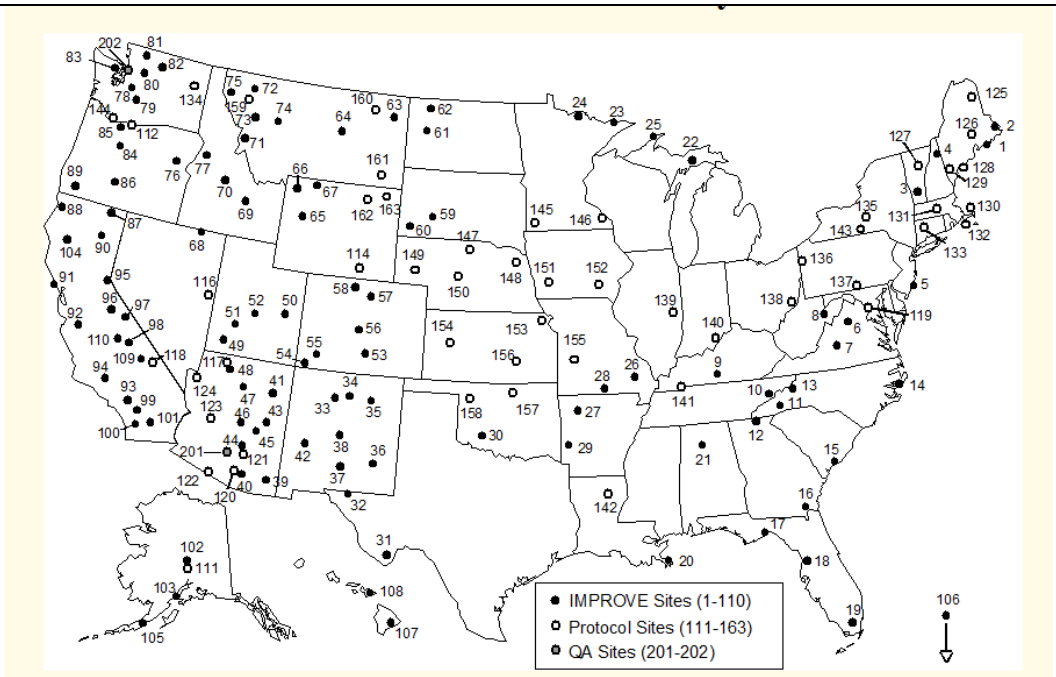


Figure 8-3. Locations of IMPROVE monitoring sites (source: http://vista.cira.colostate.edu/IMPROVE/)

67 http://vista.cira.colostate.edu/IMPROVE/

CASTNet Monitoring Network: The Clean Air Status and Trends Network (CASTNet[68]) 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.

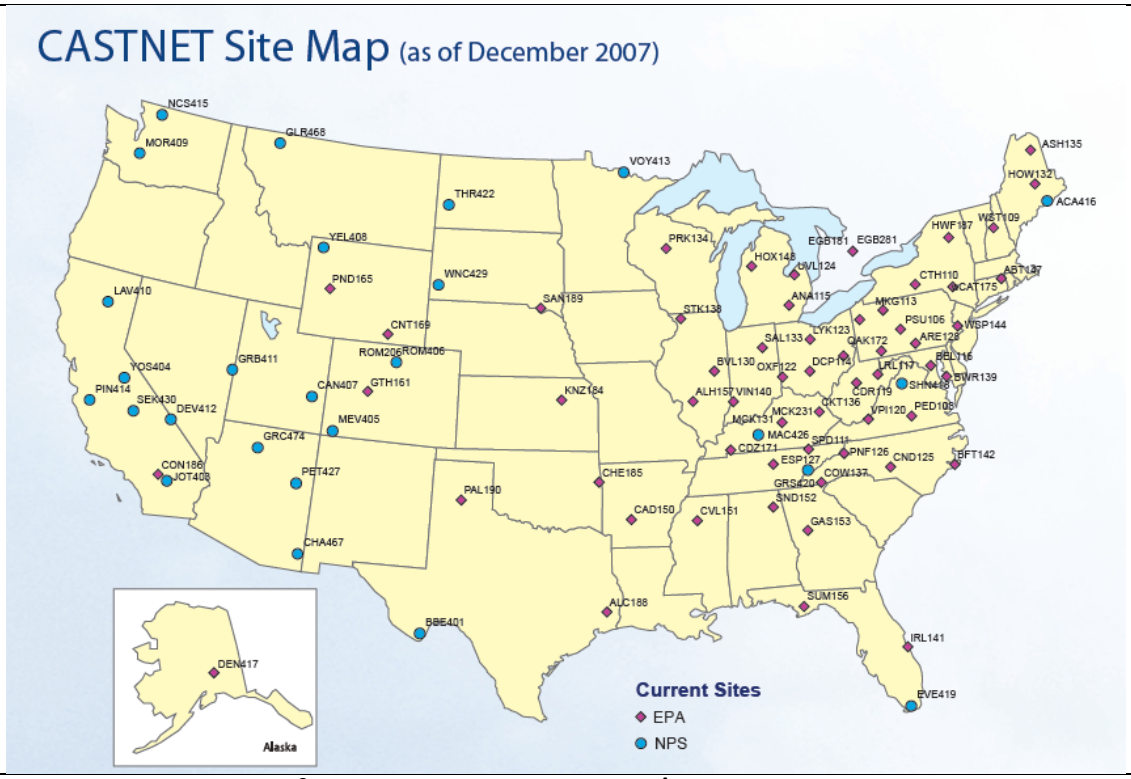


Figure 8-4. Locations of CASTNet monitoring sites (source: http://epa.gov/castnet/javaweb/index.html).

68 http://java.epa.gov/castnet/

NADP Network: The National Acid Deposition Program (NADP[69]) 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[70] throughout the world that measure the vertical structure of ozone concentrations throughout the troposphere and into the lower stratosphere. Ozonesonde monitoring sites within the WestJumpAQMS modeling domain include: (1) Trinidad Head on the coast in northern California; (2) Boulder, Colorado; and (3) at the University of Alabama at Huntsville.

69 http://nadp.sws.uiuc.edu/NADP/
70 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 WestJumpAQMS 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 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.

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)	$\frac{P - O_{peak}}{O_{peak}}$	Comparison of the peak observed value (O_{peak}) with the predicted value at same time and location
Coefficient of determination (r2)	$\frac{\left[\sum_{i=1}^{N}(P_i - \overline{P})(O_i - \overline{O})\right]^2}{\sum_{i=1}^{N}(P_i - \overline{P})^2 \sum_{i=1}^{N}(O_i - \overline{O})^2}$	Pi = prediction at time and location i; Oi = observation at time and location i; $\overline{P}$ = arithmetic average of Pi, i=1,2,…, N; $\overline{O}$ = arithmetic average of Oi, i=1,2,…,N
Normalized Mean Error (NME)	$\frac{\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\sum_{i=1}^{N} O_i}$	Reported as %
Root Mean Square Error (RMSE)	$\left[\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2\right]^{1/2}$	Reported as %
Fractional Gross Error (FE)	$\frac{2}{N}\sum_{i=1}^{N}\left\lvert\frac{P_i - O_i}{P_i + O_i}\right\rvert$	Reported as % and bounded by 0% to 200%
Mean Absolute Gross Error (MAGE)	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert$	Reported as concentration (e.g., µg/m^3)
Mean Normalized Gross Error (MNGE)	$\frac{1}{N}\sum_{i=1}^{N}\frac{\lvert P_i - O_i\rvert}{O_i}$	Reported as %
Mean Bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$	Reported as concentration (e.g., µg/m^3)
Mean Normalized Bias (MNB)	$\frac{1}{N}\sum_{i=1}^{N}\frac{(P_i - O_i)}{O_i}$	Reported as %
Mean Fractionalized Bias (Fractional Bias, FB)	$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$	Reported as %, bounded by -2005 to +200%
Normalized Mean Bias (NMB)	$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N} O_i}$	Reported as %
Bias Factor (BF)	$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{P_i}{O_i}\right)$	Reported as BF:1 or 1: BF or in fractional notation (BF/1 or 1/BF).

