



## **Three-State Air Quality Modeling Study (3SAQS)**

### **Final Modeling Protocol 2011 Emissions & Air Quality Modeling Platform**

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## CONTENTS

<b>1.0 INTRODUCTION</b>	<b>1</b>
1.1 Background	2
1.2 Air Quality Standards and Air Quality Related Values	2
1.3 Organization of the Modeling Protocol	6
1.4 Project Participants	7
1.5 Related Studies	7
1.6 Overview of 3SAQS 2011 Modeling Approach	15
<b>2.0 Model Selection</b>	<b>17</b>
2.1 Justification and Overview of Selected Models	17
<b>3.0 EPISODE SELECTION</b>	<b>23</b>
3.1 Episode Selection Criteria	23
3.2 Episode Selection Results	23
<b>4.0 DOMAIN SELECTION</b>	<b>25</b>
4.1 Horizontal Modeling Domain	25
4.2 Vertical Domain Structure	28
<b>5.0 METEOROLOGICAL MODELING</b>	<b>30</b>
5.1 Model Selection and Application	30
5.2 WRF Domain Definition	30
5.3 Topographic Inputs	30
5.4 Vegetation Type and Land Use Inputs	30
5.5 Atmospheric Data Inputs	31
5.6 Water Temperature Inputs	31
5.7 FDDA Data Assimilation	32
5.8 WRF Physics Options	32
5.9 Application Methodology	33
5.10 Evaluation Approach	33
5.11 Reporting	33
<b>6.0 EMISSIONS</b>	<b>34</b>
6.1 Base Year 2011 Emissions	34

6.2 Future Year 2020 Emissions	47
6.3 Emissions Processing	51
6.4 Quality Assurance and Quality Control	56
<b>7.0 PHOTOCHEMICAL MODELING</b>	<b>58</b>
7.1 CAMx AND CMAQ Science and Input Configurations	58
<b>8.0 MODEL PERFORMANCE EVALUATION</b>	<b>62</b>
8.1 Overview of Model Performance Evaluation	62
8.2 Available Aerometric Data for the model Evaluation	62
8.3 Model Performance Statistics, Goals and Criteria	68
8.4 Subregional Evaluation of Model Performance	72
8.5 Example Model Performance Displays	72
8.6 Summary of Model Performance	78
<b>9.0 WEBSITE REPORTING AND SOURCE APPORTIONMENT MODELING</b>	<b>79</b>
9.1 Interactive Website	79
9.2 Reports	79
9.3 Source Apportionment Modeling	79
<b>10.0 ACRONYMS</b>	<b>81</b>
<b>11.0 REFERENCES</b>	<b>84</b>
 <b>TABLES</b>	
<b>Table 1-1. Key contacts for the 3SAQS 2011 modeling platform.</b>	<b>7</b>
<b>Table 1-2. List of State Specific Oil and Gas Regulations by Source Category.</b>	<b>9</b>
<b>Table 4-1. Projection parameters for the 3SAQS modeling domains.</b>	<b>26</b>
<b>Table 4-2. 37 Vertical layer interface 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).</b>	<b>29</b>
<b>Table 6-1. 3SAQS anthropogenic (+fires) inventory sectors</b>	<b>35</b>
<b>Table 6-2. List of Additional Controls Applied to 2011 Area Sources Emissions.</b>	<b>42</b>
<b>Table 6-3. List of Controls Applied to 2020 Area Sources Emissions</b>	<b>50</b>
<b>Table 6-4. 3SAQS 2011-based emissions processing categories.</b>	<b>54</b>
<b>Table 7-1. CAMx (Version 6.10) model configurations for 3SAQS.</b>	<b>60</b>

<b>Table 7-2. CMAQ (Version5.0.2) model configurations for 3SAQS.</b>	<b>61</b>
<b>Table 8-1. PM model performance goals and criteria.</b>	<b>69</b>
<b>Table 8-2. Definition of model performance evaluation statistical measures used to evaluate the CTMs.</b>	<b>71</b>

## FIGURES

<b>Figure 1-1. Current ozone nonattainment areas under the March 2008 8-hour ozone 0.075 ppm NAAQS.</b>	<b>4</b>
<b>Figure 1-2. Counties that are violating the 1997 15.0 <math>\mu\text{g}/\text{m}^3</math> <math>\text{PM}_{2.5}</math> NAAQS and additional counties that would violate a 13.0 <math>\mu\text{g}/\text{m}^3</math> (dark green) and the new December 2012 12.0 <math>\mu\text{g}/\text{m}^3</math> <math>\text{PM}_{2.5}</math> NAAQS based on 2008-2010 observations (source: <a href="http://www.epa.gov/pm/actions.html#jun12">http://www.epa.gov/pm/actions.html#jun12</a>).</b>	<b>5</b>
<b>Figure 1-3. 156 mandatory Class I areas in the contiguous U.S.</b>	<b>6</b>
<b>Figure 4-1a. 36 km CONUS, 12 km WESTUS, and 4 km 3SAQS processing domain used for developing PGM inputs.</b>	<b>26</b>
<b>Figure 4-1b. 3SAQS 2011 4 km modeling domain showing locations of Class I areas (labeled), sensitive Class II areas (unlabeled), urban areas and 2011 oil and gas wells.</b>	<b>27</b>
<b>Figure 5-1. WRF 36/12/4 km grid structure for the WestJumpAQMS meteorological modeling.</b>	<b>31</b>
<b>Figure 6-1. Fugitive and road dust vegetation scavenging factors gridded to the 3SAQS modeling domains</b>	<b>40</b>
<b>Figure 6-2. List of counties in the three-state study region where targeted emission improvements were made.</b>	<b>44</b>
<b>Figure 6-3. 3SAQS 2011 residential natural gas consumption monthly temporal profiles</b>	<b>46</b>
<b>Figure 6-4. Colorado roadway spatial data improvement plots. Left: TIGER 2010 Shapefile of urban/rural primary/secondary roads. Right: CO 2008 VMT-based roadways</b>	<b>46</b>
<b>Figure 6-5. Wyoming and Utah CAFO locations. Colorado CAFO locations developed from the NPS RoMANS study are also being used in the 3SAQS</b>	<b>47</b>
<b>Figure 8-1. Locations of FRM <math>\text{PM}_{2.5}</math> mass monitoring sites showing active and inactive (with black dot) sites (source: <a href="http://www.epa.gov/airquality/airdata/ad_maps.html">http://www.epa.gov/airquality/airdata/ad_maps.html</a>).</b>	<b>63</b>

<b>Figure 8-2. Locations of CSN speciated PM<sub>2.5</sub> monitoring sites (source: <a href="http://www.epa.gov/ttn/amtic/speciepg.html">http://www.epa.gov/ttn/amtic/speciepg.html</a>).</b>	<b>64</b>
<b>Figure 8-3. Locations of IMPROVE monitoring sites (source: <a href="http://vista.cira.colostate.edu/IMPROVE/">http://vista.cira.colostate.edu/IMPROVE/</a>)</b>	<b>65</b>
<b>Figure 8-4. Locations of CASTNet monitoring sites (source: <a href="http://epa.gov/castnet/javaweb/index.html">http://epa.gov/castnet/javaweb/index.html</a>).</b>	<b>66</b>
<b>Figure 8-5. Locations of NADP monitoring sites (source: <a href="http://nadp.sws.uiuc.edu/">http://nadp.sws.uiuc.edu/</a>).</b>	<b>67</b>
<b>Figure 8-6. Example model performance evaluation scatterplots for predicted and observed daily maximum 8-hour ozone concentrations using Excel (left) and July 2008 monthly averaged predicted and observed sulfate at all Colorado sites using AMET (right).</b>	<b>73</b>
<b>Figure 8-7. Example time series plots using AMET for O<sub>3</sub> at all Colorado AQS sites for July 2008 12 km CAMx modeling results (left) and using Excel for a CAMx 2008 4 km simulation and two sites in the Denver area.</b>	<b>74</b>
<b>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).</b>	<b>75</b>
<b>Figure 8-9. Example soccerplots comparing monthly PM<sub>2.5</sub> 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).</b>	<b>76</b>
<b>Figure 8-10. Example spatial distribution model performance evaluation displays showing 3SAQS CAMx 12-km daily max O<sub>3</sub> performance on July 19, 2008 using PAVE (top left); July 2008 monthly mean error for O<sub>3</sub> at different monitors using AMET (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).</b>	<b>77</b>
<b>Figure 8-11. Example plots comparing hourly July 2008 AQS O<sub>3</sub> for the 3SAQS 2008 CAMx application. A cumulative density function plot organizes the model and observations by the cumulative fraction of values below different concentration bins (left); a Q-Q plot displays an unpaired numerical sorting of the model results and observations (right).</b>	<b>78</b>

## 1.0 INTRODUCTION

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

The objectives of the 3SAQS are as follows:

- Create a standard modeling database in the Three State Data Warehouse (3SDW) for use in air quality planning including National Environmental Policy Act (NEPA) analyses in Colorado, Utah, and Wyoming.
- Engage oil and gas development stakeholders to participate in the NEPA process through contributing and reviewing model input data, modeling results, and technical support documentation
- Periodically evaluate the air quality impacts of all known proposed development projects in the three state region
- Provide a modeling platform to address the next generation of air quality issues including those related to oil and gas development, including ozone, PM (PM<sub>2.5</sub> and PM<sub>10</sub>, including both primary and secondary PM), visibility, nitrogen and sulfur (acid) deposition, air toxics, and greenhouse gases.

The goals of the 3SAQS include the following:

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

The 3SAQS started with the 2008 modeling year for assessing the impacts of oil and gas development on local and regional air quality. The year 2008 was selected for the 3SAQS to leverage work completed during the West-wide Jumpstart Air Quality Modeling Study ([WestJumpAQMS](#)). With the release of the year 2011 EPA National Emission Inventory (NEI), the availability of new ozone monitoring data in oil and gas basins in the three-state region, and updates to the oil and gas emission inventories, the 3SAQS is creating new 2011 base year modeling platform. Like in the 2008 3SAQS modeling platform, emission projections to the year 2020 will be used for estimating the impacts of development in future years using the 2011 modeling platform. This document is a Modeling Protocol for the 3SAQS meteorological, emissions and PGM modeling to develop a 2011 base year modeling platform that will be used for modeling the 2011 and 2020 base case emissions scenarios. The Modeling Protocol details the modeling inputs/outputs, modeling procedures, and evaluation procedures that will be used by the 3SAQS team for the 2011 and 2020 base-case modeling. This is the second draft of the 3SAQS 2011 Modeling Protocol. The first draft Modeling Protocol was dated April 2014. Based on comments received from the 3SAQS cooperators, a Response-to-Comments document was prepared and the Modeling Protocol was updated.