8.4 SUBREGIONAL EVALUATION OF MODEL PERFORMANCE

The initial evaluation of the CAMx and CMAQ 36/12 km base case simulations would be performed over large regions on a monthly, quarterly and annual basis. At first we would use the definitions of the five RPOs (WRAP, CENRAP, MWRPO, VISTAS and MANE-VU) for the evaluation to get a regional perspective of the model performance. We would then zero in on the western U.S. and perform a subregional model performance evaluation by Impact Assessment Domain (IAD) and Detailed Source Apportionment Domain as discussed in Chapter 4 and by state. We would 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 WestJumpAQMS 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[71]) and Visualization Environment for Rich Data Interpretation (VERDI[72]) 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.
- SURFER: The Golden Software SURFER package is commercial software used primarily for generating spatial displays of modeling results under the Windows environment. Although not free, like PAVE and VERDI, it can generate high quality displays for reports. Unlike the UCR, PAVE and VERDI tools that operate directly on the model output under Linux, there is more work involved in

71 http://www.cmascenter.org/index.cfm?model=pave
72 http://www.epa.gov/AMD/EcoExposure/verdi.html

processing the model output to get the results into SURFER. However, once in SURFER the user has a lot more control in how the results are displayed.

- 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[73]) 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.

In the following sections we present examples of model performance evaluation graphics using the above tools like we will use in the WestJumpAQMS 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.

73 http://www.epa.gov/AMD/ModelEvaluation/performance.html

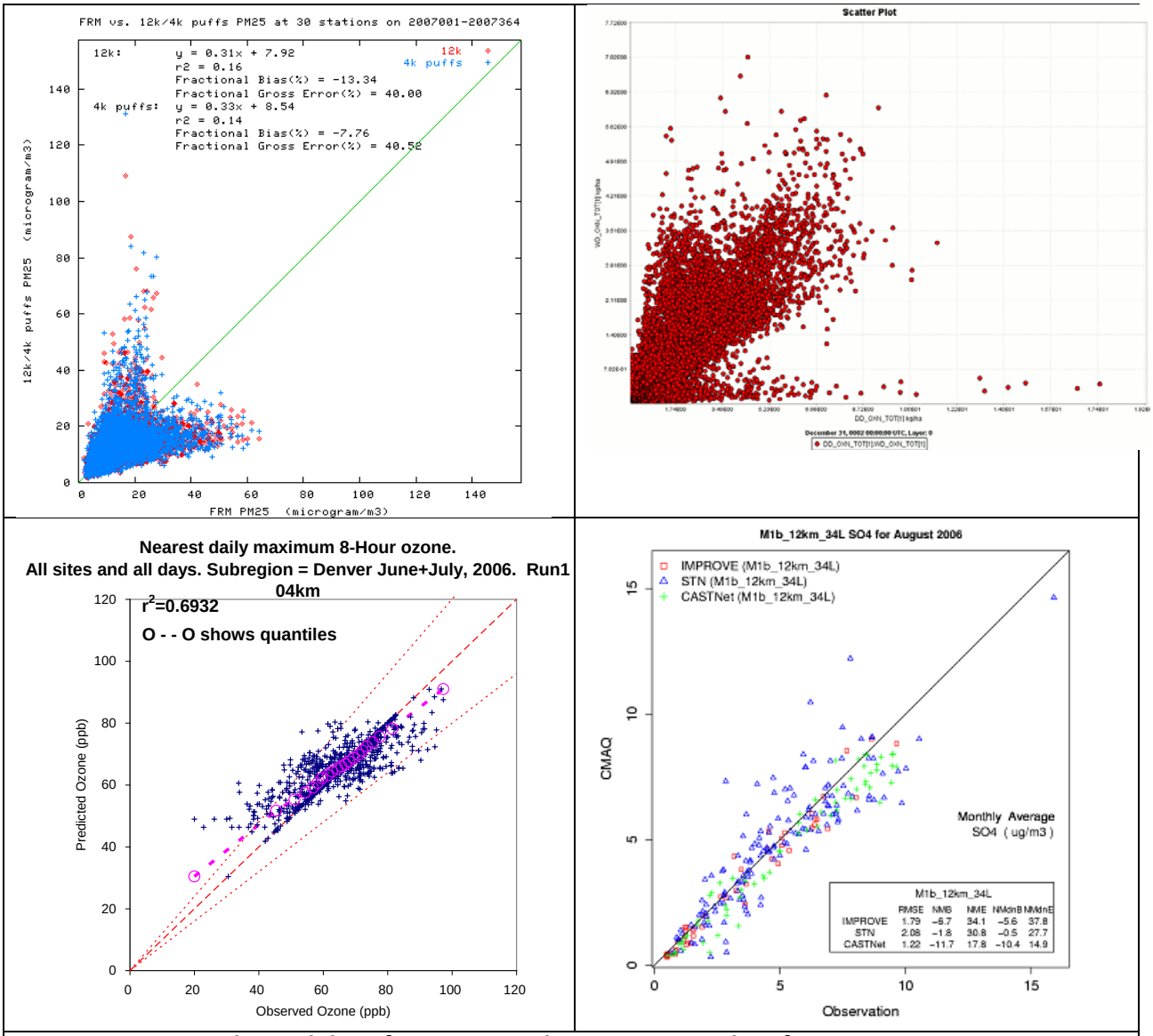


Figure 8-6. Example model performance evaluation scatterplots for FRM $PM_{2.5}$ using UCR Analysis Tool,(top left), annual oxidized nitrogen wet deposition versus oxidized nitrogen dry deposition using VERDI (top right), predicted and observed daily maximum 8-hour ozone concentrations using Excel (bottom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

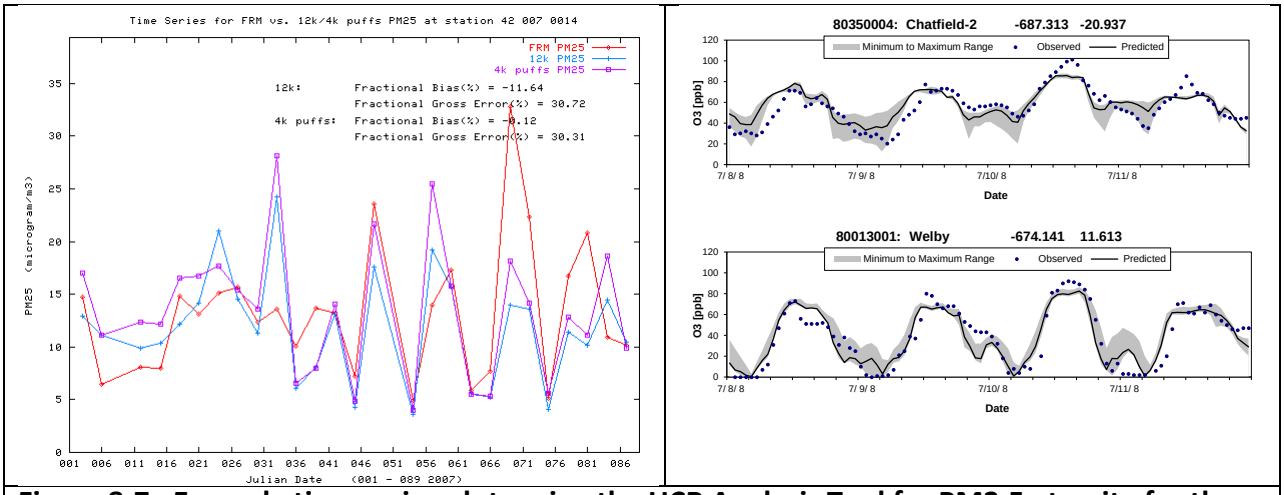


Figure 8-7. Example time series plots using the UCR Analysis Tool for PM2.5 at a site for the first quarter of 2007 using 4 km and 12 km CAMx modeling results (left) and using Excel for a CAMx 2008 4 km simulation and two sites in the Denver area.

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.