## 1.1 Background

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

## 1.2 Air Quality Standards and Air Quality Related Values

The United State (U.S.) Environmental Protection Agency (EPA) sets National Ambient Air Quality Standards (NAAQS) for six regulated air quality pollutants: ozone (O<sub>3</sub>), particulate matter (PM), sulfur dioxide (SO<sub>2</sub>), nitrogen dioxide (NO<sub>2</sub>), carbon monoxide (CO) and lead (Pb). After promulgation of a NAAQS, EPA designates nonattainment areas (NAAs) and States are required to submit State Implementation Plans (SIPs) to EPA that contain emission control plans and a demonstration that the NAA will achieve the NAAQS by the required date.

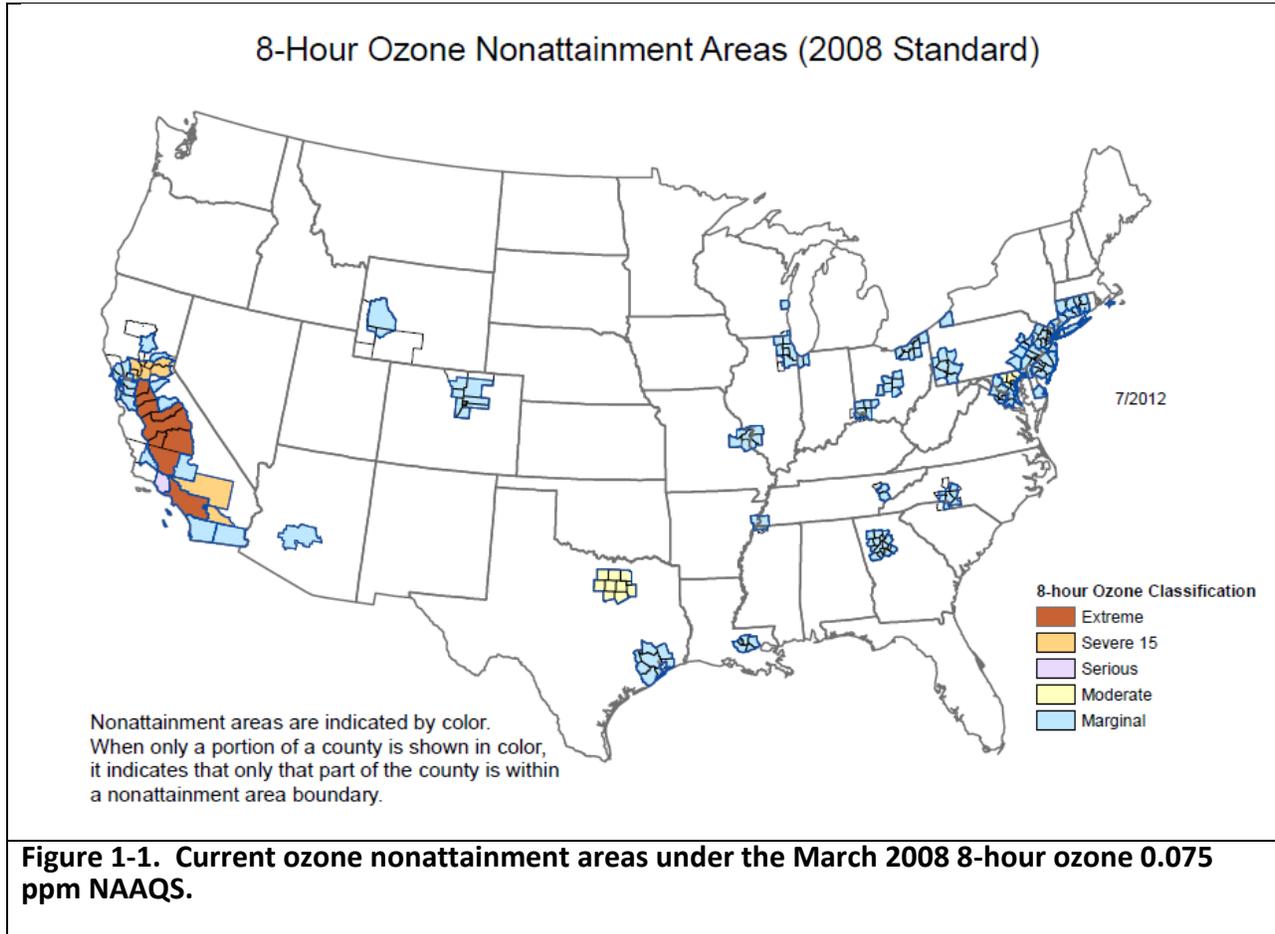
In 1997, EPA promulgated the first 8-hour ozone NAAQS with a threshold of 0.08 ppm (84 ppb). On March 12, 2008, EPA promulgated a more stringent 0.075 ppm (75 ppb) 8-hour ozone NAAQS. Figure 1-1 displays the locations of ozone nonattainment areas under the 2008 ozone NAAQS. EPA is currently re-evaluating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

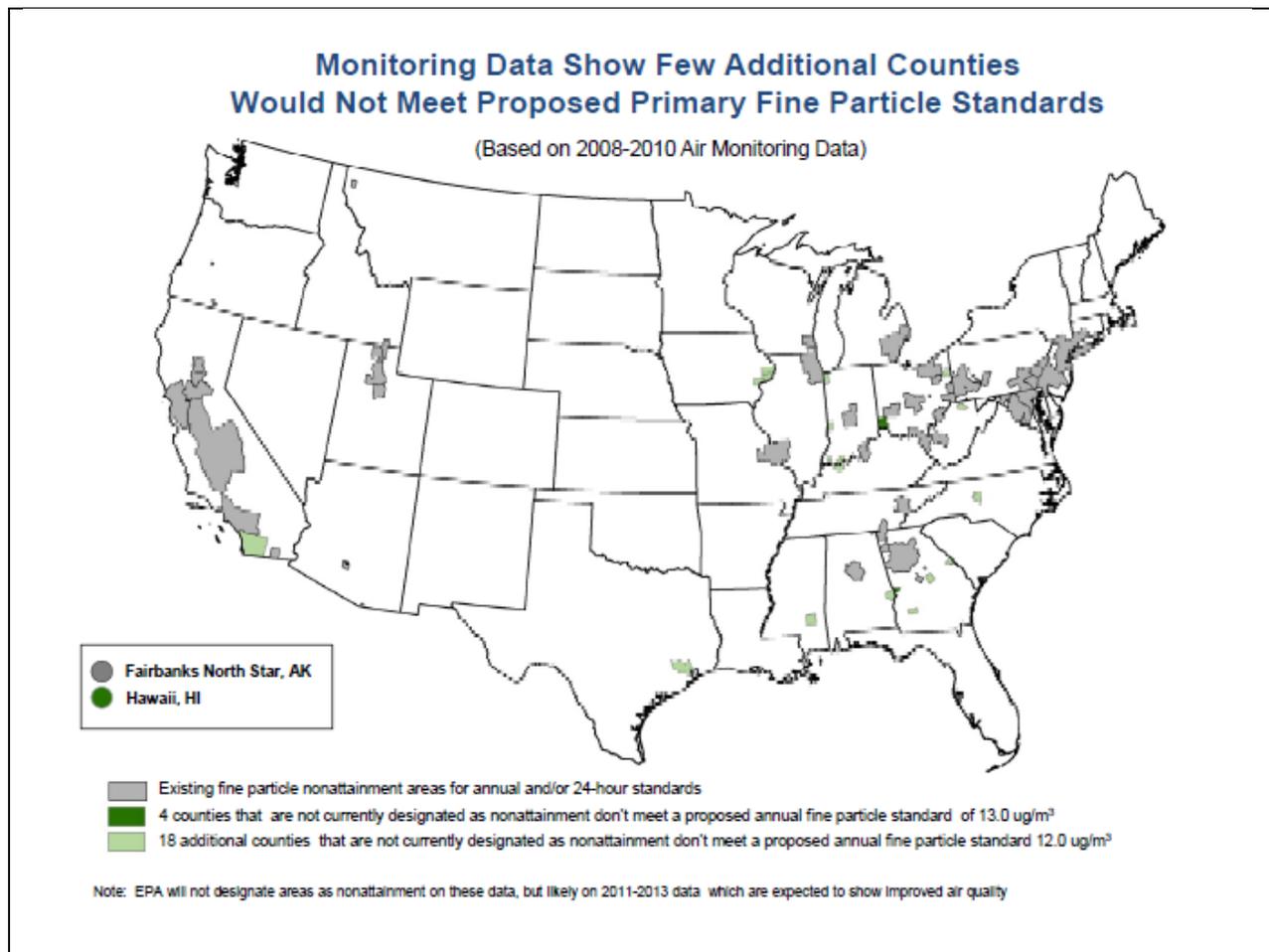
On December 14, 2012, EPA revised the [PM<sub>2.5</sub> primary NAAQS](#) by lowering the annual PM<sub>2.5</sub> NAAQS threshold from 15.0 µg/m<sup>3</sup> to 12.0 µg/m<sup>3</sup>. EPA is retaining the 24-hour PM<sub>2.5</sub> primary NAAQS at 35 µg/m<sup>3</sup>. The 24-hour coarse PM NAAQS (PM<sub>10</sub>) is also retained at 150 µg/m<sup>3</sup>. EPA considered the adoption of a secondary PM<sub>2.5</sub> NAAQS to protect against visibility impairment in urban areas with a proposed threshold in the 28 to 30 deciview range and an averaging time in the range of 4 to 24 hours. However, EPA determined that the 35

$\mu\text{g}/\text{m}^3$  24-hour  $\text{PM}_{2.5}$  secondary NAAQS provides visibility protection equal to or better than a 30 deciview (dv) standard. Figure 1-2 displays counties that are violating the old  $15.0 \mu\text{g}/\text{m}^3$  annual  $\text{PM}_{2.5}$  NAAQS and the additional counties that would violate a proposed  $13.0$  and the new  $12.0 \mu\text{g}/\text{m}^3$  annual  $\text{PM}_{2.5}$  NAAQS based on 2008-2010 measurements. There would be no new  $\text{PM}_{2.5}$  nonattainment counties in the western U.S. under the new annual  $\text{PM}_{2.5}$  NAAQS  $12 \mu\text{g}/\text{m}^3$  level based on 2008-2010 air quality observations.

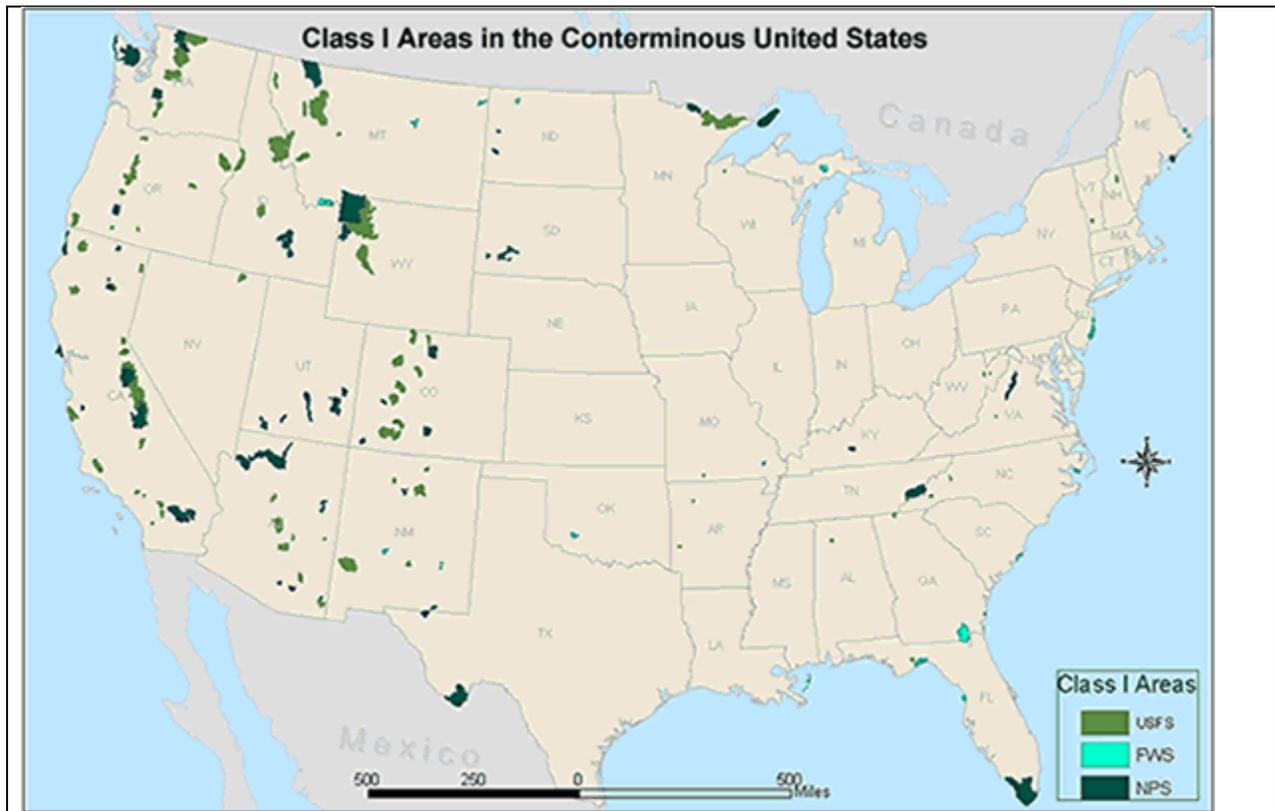
In February 2010, EPA issued a new 1-hour  $\text{NO}_2$  NAAQS with a threshold of 100 ppb and a new 1-hour  $\text{SO}_2$  NAAQS was promulgated in June 2010 with a threshold of 75 ppb. EPA has not yet designated the nonattainment areas for the 1-hour  $\text{NO}_2$  and 1-hour  $\text{SO}_2$  NAAQS. As of September 27, 2010 all NAAs for Carbon Monoxide have been redesignated as maintenance areas. A new lead NAAQS was issued in 2008 and, except for Los Angeles, all of the NAAs reside in the eastern or central U.S or Alaska.

The Clean Air Act Amendments (CAAA) designated 156 Class I areas consisting of National Parks and Wilderness Areas that are offered special protection for air quality and air quality related values (AQRVs). The Class I areas, compared to Class II areas, have lower Prevention of Significant Deterioration (PSD) air quality increments that new sources may not exceed, and are protected against excessive increases in several AQRVs including visibility impairment, acid (sulfur and nitrogen) deposition and nitrogen eutrophication. The Regional Haze Rule (RHR) has a goal of natural visibility conditions by 2064 at Class I areas, and States must submit RHR SIPs that demonstrate progress towards that goal. Figure 1-3 displays the locations of the 156 mandatory Class I areas, most of which are in the western U.S., including many in the states of Colorado, Utah and Wyoming.





**Figure 1-2. Counties that are violating the 1997 15.0  $\mu\text{g}/\text{m}^3$   $\text{PM}_{2.5}$  NAAQS and additional counties that would violate a 13.0  $\mu\text{g}/\text{m}^3$  (dark green) and the new December 2012 12.0  $\mu\text{g}/\text{m}^3$   $\text{PM}_{2.5}$  NAAQS based on 2008-2010 observations (source: <http://www.epa.gov/pm/actions.html#jun12>).**



**Figure 1-3. 156 mandatory Class I areas in the contiguous U.S.**

### 1.3 Organization of the Modeling Protocol

This document represents the 3SAQS Modeling Protocol for emissions and Photochemical Grid Model (PGM) modeling for the 2011 calendar year and 2020 future year emissions scenario. The year 2011 3SAQS meteorology data are documented in the 3SAQS 2011 WRF modeling protocol and performance evaluation reports (UNC and ENVIRON, 2014). Although the 3SAQS modeling analysis is not currently being performed to fill any particular regulatory requirement, such as a State Implementation Plan (SIP) attainment demonstration, EIA, or Resource Management Plan (RMP) as part of the National Environmental Policy Act (NEPA), it is being conducted with the same level of technical rigor as a SIP-type analysis and may ultimately be used as a basis for regulatory air quality modeling. This 3SAQS Modeling Protocol has the following sections:

1. Introduction: Presents a summary of the background, purpose and objectives of the study.
2. Model Selection: Introduces the models selected for the study
3. Episode Selection: Describes the modeling period for the study.
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 emissions input data, how the emissions modeling will be conducted, and the procedures for evaluating and validating the emissions processing results.
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. Website: web location for finding supporting project information
10. Acronyms: Definitions of acronyms used in this document
11. References: References cited in the document

## 1.4 Project Participants

The 3SAQS is conducted by the states of Colorado, Utah and Wyoming, several Federal agencies including National Park Service, (NPS), United States Forest Service (USFS), Fish and Wildlife Service (FWS), Bureau of Land Management (BLM) and Region 8 of the Environmental Protection Agency (EPA) as well as several contractors. The 3SAQS year 2011 and 2020 emissions and air quality modeling is being conducted by UNC and ENVIRON. Key contacts and their roles in the 3SAQS are listed in Table 1-1.

**Table 1-1. Key contacts for the 3SAQS 2011 modeling platform.**

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

## 1.5 Related Studies

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

### **1.5.1 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 may extend the program to the western U.S. The following is a list of federal regulatory actions that would likely lead to emission reductions in the western U.S.

- Tier 2 Vehicle Standards
- Heavy-duty Gasoline and Diesel Highway Vehicle Standards
- Non-Road Spark-ignition Engines and Recreational Engines Standards
- Large Non-Road Diesel Engine Rule
- Mercury and Air Toxics Standards (MATS)
- VOC MACT
- Federal Reformulated Gasoline
- Federal Non-Road Spark-Ignition Engines and Equipment
- Locomotive Engines and Marine Compression-Ignition Engines Final Rule
- Clean Air Act Title IV - Acid Rain Program
- Low-Sulfur Fuels
- Clean Air Visibility Rule (CAVR)
- Oil and Gas New Source Performance Standards (NSPS, August 16, 2012)

### **1.5.2 State Rulemakings that affect Oil and Gas Development Emissions**

State regulations have been implemented that would reduce emissions from oil and gas sources in the three-state region and result in improvements in air quality in the future. Table 1-2 below summarizes state rulemakings in the 3SAQS domain that affect oil and gas sources.

**Table 1-2. List of State Specific Oil and Gas Regulations by Source Category.**

Source Category	States Regulations			
	Colorado	New Mexico	Utah	Wyoming
Drill Rigs	<p><b>Reg. 3 Part A, I.B.31</b></p> <p>Requires Nonroad Engines &gt;1200 HP operating &gt;4380 Hr/Yr w/ 100 TPY NOx (40 TPY @ existing major source) to obtain a state permit w/ conditions to comply w/ CAAQS</p> <p>Nonroad Mobile Tier Standards take precedence</p>	-	-	<p>Wyoming has no separate state restrictions for temporary CI or SI-ICE</p> <p>Nonroad Mobile Tier Standards take precedence</p> <p>Wyoming has an Interim Policy for the GRB Ozone Non-Attainment area allowing operators to voluntarily permit temporary drill rig engines w/ BACT control in return for future emission credits</p>
Workover Rigs		-	-	
Well Completions	<p><b>COGCC HB-07-1341, Section 805.b(3)</b></p> <p>Green completions shall be used when technically and economically feasible. If not feasible, Best Management Practices shall be used</p>	NONE	NONE	<p><b>C6 S2 O&amp;G Permitting Guidance</b></p> <p>Wyoming has 4 area categories; 1) Concentrated Development Areas (CDA), 2) Upper Green River Basin (UGRB) 3) Jonah and Pinedale Anticline Development Area and Normally Pressured Lance (JPAD/NPL) &amp; 4) Statewide refers to all facilities not located in CDA, UGRB or JPAD/NPL</p> <p>Green completions are required in the JPAD/NPL area and CDA's in Wyoming as of July, 2014.</p>
Compression	NONE	NONE	NONE	NONE
Pneumatic Controllers	<p><b>Reg. 7, XVIII.C.1</b> No or low-bleed pneumatic devices required for all new &amp; existing applications.</p> <p><b>COGCC HB-07-1341, Section 805.b(2)E</b> No or low-bleed required for new, repaired or replaced devices where technically feasible</p>	NONE	NONE	<p><b>C6 S2 O&amp;G Permitting Guidance</b></p> <p>Install low or no-bleed at all new facilities. Upon modification of facilities, new pneumatic controllers must be low/no-bleed and within 60 days of modification, existing controllers must be replaced with no/low-bleed. (well site facilities only - not gas plants)</p>
Condensate & Crude Oil Tanks	<p><b>(Reg. 7, XII.G.2)</b> 95% VOC reduction @ gas processing plants if uncontrolled emissions from condensate tanks are <math>\geq</math> 2 tpy (only applies in ozone non-attainment areas)</p> <p><b>(Reg. 7, XVII.C)</b> 95% VOC</p>	NONE	<p><b>R307-327 Ozone Nonattainment Area</b></p> <p>Volatile Petroleum Liquid Tanks (&gt; 40,000 gallons, true vapor pressure [TVP] &gt; 1.52 psia at storage temperature) shall be controlled to minimize vapor loss. New tanks</p>	<p><b>C6 S2 O&amp;G Permitting Guidance</b></p> <p>Wyoming has 4 area categories; 1) Concentrated Development Areas (CDA), 2) Upper Green River Basin (UGRB), 3) Jonah and Pinedale Anticline Development Area and Normally Pressured Lance (JPAD/NPL) &amp; 4) Statewide refers to all facilities not located in CDA, UGRB or JPAD/NPL</p>