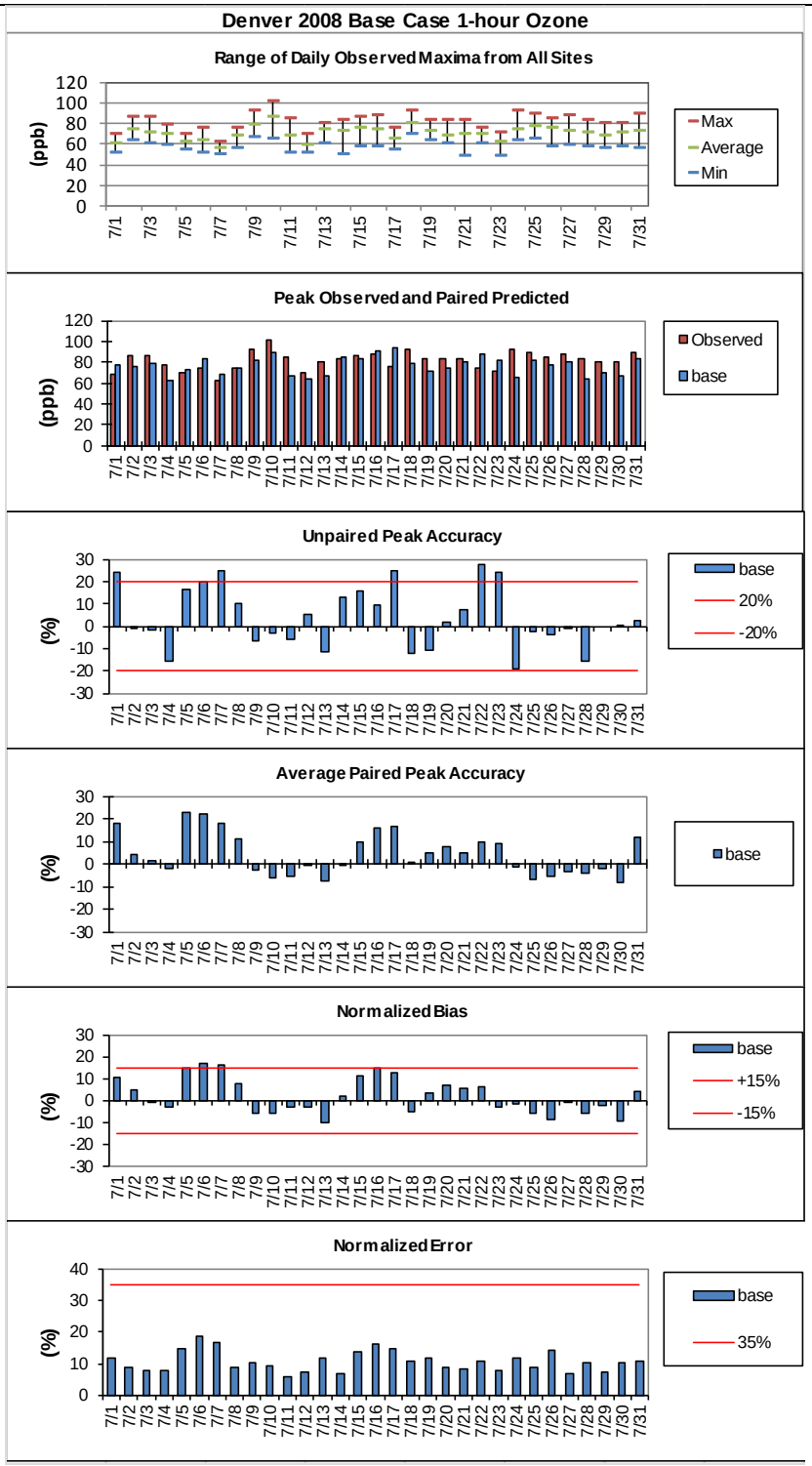


Figure 8-8. Example of hourly ozone model performance statistics comparing the UPA, MNB and MNGE statistics with EPA's 1991 ozone performance goals (red lines)..

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.

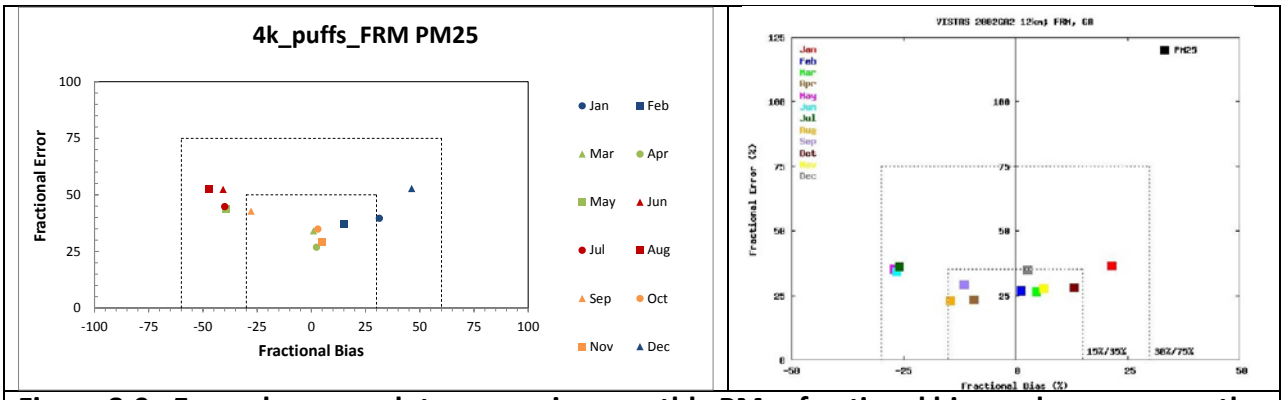


Figure 8-9. Example soccerplots comparing monthly $PM_{2.5}$ fractional bias and error versus the PM Performance Goals and Criteria (Table 8-1) for a 2007 Midwest CAMx application (left) and the VISTAS/ASIP 2002 CMAQ application for Georgia (right).

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.

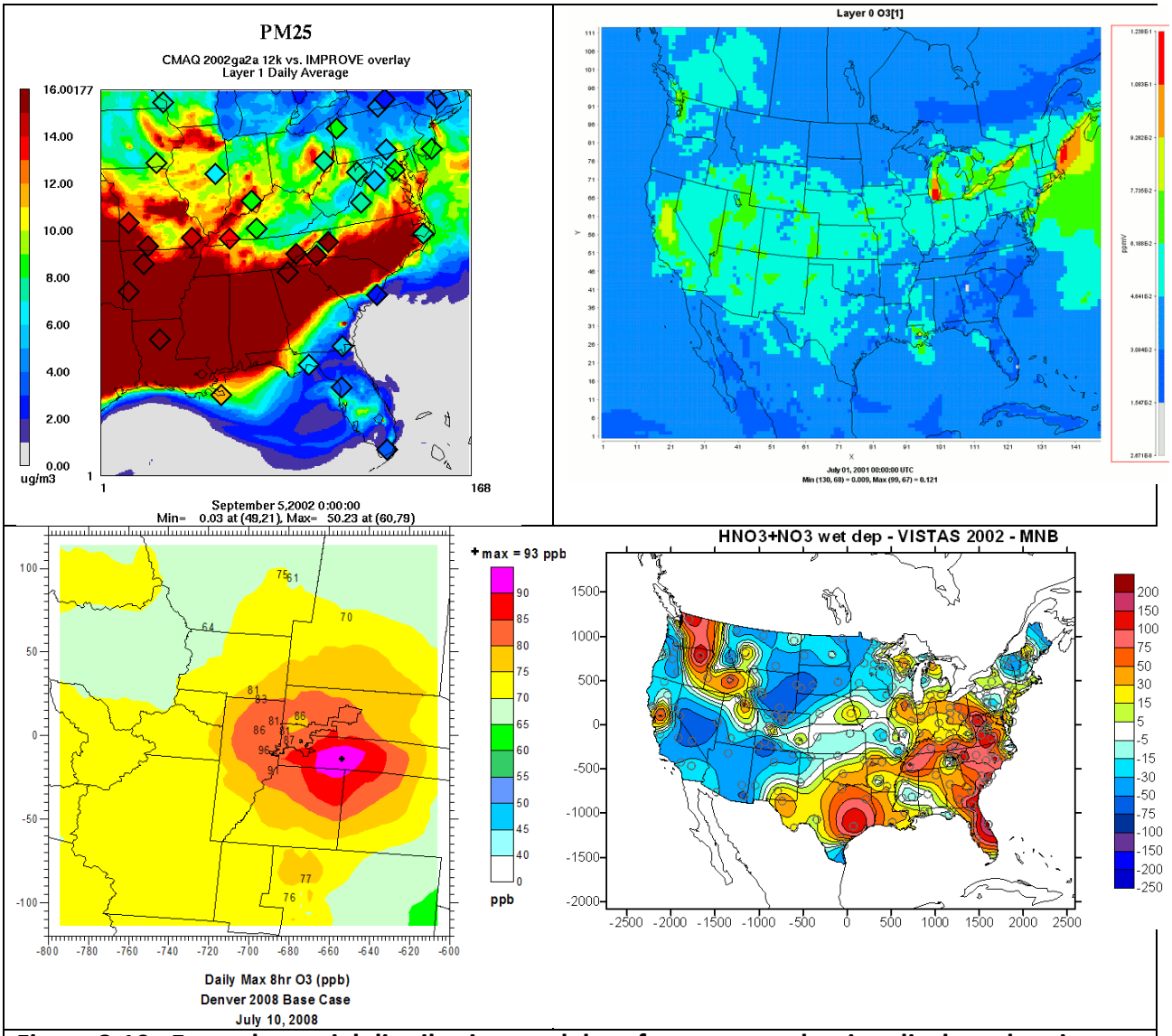


Figure 8-10. Example spatial distribution model performance evaluation displays showing VISTAS CMAQ $PM_{2.5}$ performance on September 5, 2002 using PAVE (top left) an ozone spatial display using VERDI (top right), Denver 8-hour ozone performance for July 10, 2008 using SURFER (bottom left) and spatial distribution of VISTAS wet nitrogen depositions Mean Normalized Bias (MNB; bottom right).