Source Category	States Regulations			
	Colorado	New Mexico	Utah	Wyoming
	<p>reduction for condensate storage tanks if uncontrolled emissions <math>\geq</math> 6 tpy (and if using a combustion device, the device must be designed to achieve 98% control)</p> <p><b>(Reg.. 7)</b> Storage tanks subject to system-wide controls in Section XII.D.2., and storage tanks with VOC emissions <math>\geq</math> 6 tpy to develop and employ Storage Tank Emission Management (“STEM”) plans to meet the “operate without venting” standard, which includes Approved Instrument Monitoring Method (“AIMM”) inspections. <b>(COGCC HB-07-1341,</b> Section 805.b(2)A) 95% VOC reduction for liquids condensate &amp; crude oil tanks if uncontrolled emissions <math>\geq</math> 5 tpy within 1/4 mile of an affected building (applies only to Garfield, Mesa &amp; Rio Blanco Counties)</p>		<p>shall be fitted with an internal floating roof resting on the liquid surface with the space (roof edge to tank wall) sealed.</p> <p>Owner/operator shall maintain records of the liquid type/maximum TVP. Records required of average monthly storage temperature, the liquid type, throughput and maximum TVP for tanks not subject to above (petroleum liquid TVP &gt; 1.0 psia)</p>	<p><b>JPAD/NPL</b> - 98% control of all new/modified tank emissions upon startup/modification</p> <p><b>CDA</b> PAD Facilities- 98% control upon startup/modification</p> <p>Single Well Facilities - 98% control of all new/modified tank emissions <math>\geq</math>8 tpy VOC within 60 days of startup/modification</p> <p><b>Statewide</b> 98% control of all new/modified tank emissions <math>\geq</math>10 tpy VOC within 60 days of startup/modification</p> <p><b>UGRB</b> PAD Facilities- 98% control upon startup/modification</p> <p>Single Well Facilities - 98% control of all new/modified tank emissions <math>\geq</math>4 tpy VOC within 60 days of startup/modification</p>
Gas Processing Plants	<p>Colorado has adopted NSPS Subpart KKK on LDAR under <b>Reg. 7, XII.G.1</b> (KKK applies at gas processing plants located in ozone non-attainment areas regardless of the date of construction of the affected facility)</p>	<p>New Mexico has adopted NSPS Subpart KKK on LDAR</p>	<p>Utah has adopted NSPS Subpart KKK on LDAR</p>	<p>Wyoming has adopted NSPS Subpart KKK on LDAR</p>
Glycol Dehydrators	<p><b>Reg. 7, XII.H and XVII.D</b> 95% reduction of VOCs where uncontrolled emissions &gt;2 tpy (and if using combustion device, the device must be designed to achieve 98% control). Glycol natural gas dehydrators</p>	NONE	NONE	<p><b>C6 S2 O&amp;G Permitting Guidance</b> Wyoming has 4 area categories; 1) Concentrated Development Areas (CDA), 2) Upper Green River Basin (UGRB) 3) Jonah and Pinedale Anticline Development Area and Normally Pressured Lance (JPAD/NPL) &amp; 4) Statewide refers to all facilities not located in CDA, UGRB or</p>

Source Category	States Regulations			
	Colorado	New Mexico	Utah	Wyoming
	<p>constructed before May 1, 2015, with VOC emissions greater than 6 tpy, or 2 tpy if located within 1,320 feet of a building unit or designated outside activity area, to control by 95% (and similarly meet a 98% design control efficiency) <b>COGCC HB-07-1341</b>, Section 805.b(2)C) 90% reduction of VOCs required where uncontrolled VOC emissions ≥ 5 tpy within 1/4 mile of an affected building (applies only to Garfield, Mesa &amp; Rio Blanco Counties)</p>			<p>JPAD/NPL</p> <p><b>JPAD/NPL</b> 98% control of all new/modified dehydrator VOC/HAP emissions at start up</p> <p><b>CDA &amp; Statewide</b> PAD Facilities - 98% control upon startup/modification</p> <p>SINGLE Well Facilities - 98% control within 60 days of startup/modification for VOC emissions ≥6 OR 98% control within 30 days of startup/modification for VOC emissions ≥8 tpy</p> <p><b>UGRB</b> PAD Facilities - 98% control upon startup/modification</p> <p>SINGLE Well Facilities - 98% control within 60 days of startup/modification for VOC emissions ≥4 tpy</p>
Minor Source Permitting	<p><b>Reg. 3 Part B, II.D</b> Minor Source permitting required for sources with thresholds that vary by pollutant and area (generally required in non-attainment areas for criteria emissions &gt; 1-5 tpy – required statewide for criteria emissions &gt; 5-10 tpy – thresholds depend on the pollutant)</p>	<p><b>20.2.72 NMAC</b> requires permits for all sources &gt;25 tpy of a criteria pollutant. <b>20.2.73 NMAC</b> requires Notices of Intent for all sources &gt;10 tpy of a criteria pollutant</p>	<p><b>UAC Rule 307-401-9</b> NSR permitting exempted for sources with controlled emissions below de minimis levels: PTE&lt; 5 tpy each PM10, NOx, SOx, CO, VOCs, or single HAP &lt; 500 lbs per year, combined HAP &lt; 1 tpy</p>	<p>Emissions from minor sources must be approved through permitting applied through the WAQSR <b>Chapter 6 Section 2(a)(i) O&amp;G Permitting Guidance</b>. For VOC emissions ≥8 tpy from sources other than tanks, dehydrators, pneumatic controllers and pumps, water tanks, BACT is considered on case-by-case basis.</p>
Point Source Permitting Threshold	<p>Colorado has a 10 TPY permitting threshold (5 TPY in non-attainment areas) but sources don't undergo BACT analysis unless the source reaches PSD emission levels</p>	<p>Sources &gt; 25 TPY permitting threshold undergo BACT analysis</p>	<p>Sources &gt; 5 TPY permitting threshold undergo BACT analysis</p>	<p>Wyoming has no de minimus permitting threshold outside of their <b>C6 S2(k)</b> exemptions, thus all sources not waived by the Administrator are permitted and undergo BACT analysis</p>

Source Category	States Regulations			
	Colorado	New Mexico	Utah	Wyoming
Pneumatic Pump	NONE	NONE	NONE	<p><b>C6 S2 O&amp;G Permitting Guidance</b> Wyoming has 4 area categories; 1) Concentrated Development Areas (CDA), 2) Upper Green River Basin (UGRB) 3) Jonah and Pinedale Anticline Development Area and Normally Pressured Lance (JPAD/NPL) &amp; 4) Statewide refers to all facilities not located in CDA, UGRB or JPAD/NPL</p> <p><b>JPAD/NPL</b> - 98% control of all new/modified pneumatic pump VOC/HAP emissions at startup/modification or the pump discharge streams shall be routed into a closed loop system at startup/modification</p> <p><b>CDA &amp; Statewide</b> PAD Facilities - pneumatic pumps shall be controlled by at least 98% or the pump discharge streams shall be routed into a closed loop system at startup/modification</p> <p>SINGLE Well Facilities - 98% control within 60 days of startup/modification for sites with combustion units installed OR solar, electric or air-driven pumps for sites without combustion units installed</p> <p><b>UGRB</b> 98% control of all new/modified facilities at startup/modification or the pump discharge streams shall be routed into a closed loop system at startup/modification.</p>

### 1.5.3 2008 Denver Ozone SIP Modeling

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

demonstrate that the DMA/NFR region would attain the 1997 8-hour ozone NAAQS by 2010. Details on the 2008 Denver 8-hour ozone SIP modeling can be found at:

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

#### **1.5.4 Denver Modeling of a 2008 Episode**

The Denver RAQC conducted modeling using WRF meteorological, SMOKE emissions and CAMx photochemical grid models for the same 2008 modeling year as used by 3SAQS only for just the May through August ozone season of the 3SAQS 2008 modeling year. As in the 2008 Denver Ozone SIP, on-road mobile sources in the Denver area were estimated using CONCEPT MV with link-based TDM data, except the MOVES mobile source emissions factor model was used instead of MOBILE6. The Modeling Protocol and preliminary model performance evaluation (MPE) results for the current 2008 Denver ozone modeling can be found at:

[http://www.ozoneaware.org/postfiles/documentsandpresentations/modeling/documents/Denver\\_Model\\_Protocol\\_Draft3\\_080211.pdf](http://www.ozoneaware.org/postfiles/documentsandpresentations/modeling/documents/Denver_Model_Protocol_Draft3_080211.pdf)

[http://raqc.org/postfiles/ozone\\_modeling/modeling\\_forum/Denver\\_2008\\_Prelim\\_MPE\\_080912.pdf](http://raqc.org/postfiles/ozone_modeling/modeling_forum/Denver_2008_Prelim_MPE_080912.pdf)

The Denver RAQC is moving toward using a 2011 modeling platform and plan to leverage the 3SAQS.

#### **1.5.5 WRAP Regional Modeling Center Modeling**

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

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

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

<http://www.wrapair.org/>

<http://www.wrapair2.org/>

#### **1.5.6 Four Corners Air Quality Task Force**

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

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

### **1.5.7 Environmental Impact Statements (EISs) and Resource Management Plans (RMPs)**

Photochemical grid models are also being applied in the Rocky Mountain States as part of the development of Environmental Impact Statements (EISs) for oil and gas development projects and Resource Management Plans (RMPs) for Bureau of Land Management (BLM) Field Offices. Most of these EIS/RMP studies have been or are being performed by the BLM under the National Environmental Policy Act (NEPA), although the United States Forest Service (USFS) and Tribes have also led some EISs. The main focus of these activities is on the air quality and air quality related value (AQRV; i.e., visibility and deposition) impacts due to oil and gas development activities, although RMPs can also address mining, grazing, off-highway vehicles and other activities. Such EIS/RMP activities have occurred or are undergoing air quality modeling for projects in Colorado, New Mexico, Utah and Wyoming with more information found on the BLM websites:

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

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

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

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

The most recently completed BLM oil and gas EIS is the Continental Divide-Creston gas infill development project in southwest Wyoming centered on the town of Wamsutter. The CD-C used a 2005 and 2006 modeling platform. The CD-C draft EIS was released in December 2012 and is available at:

[http://www.blm.gov/wy/st/en/info/NEPA/documents/rfo/cd\\_creston.html](http://www.blm.gov/wy/st/en/info/NEPA/documents/rfo/cd_creston.html)

### **1.5.8 RoMANS**

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

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

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

### **1.5.9 WestJumpAQMS**

The West-wide Jump-start Air Quality Modeling Study (WestJumpAQMS) conducted meteorological, emissions and photochemical grid modeling of the western U.S. for the 2008 calendar year to investigate source-receptor relationships for ozone, particulate matter, visibility and deposition. WRF meteorological and SMOKE emissions modeling was conducted for a 36 km continental U.S., 12 km western U.S., and 4 km inter-mountain west domain. Ozone and PM source apportionment modeling was also conducted with CAMx to examine state-specific and source category-specific air quality impacts. The WestJumpAQMS 2008 36/12 km modeling platform was adapted by 3SAQS for their preliminary modeling using the 2008 year. Details on the WestJumpAQMS can be found at:

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

### 1.5.10 2008 3SAQS Modeling

Year 2008 emissions and PGM modeling was conducted for the 3SAQS to provide initial results to use in near-term NEPA modeling analyses. The WRF meteorological input data for the PGM simulations were taken directly from the WestJumpAQMS. The majority of the SMOKE emissions input data were also taken from the WestJumpAQMS with the exception of the on-road mobile sector where 3SAQS used SMOKE-MOVES as compared to running MOVES in the inventory mode in WestJumpAQMS. The 3SAQS 2008 emissions also included targeted ancillary data improvements for some inventory sectors, including livestock ammonia, non-point, and residential wood combustion. PGM modeling for the 3SAQS 2008 modeling platform was conducted for a 36 km continental U.S. and a 12 km western U.S. domains. These data are being distributed to cooperators in the 3SAQS via the Three-State Data Warehouse (3SDW). Details on the 3SAQS and 3SDW can be found at:

<http://vista.cira.colostate.edu/tsdw>

## 1.6 Overview of 3SAQS 2011 Modeling Approach

The procedures for the 3SAQS 2011 modeling will follow those performed for the 2008 3SAQS and WestJumpAQMS modeling and include updated meteorology, emissions, and PGM input data. Unlike the 3SAQS 2008 modeling platform, which only included 36 and 12 km modeling domains, the 3SAQS 2011 modeling platform will include 36, 12 and 4 km modeling domains. The 3SAQS 2011 4 km domain was designed to encompass the entirety of Colorado, Utah, and Wyoming. The 3SAQS 2011 modeling data will be used to run and evaluate the CMAQ and CAMx PGMs, conduct source apportionment modeling and perform targeted sensitivity tests including for wintertime elevated ozone events. These extensions to the standard 2011 modeling platform will be explored following an initial model performance evaluation of the base 2011 modeling. A summary of the 3SAQS 2011 modeling approach is given below, with more details provided in the chapters of this modeling protocol.

- The 2011 calendar year was selected for the 3SAQS emissions modeling period.
- Year 2011 and 2020 inventories will be used to estimate base and future year emissions for the 3SAQS
- A 36 km continental U.S. (CONUS) domain, 12 km western U.S. (WESTUS) domain, and 4 km three-state domain will be used.
- Year 2011 Weather Research Forecasting (WRF) modeling results generated by the 3SAQS are being used to provide meteorology inputs for the 3SAQS 2011 PGM modeling platform.
- Emissions modeling is primarily conducted using the Sparse Matrix Operator Kernel Emissions ([SMOKE](#)) modeling system using mainly emissions data from the EPA 2011-based modeling platform ([2011v6](#)).
- Photochemical grid modeling is based on the Comprehensive Air-quality Model with extensions ([CAMx](#)) version 6.10 and the Community Multiscale Air Quality ([CMAQ](#)) modeling system version 5.0.2. The Carbon Bond 6 revision 2 ([CB6r2](#)) photochemical mechanism with active local methane emissions and chemistry will be used for the 3SAQS CAMx 2011 modeling. If the CB6r2 chemical mechanism is not available in CMAQ at the time of the CMAQ modeling, then the CB05 chemical mechanism will be used with CMAQ.
- Day-specific Boundary conditions (BCs) for the lateral boundaries of the 36 km CONUS domain are initially based on the MOZART global chemistry model (GCM). Sensitivity tests using BCs based on an alternative GCM will be performed if available.

- Model evaluation is being conducted for ozone, particulate matter (PM) mass and speciation and ozone and PM precursor and product species as well as for visibility and deposition.
- Diagnostic sensitivity tests will be conducted to determine sensitivity of the PGM model estimates to key parameters. The PGM diagnostic sensitivity tests will be developed with consultation of the 3SAQS technical committee.

## 2.0 MODEL SELECTION

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

- Technical formulation, capabilities and features;
- Pertinent peer-review and performance evaluation history;
- Public availability; and
- Demonstrated success in similar regulatory applications.

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

### 2.1 Justification and Overview of Selected Models

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

- Meteorological Models (MM)
- Emissions Models (EM)
- Photochemical Grid Models (PGM)

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

#### 2.1.1 Meteorological Model

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

- The fifth generation Mesoscale Model (MM5); and
- The Weather Research Forecasting (WRF) model.

Both MM5 and WRF were developed by the community with the National Center for Atmospheric Research (NCAR) providing coordination and support. For many years the MM5 model was widely used by both the meteorological research as well as the air quality modeling community. Starting around the year 2000, the WRF model started to be developed as a technical improvement and replacement to MM5 and today NCAR no longer supports MM5. The 3SAQS is using 2011 meteorology fields developed by 3SAQS. Based on the four selection criteria, the WRF was selected as the 3SAQS 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:** 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 than MM5. WRF is amassing a rich publication and application history.
- **Public Availability:** WRF is publicly available and can be downloaded from the WRF website with no costs or restrictions. MM5 is also publicly available.
- **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:** The non-hydrostatic version of the Advanced Research version of the Weather Research Forecast (WRF-ARW<sup>1</sup>) 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 Processing Systems

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

- [Sparse Matrix Operator Kernel Emissions \(SMOKE\) processor, version 3.0](#) – software system that prepares emission inventory data for input to a PGM; primary functions include spatial, temporal, and chemical conversion of emission inventory data to the terms required by a PGM
- [Model of Emissions of Gases and Aerosols from Nature \(MEGAN\), version 2.10 \(Guenther et al., 2012\)](#) – biogenic emissions model; primary function is to estimate gridded gas-phase emissions from plants and soils
- WRAP Windblown Dust Model ([WRAP-WBD](#); Mansell et al., 2006) - software to estimate wind-driven dust emissions

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<sup>1</sup> All references to WRF in this document refer to the WRF-ARW

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

- The Consolidated Community Emissions Processing Tool (CONCEPT);
- The Emissions Modeling System (EMS); and
- The Sparse Matrix Operator Kernel Emissions (SMOKE) system.

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

- Technical: SMOKE is undergoing the most active development and updates of all of the three processors listed above. It is updated annually to add new capabilities and features and to address bugs and inefficiencies. SMOKE is widely used for regulatory modeling studies and is the only emissions processor in use by EPA.
- Performance: SMOKE is designed to be efficient in how it processes large quantities of data. It has been used in countless research and regulatory studies worldwide and is most likely the emissions processor in recently published regional modeling studies that used either the CMAQ or CAMx PGM.
- Public Availability: SMOKE is publicly available and can be downloaded from the Community Modeling and Analysis System Center with no costs or restrictions.
- Demonstrated Success: The RoMANS study, Denver 2008 SIP modeling, all of the EIS projects that used CMAQ or CAMx, and the WestJumpAQMS all used SMOKE for preparing the PGM emissions. While some of the deficiencies in the model performance in all of these studies may be partially traced to flaws in the emissions data, SMOKE has proven to be a reliable system for processing the data into the gridded hourly and chemically speciated emission inputs needed for PGM modeling.

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

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

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

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

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

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

**MOVES:** The MOrtor 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 current version is MOVES2010b that was released 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. Note that a new version of MOVES is scheduled to be released in July 2014. MOVES2014 will include the new light duty vehicle Tier 3 tailpipe standards and fuels starting in 2017 and other regulations as well as other changes. Because it wasn't available when emissions processing needed to be performed, MOVES2014 will not be used for this round of 3SAQS 2011 and 2020 modeling, but may be added to the study in the future.

**MEGAN:** The Model of Emissions of Gases and Aerosols in Nature ([MEGAN](#)) is a modeling system for estimating the net emission of gases and aerosols from terrestrial ecosystems into the atmosphere (Jiang et al., 2012; Wiedinmyer, Sakulyanontvittaya and Guenther, 2007). 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).

### 2.1.3 Photochemical Grid Model

There are two PGMs that are widely used for ozone, PM<sub>2.5</sub> 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<sub>2.5</sub>, air toxics, visibility and other air quality issues within a single platform. CMAQ has some more recent treatment in its aerosol modules, whereas CAMx has a more recent gas-phase photochemical mechanism.

- **Technical:** Both CMAQ and CAMx represent state-of-science one-atmosphere PGMs. Both models were selected for use in the 3SAQS. CAMx was selected for the initial 3SAQS applications because it supports two-way grid nesting; a feature needed for the 3SAQS source apportionment modeling that is not present in CMAQ.
- **Performance:** A peer-review of the CAMx and CMAQ source apportionment algorithms found CAMx to be technically and operationally superior to CMAQ. CAMx also tends to run a little faster than CMAQ.
- **Public Availability:** CMAQ and CAMx are both publicly available.
- **Demonstrated Success:** Both CMAQ and CAMx have had many successful model performance applications. CAMx has been applied more frequently in the Rocky Mountain region for NEPA studies and the Denver ozone SIP modeling.

The CAMx and CMAQ models are summarized below.

**CAMx:** 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, 2014). 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<sub>2.5</sub> and PM<sub>10</sub> 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<sub>x</sub> SIP Call, etc.).

**CMAQ:** 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.

The CAMx PGM will initially be applied in the 3SAQS project. To take advantage of the active methane chemistry in the CB6r2 photochemical mechanism, CAMx Version 6.10 (April 2014) will be used for the initial 3SAQS modeling. CMAQ will be applied as part of the 2015 3SAQS work effort starting in October 2014. The WRF meteorological model Version 3.5.1 (September 2013) was applied for the 2011 modeling episode and grid structure. The WRF output was processed using the WRFCAMx program to generate meteorological inputs for the CAMx model.

Boundary Conditions (BCs) for the 36 km CONUS domain are based on output from a global chemistry model (GCM). The current plan is to initially use results from the MOZART GCM. Sensitivity tests using an alternative GCM (e.g., GEOS-Chem) are planned to be performed if GCM output for 2011 are available. The interaction between the GCM with the regional models (CAMx and CMAQ) is performed through processors that perform the following activities:

- For each BC horizontal grid cell in the 36 km CONUS domain, identify the appropriate grid cell of the GCM where it resides.
- Mass consistent interpolation GCM species in the GCM vertical layer structure to the vertical layer structure used by CAMx/CMAQ.
- Mapping of species in the GCM chemical mechanism to the species used in CAMx or CMAQ.