8.6 SUMMARY OF MODEL PERFORMANCE

An initial model performance of the CAMx and CMAQ 36/12 2008 base case simulations will be conducted for ozone, $PM_{2.5}$ and speciated $PM_{2.5}$ concentrations and wet sulfur and nitrogen depositions over large regions (e.g., RPO domains). 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. These more refined model evaluations will be expanded to include ozone and PM precursor and product species, visibility and deposition. 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 SOURCE APPORTINMENT MODELING

The CAMx and CMAQ photochemical grid models contain several "Probing Tools" that can provide different types of information regarding source-receptor relationships and model sensitivity in a photochemical grid model simulation. For the WestJumpAQMS, we will use the CAMx Ozone Source Apportionment Technology (OSAT) and the Particulate Source Apportionment Technology (PSAT) Probing Tools to better understand the ozone and fine particulate matter ($PM_{2.5}$) source-receptor relationships in the western U.S. OSAT and PSAT are source apportionment methods that provide the contributions of user selected Source Groups to downwind ozone and PM concentrations for a given photochemical grid model simulation. Note that the concept of source apportionment is different than determining the response of the model to changes in emissions from a particular Source Group for which a sensitivity method is required. The different Probing Tools available in the CAMx/CMAQ photochemical grid models and what kinds of information they can provide is described next followed by a description of the ozone and PM source apportionment modeling methodology for the WestJumpAQMS.

9.1 PROBING TOOLS

The CAMx/CMAQ models contain several different Probing Tools that can provide different kinds of information on the internal workings of the model, model sensitivity and source apportionment.

Brute Force Sensitivity: The Brute Force Sensitivity modeling can be performed using any photochemical model and involves the application of the model for a base case and then for a sensitivity simulation that has a perturbation in the model or model inputs. The difference in concentrations between the base case and sensitivity simulation is the sensitivity of the model to the selected perturbation. Although a brute force sensitivity simulation can be performed for any model attribute, it is most frequently applied to changes in emissions. For example, multiple brute force simulations off across-the-board VOC and or NO_X emission reductions can be performed to develop an ozone isopleth (EKMA) diagram that can be used to help identify a VOC/NO_X emissions control path toward ozone attainment. Another example of Brute Force Sensitivity applications is the sequence of control measures that are used to ultimately demonstrate attainment of the ozone standard as part of the development of a SIP control plan. Brute force Sensitivity simulations have been used to completely eliminate (zero-out) emissions from a specific source sector (e.g., on-road mobile sources) and the differences between the base case and the specific source sector zero-out case has been interpreted as the contributions of that source sector. However, for reactive pollutants the zero-out approach is a sensitivity and not a source apportionment method. For example, the sum of the ozone contributions due to the zero-out modeling of all Source Groups does not add up to the base case ozone concentrations because the effect of altering the emissions in the zero-out runs changes the chemistry in the photochemical model simulation thereby altering the source-receptor relationships from those in the base case.

CAMx Ozone and PM Source Apportionment: CAMx contains two versions of an ozone source apportionment tool, the Ozone Source Apportionment Technology (OSAT) and the Anthropogenic Precursor Culpability Assessment (APCA). The CAMx also contains the Particulate Source Apportionment Technology (PSAT) that estimates source apportionment for particulate matter (PM) species. All three source apportionment techniques use reactive tracers (also called tagged species) that run in parallel to the host model to determine the contributions of ozone and PM to user selected Source Groups. A Source Group is typically defined as the intersection between a geographic Source Regions (e.g., grid cell definitions of states) and user selected Source Categories

(e.g., Point Sources, On-Road Mobile, etc.). The intersection of the Source Regions and the Source Categories defines the Source Groups (e.g., on-road mobile sources from California) for which individual source apportionment contributions are obtained. Source apportionment provides contributions of emissions within each Source Group to concentrations/depositions under the current model simulation conditions, but does not necessarily estimate what would be the effect that controls on a given Source Group would have on the concentrations, which is a sensitivity question.

- Ozone Source Apportionment: The OSAT method follows VOC and NO_X emissions from each Source Group and when ozone is formed OSAT estimates whether ozone formation was more VOC-limited or NO_X-limited and then allocates the ozone formed to Source Groups based on their relative contributions of the limiting precursor. The APCA ozone source apportionment technique differs from OSAT in that it recognizes that some emissions are not controllable (e.g., biogenic emissions) so focuses ozone source apportionment on controllable emissions. In the case when ozone is formed due to the interaction of biogenic VOC and anthropogenic NO_X emissions under VOC-limited conditions, a case where OSAT would assign the ozone formed to the biogenic VOC emissions, APCA redirects the ozone formed to the controllable anthropogenic NO_X emissions. Thus, in APCA the only ozone attributable to biogenic emissions is when ozone is formed due to the interaction of biogenic VOC and biogenic NO_X emissions. Ozone and PM source apportionment techniques have also been implemented in CMAQ (OPTM and PPTM), but the version of CMAQ with source apportionment is now out-of-date and a peer review of source apportionment techniques found the implementation in CAMx to be superior (Arunachalam, 2009).
- Particulate Source Apportionment: The CAMx PSAT particulate source apportionment method has five different families of tracers that can be invoked separately or together to track source apportionment of the following particulate species: Sulfur (SO4), Nitrogen (NO3/NH4), Primary PM, Secondary Organic Aerosol (SOA) and Mercury. Because PSAT needs to track the PM source apportionment from the PM precursor emissions to the PM species, the number of tracers needed to track a Source Group's source apportionment depends on the complexity of the chemistry and number of PM species involved. The Sulfur family requires only two reactive tracer species (SO_2 and SO_4) to track the formation of particulate sulfate from SO_2 emission source contributions for each Source Group. Whereas SOA family is the most expensive PSAT family with 18 reactive tracers needed for each Source Group in order to track the four VOC precursors (aromatics, isoprene, terpenes and sesquiterpenes) and the 7 condensable gas (CG) and SOA pairs.

  Sulfur (2 Tracers)

  - $SO2_i$ Primary SO_2 emissions
  - $PS4_i$ Particulate sulfate ion from primary emissions plus secondarily formed sulfate

  Nitrogen (7 Tracers)

  - RGN_i Reactive gaseous nitrogen including primary NOx ($NO + NO_2$) emissions plus nitrate radical (NO_3), nitrous acid (HONO) and dinitrogen pentoxide (N_2O_5).
  - TPN_i Gaseous peroxyl acetyl nitrate (PAN) plus peroxy nitric acid (PNA)

- NTR_i Organic nitrates (RNO_3)
- $HN3_i$ Gaseous nitric acid (HNO_3)
- $PN3_i$ Particulate nitrate ion from primary emissions plus secondarily formed nitrate
- $NH3_i$ Gaseous ammonia (NH_3)
- $PN4_i$ Particulate ammonium (NH_4)

Secondary Organic Aerosol (18 Tracers)

- ARO_i Aromatic (toluene and xylene) secondary organic aerosol precursors
- ISP_i Isoprene secondary organic aerosol precursors
- TRP_i Terpene secondary organic aerosol precursors
- SQT Sesquiterpene secondary organic aerosol precursors
- $CG1_i$ Condensable gases from aromatics (low volatility products)
- $CG2_i$ Condensable gases from aromatics (high volatility products)
- $CG3_i$ Condensable gases from isoprene (low volatility products)
- $CG4_i$ Condensable gases from isoprene (high volatility products)
- $CG5_i$ Condensable gases from terpenes (low volatility products)
- $CG6_i$ Condensable gases from terpenes (high volatility products)
- $CG7_i$ Condensable gases from sesquiterpenes
- $PO1_i$ Particulate organic aerosol associated with CG1
- $PO2_i$ Particulate organic aerosol associated with CG2
- $PO3_i$ Particulate organic aerosol associated with CG3
- $PO4_i$ Particulate organic aerosol associated with CG4
- $PO5_i$ Particulate organic aerosol associated with CG5
- $PO6_i$ Particulate organic aerosol associated with CG6
- $PO7_i$ Particulate organic aerosol associated with CG7

Mercury (3 Tracers)

- $HG0_i$ Elemental Mercury vapor
- $HG2_i$ Reactive gaseous Mercury vapor
- PHG_i Particulate Mercury

Primary Particulate Matter (6 Tracers)

- PEC_i Primary Elemental Carbon
- POA_i Primary Organic Aerosol

- o PFC_i Fine Crustal PM
- o PFN_i Other Fine Particulate
- o PCC_i Coarse Crustal PM
- o PCS_i Other Coarse Particulate

DDM Sensitivity Modeling: Another type of analysis that may be performed entails the use of the Direct Decoupled Method (DDM) sensitivity analysis. DDM, and the higher order DDM (HDDM), can produce a numerically intensive, direct sensitivity/uncertainty analysis. DDM can provide information on the sensitivity of ozone, PM or other concentrations to model inputs (e.g., IC, BC, specific emissions). For example, it was used in the Houston area to identify where locations of potential highly reactive VOC (HRVOC) emissions would be that could explain the rapid rise in ozone at a particular time and location (i.e., assuming that VOC emissions are missing from the inventory, what emissions locations would best explain observed high ozone levels?). As a sensitivity method, DDM/HDDM can estimate the effects on the base case concentrations due to a change in emissions from a specific source group. In general, DDM is reasonably accurate to estimate the change in a reactive species concentration due to a change in emissions of up to ~20%, whereas HDDM can estimate the effects of larger amounts of emissions reductions on concentrations.

Process Analysis: Process Analysis is a tool in CAMx/CMAQ to extract additional information about the various physical and chemical processes in the model that produced the ozone and other concentrations. Information on VOC-limited versus NO_X-limited ozone formation, importance of local production versus entrainment of ozone aloft and identification of the contributions of individual VOC species to ozone formation are the types of information that can be obtained with Process Analysis. It can be a powerful tool for diagnosing the causes of poor model performance.

9.2 WESTJUMPAQMS SOURCE APPORTIONMENT MODELING

Several rounds of CAMx 2008 ozone and PM source apportionment modeling will be conducted using the WestJumpAQMS 2008 modeling database. We will start with broad-brush ozone and PM source apportionment modeling using the 36/12 km domains by individual state (the Source Regions) for two source categories: anthropogenic and natural emissions (the Source Categories). The results will be analyzed in a similar fashion as EPA used in the Cross-State Air Pollution Rule (CSAPR[74]) to estimate upwind state contribution to downwind ozone and PM concentrations and Design Values.

Based on the preliminary CAMx ozone and PM source apportionment modeling linkages, we would perform more detailed source apportionment modeling that would obtain contributions by source sector in addition to geographic region (i.e., state) and use the 4 km DSAD domains as appropriate. After the preliminary 36/12 ozone and PM source apportionment model is conducted, we will prepare a detailed source apportionment modeling plan that will be submitted to WRAP and others for review. The source apportionment modeling plan would discuss three general types of source apportionment modeling: (1) assessing the contributions of emissions from upwind states to ozone and/or PM in the western U.S. (Upwind Transport); (2) assessment of the contributions of western states to downwind areas many may be out of the WRAP region (Downwind Transport); and (3) assessment of the contributions of local sources (Local Contributions). The types of issues that need to be addressed in each of these three types of source apportionment are as follows:

74 http://www.epa.gov/airtransport/

- Ozone and/or PM Source apportionment.
  - Whether OSAT or APCA ozone source apportionment is used.
  - Which families of PSAT particulate source apportionment is used.
- Boundaries, Processing Time, and Number of non-overlapping 4 km DSAD domains to be used.
- Period of modeling.
  - If focusing on ozone then only the summer ozone season is needed.
- Definitions of the Source Regions for source apportionment modeling
- Definitions of the Source Categories used for source apportionment modeling
  - For example, biogenic, EGU point, non-EGU point, on-road mobile, non-road mobile, oil and gas, area, etc.

We anticipate that there will be some iterations on the definition of the detailed source apportionment plan and that there will be some trade-offs that will have to be made between number of Source Regions and Source Categories, number of 4 km DSADs, simulation length and computer time and memory. For ozone source apportionment modeling we would select periods with high ozone in the DSAD domains as well as periods with high ozone in downwind regions. The preliminary CAMx 2008 36/12-km source apportionment simulations and 4 km DSAD sensitivity source apportionment runs will allow us to collect the benchmark data so we can make intelligent decisions regarding these tradeoffs in the source apportionment design document.

The design of the more detailed source apportionment runs would be documented and provided to WRAP and other project participants for review and comment. We anticipate there will be several levels of source apportionment modeling as described below.

9.2.1 Level 1 APCA Ozone Source Apportionment Modeling

The Level 1 ozone source apportionment will use the APCA ozone source apportionment tool to estimate the contributions of western state's anthropogenic emissions on downwind ozone concentrations to obtain a preliminary estimate of western U.S. ozone source-receptor relationships from which more detailed ozone source apportionment modeling would be designed. The attributes of the Level 1 preliminary ozone source apportionment modeling would be as follows:

- CAMx Version 5.4 (or most current version as available).
- APCA ozone source apportionment method.
- 36 km CONUS and 12 km WESTUS domains using two-way grid nesting.
- Source Regions consisting of western states (22 individual states west of Mississippi), offshore shipping, Mexico, Canada and eastern U.S. (26 Source Regions, see Figure 9-1):
  - Source region map of grid cell definitions of states; and
  - Use point source override to assure point sources assigned to the correct state.
- Two Source Categories with one consisting of all anthropogenic emissions and the other being natural sources (i.e., biogenic, fires, lightning and sea salt).
- 54 total Source Groups (=26 x 2 +2; 2 extra Source Groups for IC and BC)
- Several procedures for post-processing:

- Contributions to 8-hour ozone Design Values using procedures in CSAPR;
- Contributions to elevated (>75, 70, 65 and 60 ppb) ozone concentrations; and
- Other procedures to be determined.