### 3.0 EPISODE SELECTION

EPA's ozone, PM<sub>2.5</sub> and visibility SIP modeling guidance (EPA, 2007) contains recommended procedures for selecting modeling episodes, while also referencing EPA's 1-hour ozone modeling guidance for episode selection (EPA, 1991). This Chapter presents the modeling period selected for performing the 3SAQS and the justification and rationale for its selection.

#### 3.1 Episode Selection Criteria

EPA's modeling guidance lists primary criteria for selecting episodes for ozone, PM<sub>2.5</sub> 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<sub>2.5</sub> 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<sub>2.5</sub> exceedances in the western U.S.;
2. Choose episodes having days with monitored 8-hour daily maximum ozone and 24-hour PM<sub>2.5</sub> concentrations close to the ozone and PM<sub>2.5</sub> 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 or PM<sub>2.5</sub> 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<sub>2.5</sub> 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<sub>2.5</sub> Design Value projections.

#### 3.2 Episode Selection Results

The 2011 calendar year was selected for the 3SAQS modeling because it satisfied more of the episode selection criteria listed above than other recent years:

1. Modeling the entire year of 2011 will capture a variety of conditions that lead to elevated ozone and PM<sub>2.5</sub> concentrations in the western U.S., including wintertime ozone formation

2. There is some special study data in 2011, including ozone and precursor measurements in oil and gas development basins through the three-state region. 2011 is also a National Emissions Inventory (NEI) update year and the NEI is an important database required for modeling.
3. An annual simulation will assure sufficient days are available to analyze ozone and PM<sub>2.5</sub> 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.
4. 2011 is being used for other studies including several BLM Environmental Impact Statements (EISs) and Resource Management Plans (RMPs).
5. With an annual run, all weekend days in a year are included.

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<sub>2.5</sub>, 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, initial model simulations will not be configured to simulate the winter ozone events. However, as part of the 3SAQS 2015 work effort starting in October 2014, focused WRF meteorological and PGM sensitivity tests will be performed to simulate the winter ozone exceedance events during 2011 in the Uinta Basin, Utah and the Jonah-Pinedale Anticline Development (JPAD) area in southwest Wyoming. These focused sensitivity tests will include configuring WRF for simulating cold pooling and use of measured high snow cover albedo in the PGM modeling.

## 4.0 DOMAIN SELECTION

This Chapter summarizes the model domain definitions for the 3SAQS 2011 photochemical grid modeling (PGM), including the domain coverage, resolution, map projection, and nesting schemes for the high resolution sub-domains. The modeling domains for the WRF meteorological modeling are defined slightly larger than the PGM domains and are given in Chapter 5 with more details provided in the 3SAQS WRF Application/Evaluation Report (UNC and ENVIRON, 2014).

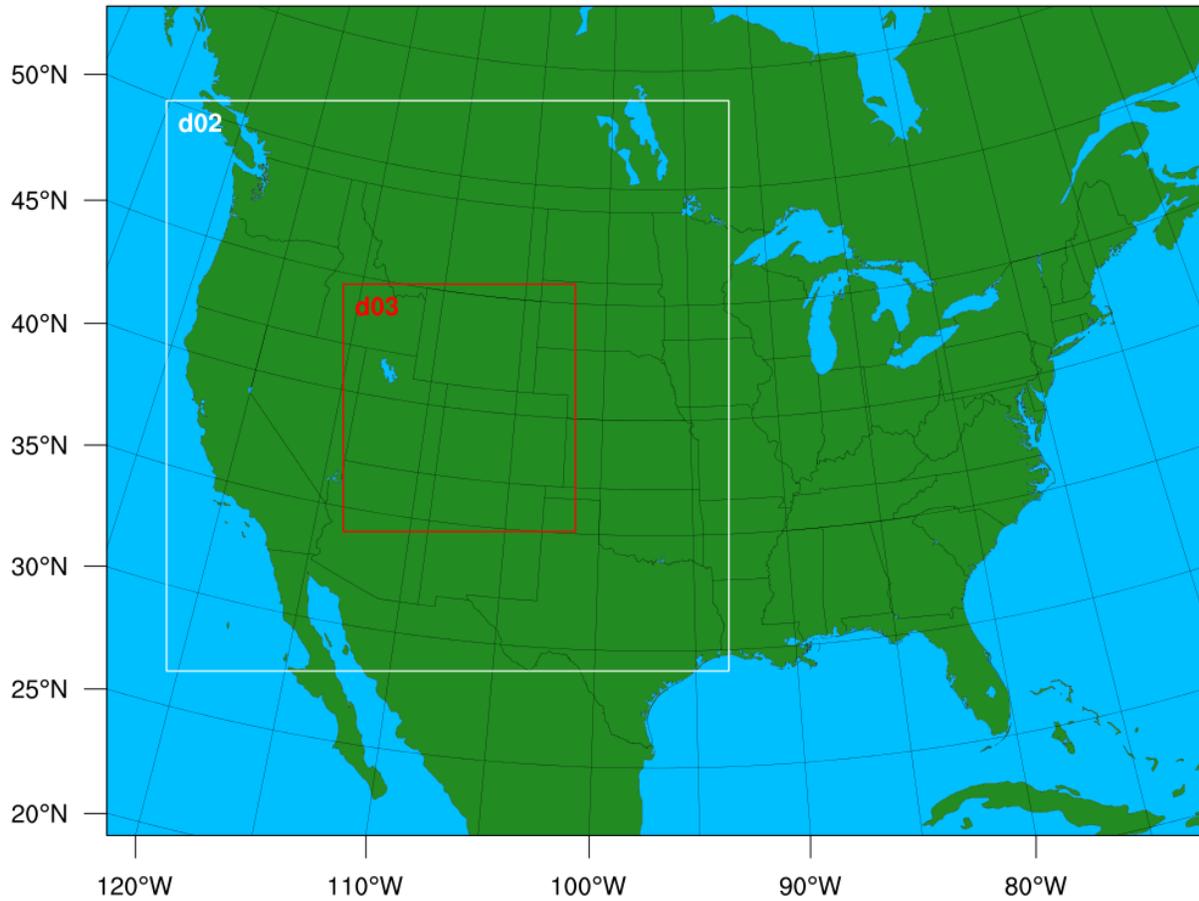
### 4.1 Horizontal Modeling Domain

The 3SAQS modeling domains were selected as a trade-off between the need to have high resolution modeling for sources in the Inter-Mountain West versus ability to perform regional ozone and particulate matter source apportionment modeling among all of the western states. The 3SAQS 2011 modeling used 36, 12 and 4 km domains. The WRF meteorological model requires use of an odd nesting ratio so the 36/12/4 km domains are using a 3:1 grid-nesting ratio. A Lambert Conformal Projection (LCP) was used for the 3SAQS 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.
- A 4 km three-state (3SAQS) domain focuses on the states of Colorado, Utah, and Wyoming.

Figure 4-1a displays the 36 km CONUS, 12 km WESTUS, and 4 km 3SAQS modeling domains and the definition of their extent. The SMOKE and MEGAN emissions and PGM modeling will be conducted on the 36/12/4 km domain grid structure shown in Figure 4-1a. The 3SAQS 4 km modeling domain is shown in Figure 4-1b along with the locations of Class I and sensitive Class II areas and oil and gas wells that were operating in 2011.

## 3SAQS 36/12/04km CAMx Domains



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

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

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

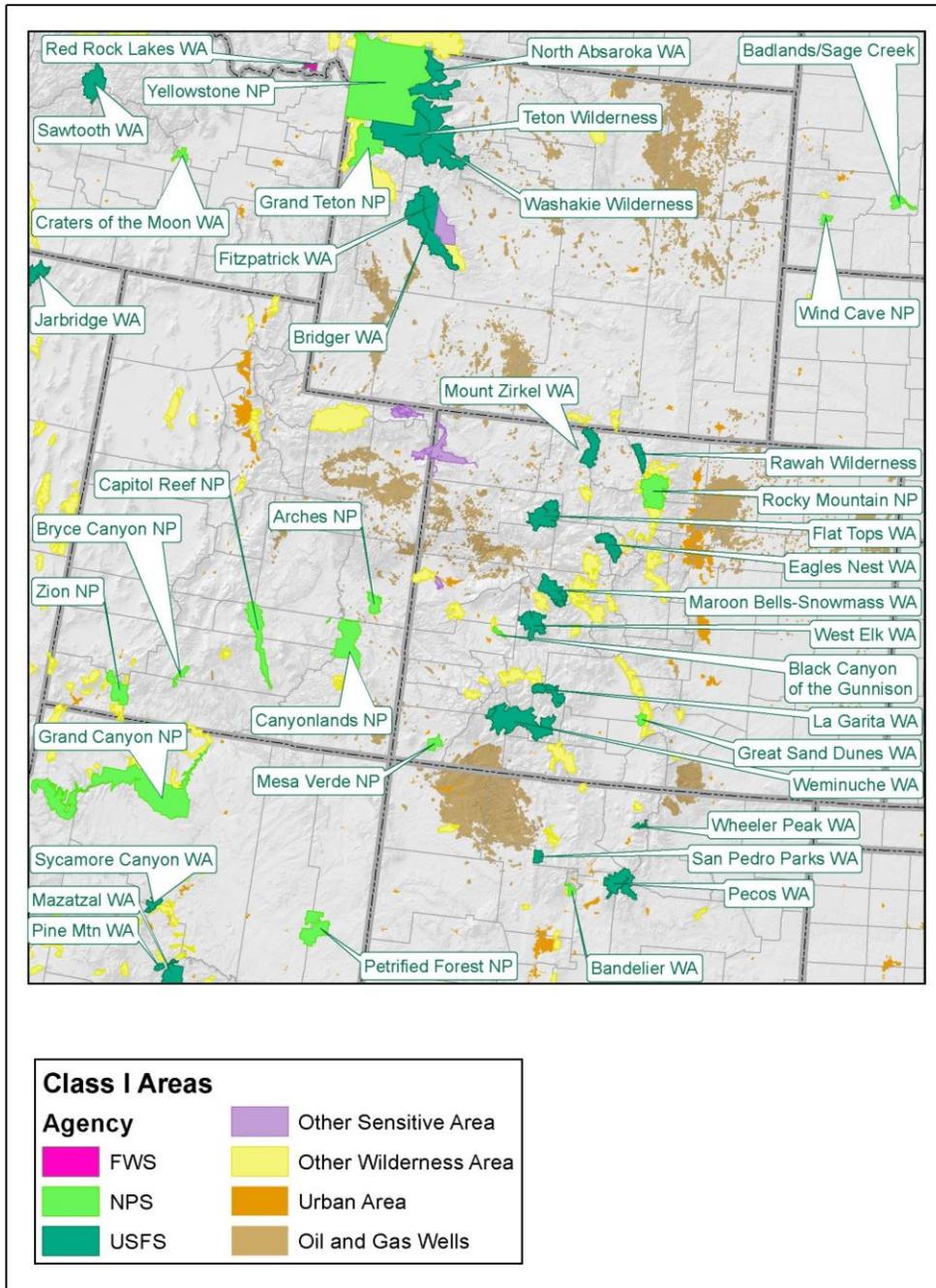


Figure 4-1b. 3SAQS 2011 4 km modeling domain showing locations of Class I areas (labeled), sensitive Class II areas (unlabeled), urban areas and 2011 oil and gas wells.

## 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) (UNC- and ENVIRON, 2014). 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/CMAQ layer to reduce the air quality model computational time. Table 4-3 displays the approach for collapsing the WRF 36 vertical layers to 25 vertical layers in CAMx. In previous modeling for WRAP and the 2008 Denver ozone SIP, 19 vertical layers were used that resulted in some very thick vertical layers near the top of the modeling domain that contributed to the too rapid transport of high ozone concentrations of stratospheric ozone origin to the ground (Emery et al., 2009a,b).

The WRF layer collapsing scheme in Table 4-2 is collapsing two WRF layers into one CAMx layer for the lowest four layers in CAMx. In the past, the lowest layers of MM5/WRF were mapped directly into CAMx with no layer collapsing. However, in those applications the MM5/WRF layer 1 was much thicker (20-40 m) than used in this WRF application (12 m). Use of a 12 m lowest layer may trap emissions in a too shallow layer resulted in overstated surface concentrations. For example, NO<sub>x</sub> emissions are caused by combustion so are buoyant and have plume rise that in reality could take them out of the first layer if it is defined too shallow. However, there is concern that layer collapsing of the lowest WRF layers may introduce uncertainties or errors in the modeling. However, use of a 12 m WRF surface layer will facilitate the WRF and PGM modeling of the winter ozone cold pooling events where higher horizontal and vertical resolution is needed.

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

**Table 4-2. 37 Vertical layer interface 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 2011 calendar year using a 36/12/4 km domain structure. The WRF modeling results for the 2011 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 (UNC-IE and ENVIRON, 2012). The WRF precipitation fields were also compared against analysis fields that were based on observations using the Parameter-elevation Relationships on Independent Slopes Model ([PRISM](#)). Snow cover will be evaluated against the Snow Data Assimilation System ([SNODAS](#)) data.

### 5.1 Model Selection and Application

The 3SAQS 2011 modeling is using meteorology fields simulated by WRF version 3.5.1. 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 nested 36/12/4-km domains depicted in Figure 4-1 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 3SAQS with the WRF 37 vertical layer structure presented previously in Table 4-2. The outer 36 km domain (D01) has 165 x 129 grid cells, selected to be consistent with existing Regional Planning Organization (RPO) and EPA modeling CONUS domain. The projection is Lambert Conformal with the "national RPO" grid projection pole of 40°, -97° with true latitudes of 33° and 45°. The 12 km domain has 256 x 253 grid cells with offsets from the 36 km grid of 15 columns and 26 rows. The 4 km domain has 301 x 361 grid cells with offsets from the 12 km grid of 75 columns and 55 rows. The nests were run together with continuous updating without feedback from the 12 km to 36 km or from the 4 km to 12 km domains.

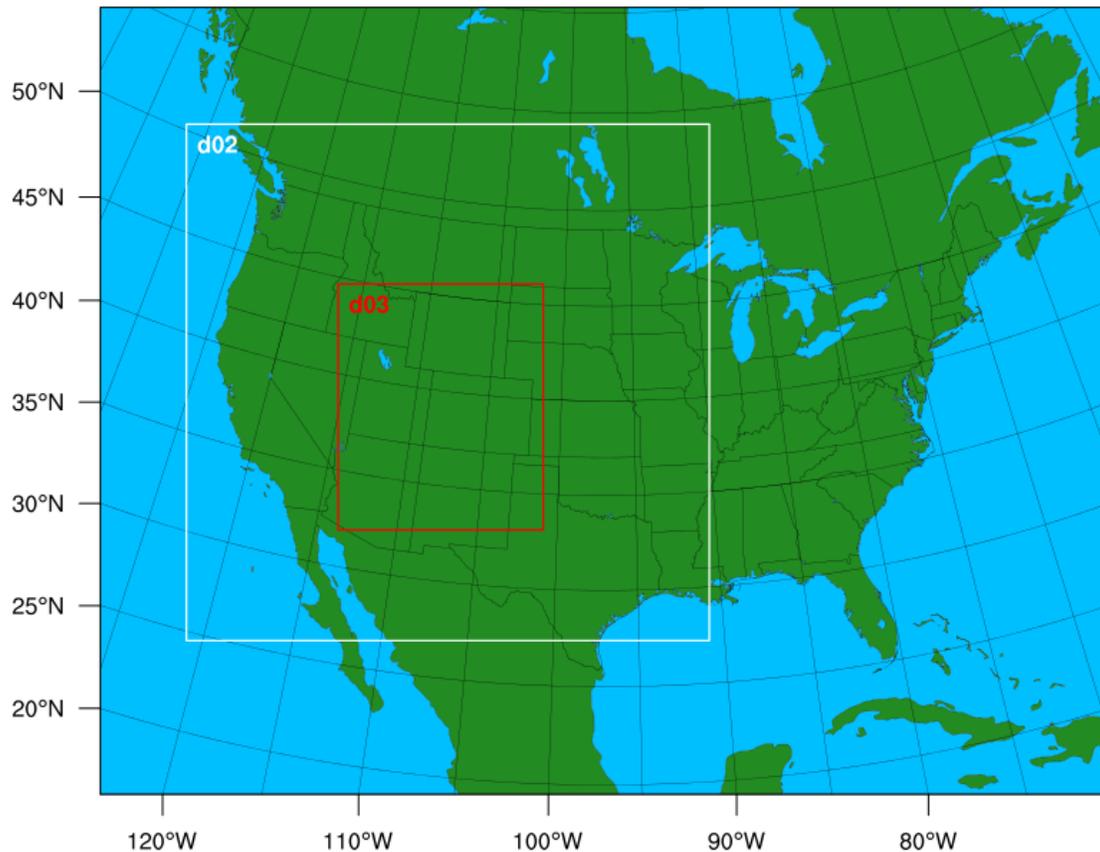
### 5.3 Topographic Inputs

Topographic information for the WRF was developed using the standard WRF terrain databases available from the National Center for Atmospheric Research ([NCAR](#)). 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 and the 4 km 3SAQS domain was based on the 30 sec (~1 km).

### 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.

## WPS Domain Configuration



**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 12 km (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  $5 \times 10^{-4}$  and  $3.0 \times 10^{-4}$  were used on the 36 and 12 km grids, respectively. For mixing ratio, analysis nudging coefficients of  $1.0 \times 10^{-5}$  were used for both the 36 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](#)) observation archive. The MADIS archive includes the National Climatic Data Center ([NCDC](#)) observations and the National Data Buoy Center ([NDBC](#)) Coastal-Marine Automated Network C-MAN stations. The observational nudging coefficients for winds, temperatures and mixing ratios were  $1.0 \times 10^{-4}$ ,  $1.0 \times 10^{-4}$ , and  $1.0 \times 10^{-5}$ , respectively and the radius of influence was set to 60 km.

## 5.8 WRF Physics Options

The WRF model contains many different physics options. WRF physics options for an initial 2011 calendar year 36/12/4 km WRF simulation were based on our extensive experience with MM5 meteorological modeling and experience with WRF modeling of the Rocky Mountains and used the NOAH land-surface model (LSM), YSU planetary boundary layer (PBL) model and the Kain-Fritsch cumulus parameterization. These simulations were performed for only the first week of January and July of 2011 to help determine the best choice for input datasets and physics options for temperature, mixing ratio, and wind speed/direction. The preliminary model performance of input datasets included choice of Initial Condition and Boundary Condition (ICBC) from the North American Model ([NAM](#)) and ECMWF Interim Reanalysis Data ([ERA-Interim](#)) and land-use land-cover data from the 2006 National Land Cover Database (NLCD; Fry et al., 2011) and US Geological Survey (USGS; Pielke et al., 1997). Evaluation revealed better overall performance for standard near surface meteorological fields using NAM ICBC and USGS land cover data. In particular, NLCD requires additional attention when considering look-up values found in METGRID.TBL and VEGPARM.TBL. An additional test changed the land surface and boundary layer options from Noah (Chen et al., 2001) -YSU (Yonsei University; Hong, Noh and Dudhia, 2006) to PX-ACM2 (Pleim/Xiu-Asymmetric-Convective Model version 2; Gilliam and Pleim, 2010; Pleim, 2007). Unfortunately, PX-ACM2 crashed for the summer case causing us to revert to Noah-YSU. However, we found Noah-YSU to outperform PX for the wintertime case and have reasonable performance during the summer relative to other recent prognostic model applications used in air quality planning. The above options of Noah-YSU with NAM ICBC and USGS land cover were then run for the entire months of January and July with additional sensitivities performed using observational nudging. Nudging too strong to observations generates too much precipitation in WRF and indicates careful attention is needed with observational nudging, especially over complex terrain. 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 3SAQS 2011 36/12/4 km WRF simulation:

- Thompson ice, snow, and graupel scheme (mp\_physics=)
- 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)
- 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 16, 2010 through January 1, 2012.

## 5.10 Evaluation Approach

The model evaluation approach was based on a combination of qualitative and quantitative analyses. The quantitative analysis was divided into monthly summaries of 2-m temperature, 2-m mixing ratio, and 10-m wind speed using the boreal seasons to help generalize the model bias and error relative to a standard benchmark. The evaluation focused on the 4 km three-state domain and the states of Colorado, Wyoming, and Utah and supplemented with select diurnal and time series analyses. Additional analysis includes a qualitative evaluation of the WRF daily and monthly precipitation fields against PRISM fields re-mapping the PRISM data to the WRF domains and grid resolution. WRF snow cover estimates will be evaluated against SNODAS data. A brief analysis of the WRF model performance for winter ozone events was also made to assist in the future design of WRF simulations for simulating elevated winter ozone concentrations, although it is recognized that the initial 2011 WRF simulation was not configured for winter ozone periods. The observed database for winds, temperature, and water mixing ratio used in this analysis was the National Oceanic and Atmospheric Administration (NOAA) Earth System Research Laboratory (ESRL) Meteorological Assimilation Data Ingest System (MADIS).

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, and on a domain-wide basis for the 36 km CONUS, 12 km WESTUS and 4 km 3SAQS modeling domains. Particular attention is paid to the model performance in the states of Colorado, Utah, and Wyoming.

## 5.11 Reporting

The 3SAQS 2011 WRF application and evaluation is documented in a report prepared by UNC and ENVIRON (2014). The model evaluation was performed for winds, temperature, humidity and precipitation for each of the three states. Details are provided in the final 3SAQS 2011 WRF Application/Evaluation report.