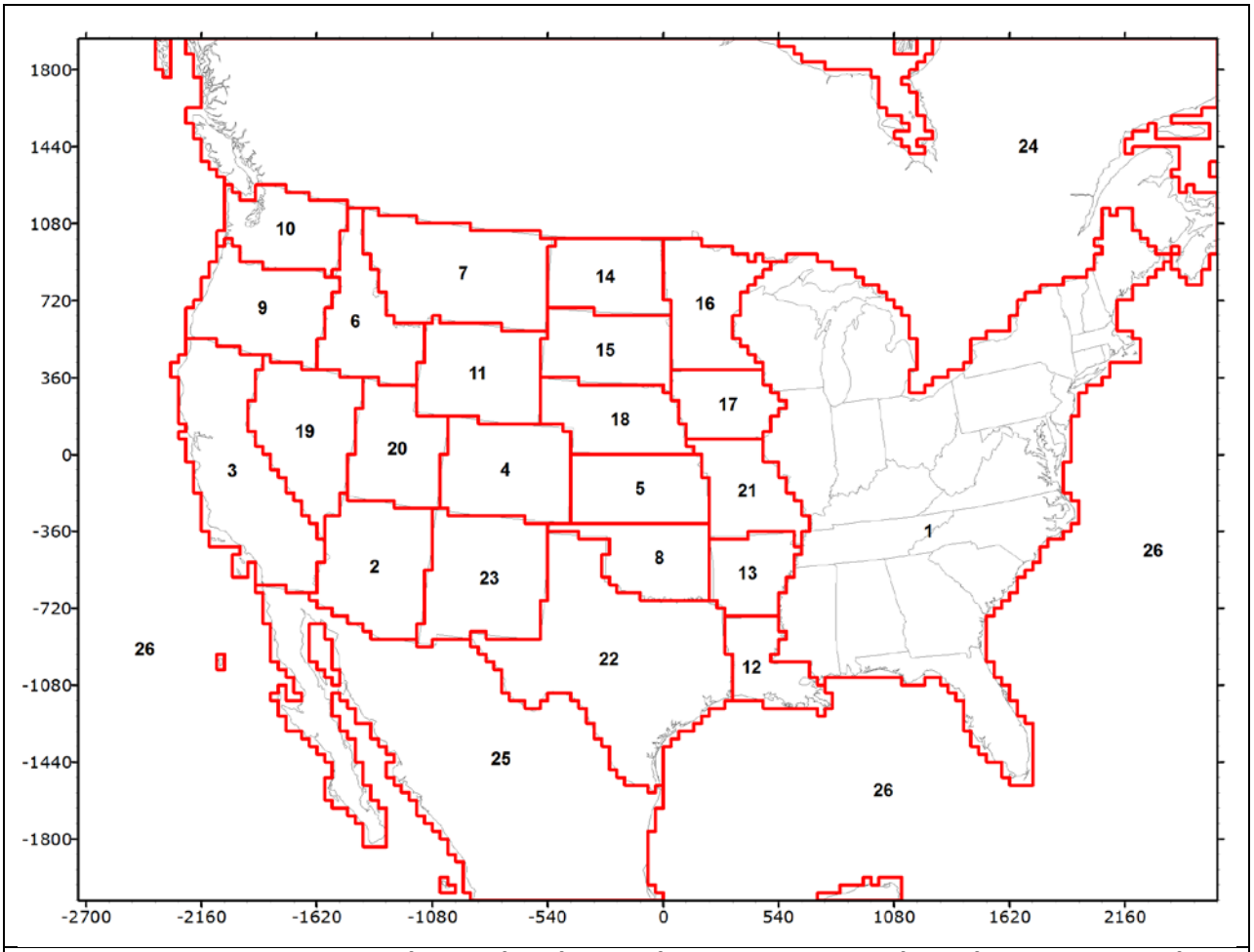


Figure 9-1. Source Regions to be used in the Level 1 APCA ozone and Level 3 PSAT particulate matter 2008 source apportionment modeling for WestJumpAQMS.

9.2.2 Level 2 OSAT Ozone Source Apportionment Modeling

The purpose of the Level 2 OSAT ozone source apportionment modeling is to learn more about VOC-limited versus NO_X-limited ozone formation in the western U.S., rather than investigate ozone source-receptor relationships. CAMx would be exercised for 2008 on the 36/12 km domains using the OSAT tool with one Source Region (i.e., no geographic source apportionment) using two Source Categories of anthropogenic and natural emissions. The CAMx OSAT results would be post-processed to estimate whether high ozone is formed more under VOC-limited or NO_X-limited conditions. The differences between OSAT and APCA source apportionment tools would also be investigated.

9.2.3 Level 3 PSAT PM Source Apportionment Modeling

The Level 3 PSAT PM source apportionment modeling would use the exact same configuration (26 Source Regions and 2 Source Categories, see Figure 9-1) as in the Level 1 APCA ozone source apportionment modeling, only using the PSAT PM source apportionment tool. For the Level 3 PSAT PM source apportionment we will use the Sulfate, Nitrogen and Primary PM PSAT source apportionment families of reactive tracers. Although SOA can be an important part of $PM_{2.5}$, especially in the summer, we have found that a majority of the SOA is due to biogenic sources. Given that the cost (memory, run time and disk space) of the SOA family is greater than the combined effects of the Sulfur, Nitrogen and Primary PM families then the small information obtained on SOA contributions is not worth the expense. However, the standard CAMx model output does have the ability to distinguish between SOA from anthropogenic versus biogenic emissions that we would use to assess the importance of the modeled anthropogenic SOA to $PM_{2.5}$ concentrations.

The Level 3 PSAT PM source apportionment results would be processed like was done for CSAPR to obtain state contributions to annual and 24-hour $PM_{2.5}$ Design Values. The role of transport versus local contributions would be examined.

9.2.4 Preliminary Results and Detailed Source Apportionment Plan

The results of the preliminary western state Level 1 APCA, Level 2 OSAT and Level 3 PSAT source apportionment modeling would be documented in an Interim Report. Based on the preliminary source apportionment results, we would also prepare a detailed source apportionment design for the next round of ozone and particulate source apportionment modeling.

Below we describe the types of source apportionment modeling that could be conducted after the preliminary analysis. Since the exact definition of these source apportionment runs will depend on the preliminary simulations, the details of the runs are not provided. However, the details in the next round of source apportionment modeling will be provided in the detailed source apportionment modeling plan prior to their execution to give WRAP and others a chance to comment on and revise the approach.

9.2.5 Level 1A APCA Ozone Source Apportionment Modeling

The Level 1A APCA ozone source apportionment modeling would extend the Level 1 APCA western states analysis to also obtain source apportionment by Source Category for selected states. Based on the Level 1 APCA analysis, several states that had anthropogenic ozone contributions to downwind elevated ozone concentrations would be selected as Source Regions and we would also obtain separate ozone source apportionment by Source Categories for the selected states as well as the remainder of the domain. The Source Categories would be selected from the pre-merged emissions modeling streams (see Table 6-3) and could consist of something like the following:

- Natural Emissions (biogenic, fires, lightning and sea salt).
- CEM Point Sources.
- Non-CEM Point Sources.
- Oil and Gas Exploration and Production Sources (point and area).
- On-Road Mobile Sources.
- Non-Road Mobile Sources.
- Area Sources.

The exact definition of the selected Source Categories will be identified in the detail source apportionment modeling plan. CAMx would be run using the 36/12 km domains and 2008 with the APCA ozone source apportionment tool.

The Level 1A APCA ozone source apportionment modeling results would be processed in a similar manner as was done for the Level 1 APCA analysis to obtain state and source sector contributions to ozone design Values and elevated ozone concentrations in the western U.S. We would also obtain the contributions to ozone concentrations by all source sector emissions, in addition to by state.

9.2.6 Level 3A PSAT PM Source Apportionment Modeling

The Level 3A PSAT analysis would be analogous to the Level 1A APCA analysis only using the PSAT PM source apportionment tool. States whose anthropogenic emissions had a significant $PM_{2.5}$, visibility or deposition impacts will be selected and we will obtain PM source apportionment results by source sector. The state-specific source category contributions to annual and 24-hour $PM_{2.5}$ Design Values and elevated concentrations as well as visibility and deposition will be obtained.

9.2.7 Level 4A APCA Ozone Source Apportionment Modeling

The objective of the Level 4A APCA ozone source apportionment modeling is to obtain more detailed information on local source contributions to elevated ozone concentrations in the Intermountain West Domain (IMWD). CAMx would be configured using a 12/4 km grid structure using the 12 km WESTUS and six 4 km Detailed Source Apportionment Domains (DSADs; see Figure 4-7). Seven Source Regions would be selected corresponding to the 6 DSADs and the remainder of the 12 km WESTUS domains. Ozone contributions would also be obtained by Source Category, such as the 7 Source Categories identified in Section 9.2.5 for the Level 1A APCA analysis. In addition to examining the contributions that local sources have on ozone within each of the 4 km DSAD domains, we would examine the contributions that emissions from the DSAD domains have on downwind ozone concentrations. Details on definition of the Level 4A APCA analysis will be contained in the detailed source apportionment modeling plan discussed previously.

9.2.8 Level 4B PSAT PM Source Apportionment Modeling

The Level 4B PSAT PM source apportionment modeling would be similar to the Level 4A APCA analysis, only using the PSAT PM source apportionment tool and the Sulfur, Nitrogen and Primary PM families of reactive tracers. The contributions of the DSAD 4 km domains by source category to $PM_{2.5}$, visibility and deposition would be obtained.

9.2.9 Online Source Apportionment Tool

The CAMx PACA/OSAT ozone and PSAT PM source apportionment modeling generates a wealth of information. It is not possible to document everything in a report. Different users will want to obtain different information for different locations from the modeling results. Thus, we will develop an on-line tool that users can use to mine the WestJumpAQMS source apportionment modeling results and generate custom graphics for locations and parameters of interest. The on-line source apportionment tool will be similar to the one developed for CENRAP from a state-specific PSAT source apportionment run for a 2018 emissions scenario using a 2002 36 km CONUS modeling database. Below we describe how the CENRAP source apportionment tool works with a few examples followed by a basic design of the data that would be available in the WestJumpAQMS source apportionment tool.

9.2.9.1 Example Results from the CENRAP Visibility Source Apportionment Visualization Tool

We envision that the WestJumpAQMS source apportionment visualization tool would be somewhat similar to the CENRAP visualization tool, only in addition to being able to visualize visibility at Class I areas the

WestJumpAQMS tool would also be able to visualize contributions to 8-hour ozone and annual and 24-hour $PM_{2.5}$ Design Values and concentrations as well as deposition and visibility impairment. Below we describe some of the features for the CENRAP visualization tool and discuss the anticipated differences with the WestJumpAQMS source apportionment visualization tool.

Figure 9-2 displays the control panel for the CENRAP source apportionment visualization tool that has the following options from top to bottom:

- Analysis: The parameter selected in Figure 9-2 is visibility extinction (Mm^{-1}) for the worst 20% days at Class I areas using the Absolute Value (as compared to percentage) of the modeling results. For WestJumpAQMS we anticipate additional variables such as ozone and $PM_{2.5}$ Design Values and nitrogen and sulfur deposition.
- Scenarios: The 2018 Future Year is selected in Figure 9-2, for WestJumpAQMS the scenario will be the 2008 Base Case.
- Options: There are two main modes for visualization the source apportionment results: (1) looking at the source contributions from multiple source regions/categories at a receptor location (One Receptor Multiple Source Regions); or (2) looking at the contributions of a given source region on multiple downwind receptors. For the example in Figure 9-2, the former approach has been selected to look at the visibility source apportionment averaged across the W20% days for the Rocky Mountains National Park (ROMO) receptor.
- Source Region: You can chose to visualize the source apportionment from all source regions (i.e., states), or manually select which ones you want to visualize.
- Source Category: The CENRAP PSAT source apportionment run obtained separate source apportionment for 8 Source Categories.
- Species: The CENRAP visualization tool can obtain visibility impairment for 6 PM species (SO4, NO3, POA, EC, SOIL and CM). Note that CENRAP did not run PSAT for the SOA species, so some of the plots also include the contributions due to SOA from all anthropogenic (SOAA) and all biogenic (SOAB) VOC precursors. We envision doing a similar approach with the WestJumpAQMS PSAT source apportionment visualization tool.
- Chart Type: There are four types of chart types that can be generated when looking at the source contributions at a given receptor (ROMO in this case) with the examples given in Figure 9-3:
    - Source Category versus Species (Figure 9-3a, left) that shows elevated point sources are the largest contributor to visibility impairment at ROMO followed by area sources.
    - Species by Source Category (Figure 9-3a, right) that shows SO_4 is the most important species at ROMO followed by NO_3 (note that since the IMPROVE equation is used then NH_4 is linked to the SO_4 and NO_3).
    - Source Regions by Species (Figure 9-3b, left) that indicate emissions from Colorado are the largest contributor to visibility impairment for the W20% days at ROMO.
    - Source Regions by Source Category (Figure 9-3b, right).
- Ranked Ordering: Clicking on the Ranked Ordering button at the bottom of the control panel in Figure 9-2 will generate a chart of the top 30 highest contributing Source Groups (Source Region by Source Category) to visibility impairment for the Worst 20% days at ROMO as shown in the left panel of Figure 9-4.

- Multiple Receptors One Source Region Option: The right panel in Figure 9-4 and left panel in Figure 9-5 display the charts generated when selecting the option to look at a Source Regions (Colorado in this case) on visibility in multiple receptor regions, where we selected Class I areas in WRAP and Colorado, respectively, in this case.
- Crossover Option: The final Option is called Crossover and plots Source Region contributions to receptors, where Class I areas in Colorado was selected in the example in the right panel of Figure 9-5.

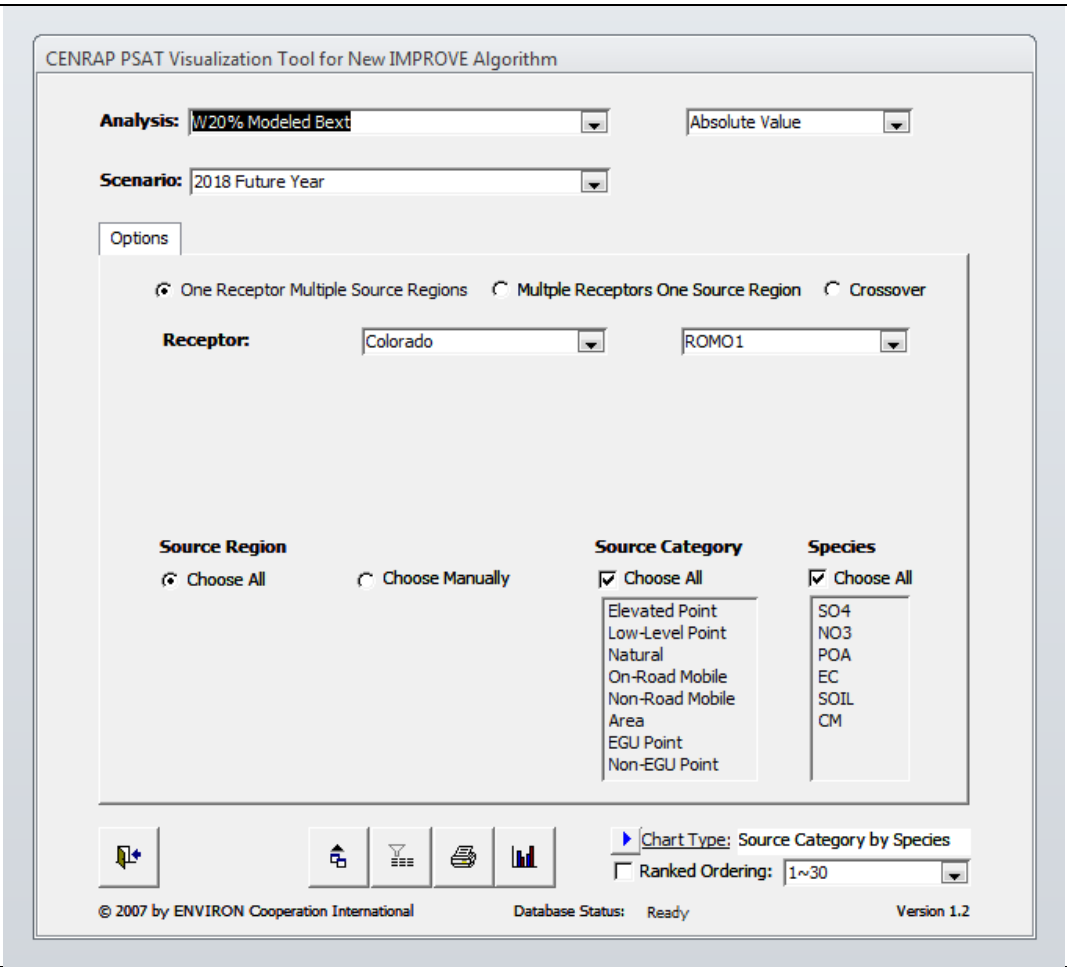
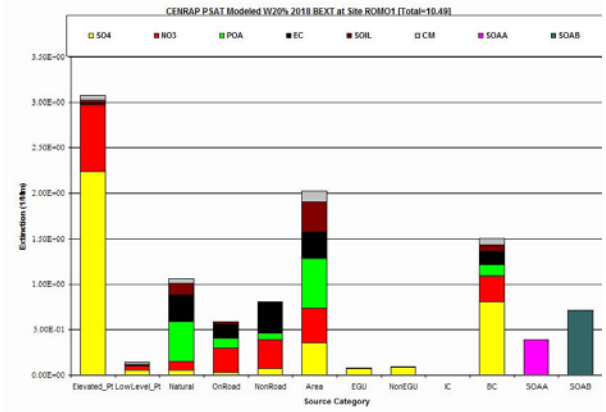


Figure 9-2. CENRAP source apportionment visualization tool control panel.



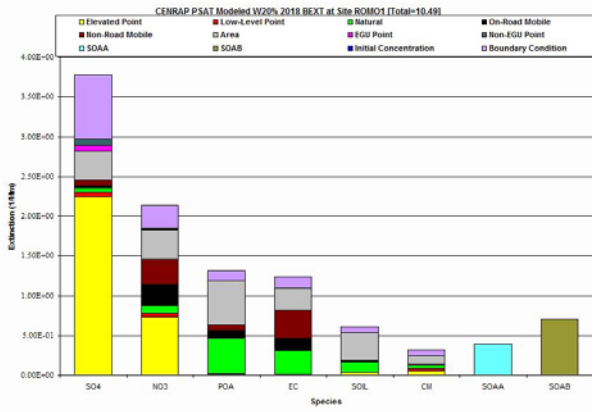
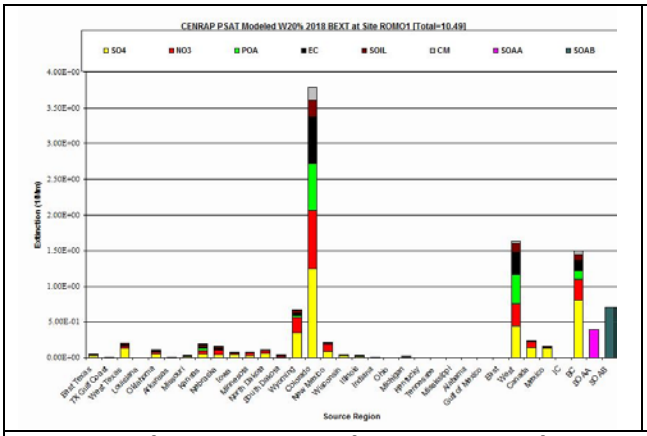


Figure 9-3a. CENRAP tool source contributions to 2018 visibility impairment for W20% days at ROMO for Source Category versus Species (left) and Species versus Source Category (right).



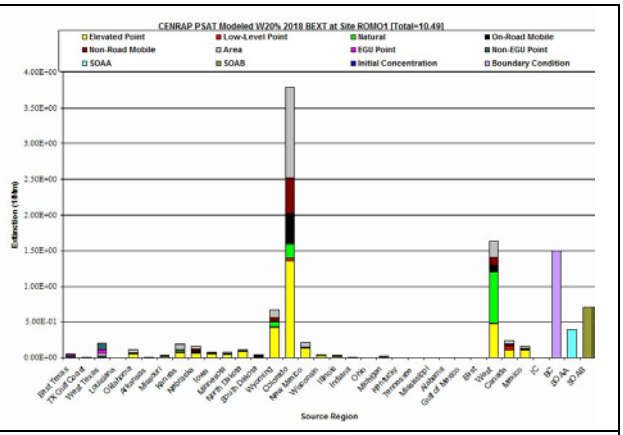
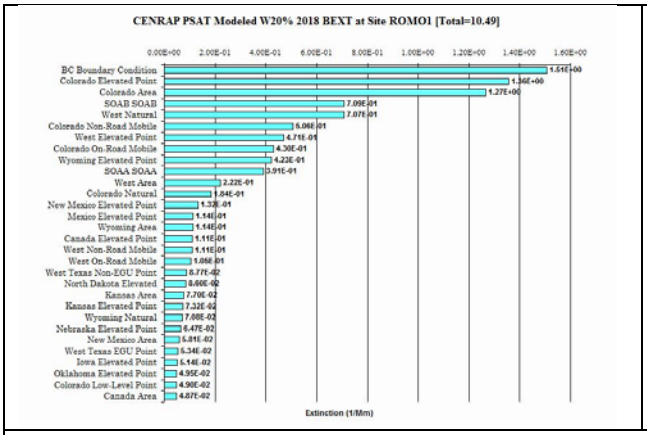


Figure 9-3b. CENRAP tool source contributions to 2018 visibility impairment for W20% days at ROMO for Source Category versus Species (left) and Species versus Source Category (right).



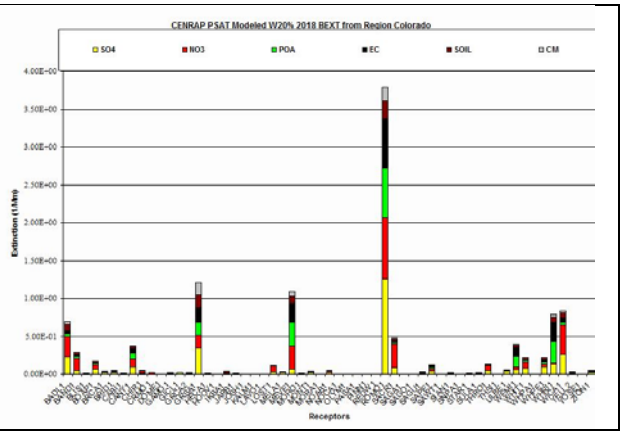


Figure 9-4. CENRAP tool ranked Source Group contributions to W20% days visibility at ROMO (left) and contributions due to emissions from Colorado to W20% visibility days at Class I areas in the WRAP region (right).

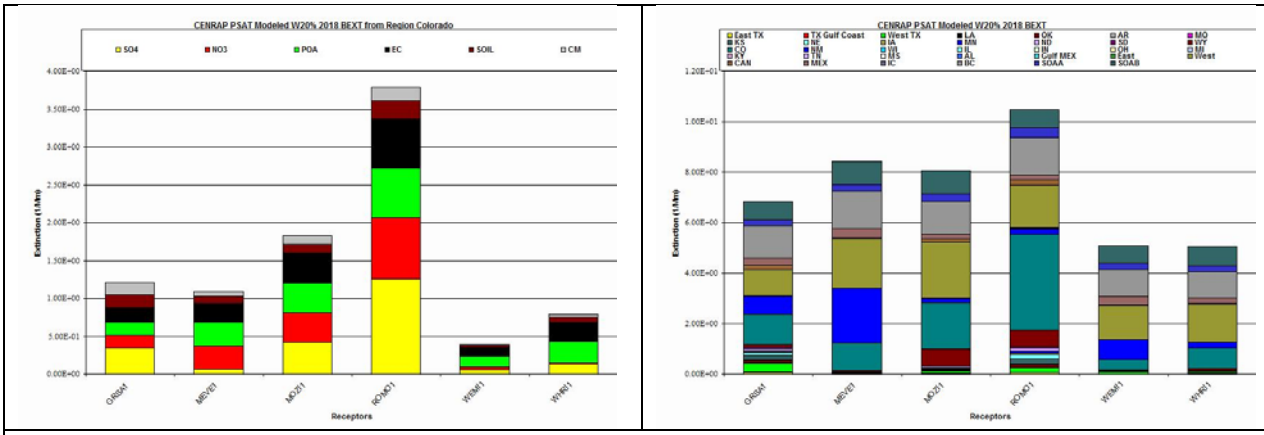


Figure 9-5. CENRAP tool contributions due to emissions from Colorado to W20% visibility days at Class I areas in Colorado (left) and contributions of emissions from Source Regions to W20% visibility days at Colorado Class I areas (right).

9.2.9.2 WestJumpAQMS Visualization Tool

We envision that the WestJumpAQMS on-line source apportionment visualization tool will operate functionally similar to the CENRAP visualization tool, only with additional air quality metrics as follows:

- 8-hour ozone Design Values at AQS sites.
- Maximum observed and modeled daily maximum 8-hour ozone concentrations at AQS sites.
- W126 at AQS sites.
- Annual and 24-hour $PM_{2.5}$ Design Values at FRM sites.
- Annual observed and modeled $PM_{2.5}$ concentrations at FRM sites.
- Maximum observed and modeled 24-hour $PM_{2.5}$ concentrations at FRM sites.
- Average visibility impairment for Worst and Best 20% days at IMPROVE sites.
- Annual nitrogen and sulfur deposition at IMPROVE sites.
- Other parameters to be determined.

8.0 WEBSITE AND REPORTING

Because of the sheer volume of information that will be generated as part of the meteorological and emissions modeling, in the model performance evaluation and from the source apportionment modeling, 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.

8.1 INTERACTIVE WEBSITE

As modeling steps and results are completed from the WestJumpAQMS 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 WestJumpAQMS project website is being developed, WestJumpAQMS reports are available on the WRAP website:

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

8.2 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 WestJumpAQMS:

- Technical Scope of Work dated July 20, 2011
  - http://www.wrapair2.org/pdf/WestJumpAQMS_SoW_July20_2011revision.pdf
- Modeling Plan dated January 23, 2012
  - http://www.wrapair2.org/pdf/WestJumpAQMS_Modeling_Plan_Final_Jan23_2012.pdf
- Thirteen Emissions Technical Memorandum discussing source of emissions and how they will be processed for photochemical modeling
  - Various stages of completion, some available on website: http://www.wrapair2.org/WestJumpAQMS.aspx
- WRF Meteorological Modeling Application/Evaluation report dated February 29, 2012
  - http://www.wrapair2.org/pdf/WestJumpAQMS_2008_Annual_WRF_Final_Report_February29_2012.pdf
- Draft Modeling Protocol dated September 2012

  - This document.
- 2008 Base Case and Model Performance Evaluation Report
  - October 2012
- Interim Report on Preliminary Source Apportionment Modeling
  - December 2012
- Detailed Refined Source Apportionment Modeling Plan
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