## 6.0 EMISSIONS

The section presents the emissions database that we will compile for the 3SAQS 2011 base and future year modeling simulations. Emissions data fall into three broad categories:

- Inventory data – county total estimates of emissions from explicit source categories that have to be processed by SMOKE to obtain the gridded hourly PGM-ready emission inputs.
- Gridded data – fluxes of emissions by grid cell or gridded data that are used to calculate emissions fluxes that are hourly and PGM-ready emissions inputs.
- Ancillary data – non-inventory emissions data that characterize the spatial/chemical/temporal patterns of emissions that are typically used with SMOKE or another emission model to generate the hourly gridded PGM-ready emissions inputs.

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

### 6.1 Base Year 2011 Emissions

The modeling periods and domains for the 3SAQS that are described in the 3SAQS 2011 WRF Modeling Protocol (UNC and ENVIRON, 2014) dictate the temporal and spatial coverage requirements of the 3SAQS 2011 emissions. We will develop an emissions modeling platform, which consists of data and software, to estimate air emissions fluxes that best represent the conditions in the 3SAQS modeling domain and modeling period. The base 2011 modeling period is annual, starting with a model spin-up period on December 16, 2010 and ending December 31, 2011. The modeling domain includes a 36 km continental US (CONUS) domain with a 12 km nest over the western U.S. and a 4-km nest that covers the states of Colorado, Utah, and Wyoming in their entirety (Figure 4-1).

The following sectors will be used to represent air pollutant emissions for the 3SAQS:

- Inventory Data
  - Aircraft/locomotive/marine
  - Off-road mobile
  - On-road mobile
  - Non-point/Area
  - Area oil and gas
  - Point oil and gas
  - Continuous Emission Monitor (CEM) point
  - Non-CEM point
  - Offshore shipping
  - Fires
  - Canada and Mexico sources
- Gridded data
  - MEGAN biogenics
  - Fires

- Windblown dust
- Sea salt
- Lightning

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

### 6.1.1 Inventory Data

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

All of the non-oil and gas (O&G) inventories for the 3SAQS are from the 2011 U.S. EPA National Emission Inventory (NEI). We will use the [2011v6 platform](#) inventories for representing the year 2011 emissions in the 3SAQS. EPA publically released the 2011v6 platform in February 2014. A complete description of the inventory, sectors, and preparation procedures for these data is available in the NEI2011v6.0 Technical Support Document (EPA, 2014).

We will break the NEI2011 inventory sectors into processing sectors to facilitate reporting, quality assurance, and special processing of the data. Table 6-1 lists the major anthropogenic emission inventory sectors used for the 3SAQS 2011 modeling. This table includes fires in addition to the anthropogenic inventories. Table 6-4 lists the more detailed inventory processing sectors that we will simulate for the 3SAQS and includes the source of the data and other details about the inventory.

**Table 6-1. 3SAQS anthropogenic (+fires) inventory sectors**

Sector	Source	Type	Inventory Period	Description
Aircraft/locomotive/marine	NEI 2011v6	Point and Nonpoint	Annual	The aircraft/locomotive/marine (ALM) sector is a subset of the non-point/area sector. It includes county-level emissions at airports (point), line haul locomotives (nonpoint), train yards (point), and class 1 and 2 in- and near-shore commercial marine; CA and MWRPO provided replacement data for the 2011v6 platform, all other state emissions from the 2011v1 platform.
Off-road mobile	NEI 2011v6	Nonpoint	Monthly	NONROAD2008a county-level inventories for recreational vehicles, logging equipment, agricultural equipment, construction equipment, industrial equipment, lawn and garden equipment, leaf and snow blowers, and recreational marine. The CA and TX NONROAD estimates were normalized to emissions values provided by these states.
On-road	NEI	MOVES	Annual and	EPA ran MOVES20110414a for 2011 in emissions

Sector	Source	Type	Inventory Period	Description
mobile	2011v6		Daily	factor mode. The MOVES lookup tables include on-network (RPD), on-network refueling (RPD_RFL), on-network for CA and TX (RPD_CATX), off-network starts/stops (RPV), off-network starts/stops refueling (RPV_RFL), off-network starts/stops for CA and TX (RPV_CATX), off-network vapor venting (RPP), and off-network vapor venting sources for CA and TX (RPP_CATX). These data include the reference county and reference fuel month assignments that EPA used for the MOVES simulation. The CA and TX MOVES estimates were normalized to emissions values provided by these states.
Non-point/ Area	NEI 2011v6	Nonpoint	Annual	County-level emissions for sources that individually are too small in magnitude or too numerous to inventory as individual point sources. Includes small industrial, residential, and commercial sources; broken out into nonpoint, residential wood combustion, livestock, and fertilizer processor sectors
Area Oil & Gas	3SAQS 2011p1 and NEI 2011v6	Nonpoint	Annual	The non-point O&G sector consists of the 3SAQS 2011 Phase I inventory and the NEI 2011v6 inventory for all areas outside of the 3SAQS inventory coverage area
Point Oil & Gas	3SAQS 2011p1 and NEI 2011v6	Point	Annual	The point O&G sector consists of the 3SAQS 2011 Phase I inventory and the NEI 2011v6 inventory for all areas outside of the 3SAQS inventory coverage area
CEM Point	2011v6 and CAMD	Point	Hourly	2011 Clean Air Markets Division (CAMD) hourly Continuous Emissions Monitor (CEM) data
non-CEM Point	2011v6	Point	Annual	Elevated and low-level combustion and industrial sources, airports, and offshore drilling platforms.
Offshore Shipping	2011v6	Point	Annual	Elevated point C3 commercial marine sources in offshore commercial shipping lanes
Fires	PMDETA L	Point	Hourly	Hourly agricultural, prescribed, and wildfire sources with pre-computed plume parameters and speciated PM.
Canada Sources	NPRI2006	Nonpoint and Point	Annual	Canadian 2006 National Pollutant Release Inventory
Mexico Sources	MNEI 2012	Nonpoint and Point	Annual	Mexican NEI 2012



### 6.1.2 Gridded Data

Several gridded datasets are used for either directly estimating air emissions or as ancillary data for processing/adjusting the emissions data. 3SAQS used the same programs and procedures as WestJumpAQMS for generating the gridded emissions data with details available on the [WestJumpAQMS website](#). The following datasets are key gridded data used for the 3SAQS.

#### *Biogenic Emissions Model Inputs*

The major components of biogenic emissions models include:

- Leaf Area Index (LAI)
- Plant Functional Type (PFT)
- Plant specific species composition data and averaging
- Emissions factors, including the effects of temperature and photosynthetically active radiation (PAR)

The gridded data for input the MEGANv2.10 biogenic model used to estimate 2011 biogenic emissions for the 3SAQS include the following:

Leaf Area Index (LAI): A gridded dataset of 46 8-day files for North America were generated for 2011 at 1-km resolution

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

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

Additional details on the development and evaluation of the gridded data used for the 3SAQS are available in the final report on the WRAP Biogenic Emissions Study (Sakulyanontvittaya, Yarwood and Guenther, 2012).

#### *Fire Emissions*

The 3SAQS used fire emissions for 2011 were generated by the Particulate Matter Deterministic and Empirical Tagging and Assessment of Impacts on Levels ([PMDetail](#)) study. PMDETAIL developed 2011 fire emission using satellite data and ground detect and burn scar and other data using a slight modification (Mavko, 2014) to the methodology used in the Deterministic and Empirical Assessment of Smoke's Contribution to Ozone Project ([DEASCO3](#)) study for the 2008 modeling year (DEASCO3, 2013). 3SAQS used a similar plume rise approach as PMDETAIL/DEASCO3 where plume rise depends on fire size and type (Mavko and Morris, 2013). The PMDETAIL 2011 fire inventory was selected over the 2011 Fire INventory from NCAR (FINN) and Smartfire 2011 inventory because it uses a more complete satellite and surface fire dataset.

#### *Windblown Dust (WBD) Emissions*

The major components of the WRAP WBD model include:

- Land use/land cover (LULC)
- Soil characteristics
- Surface roughness lengths

- Meteorology (wind-speeds and friction velocities)

The gridded data for input to the WRAP WBD Model used to estimate 2011 emissions for the 3SAQS include the following:

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

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

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

Additional details on the development and evaluation of the gridded data used for the 3SAQS are available in the final report on the WRAP WBD (Mansell et al., 2006).

#### *Sea Salt*

ENVIRON developed an emissions processor that integrates published sea spray flux algorithms to estimate sea salt PM emissions for input to CAMx. The gridded data for input to the sea salt emissions model used for the 3SAQS is a land-water mask file that identifies each modeling domain grid cell as open ocean, surf zone, or land. Additional details on the development and evaluation of the sea salt emissions processor used for the 3SAQS are available in the WestJumpAQMS Sea Salt and Lightning memo (Morris, Emery, Johnson and Adelman, 2012).

The 3SAQS will use the CAMx sea salt emissions processor with 2011 WRF data to generate sea salt emissions for the 36 and 12 km modeling domains. The 3SAQS 4 km domain is inland so will not have any sea salt emissions.

#### *Lightning*

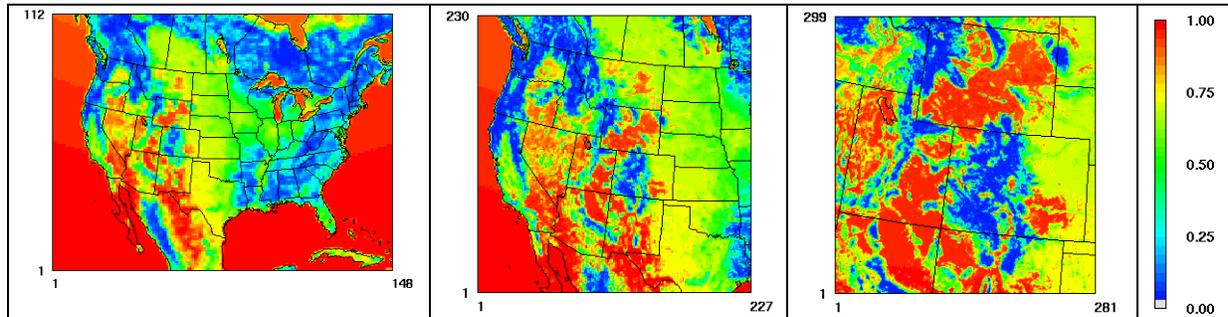
The modified lightning NO<sub>x</sub> emissions model of Koo et al. (2010) used in the WestJumpAQMS will be used to estimate lightning NO<sub>x</sub> emissions for the 3SAQS. Additional details on the development and evaluation of the lightning emissions processor used for the 3SAQS are available in the WestJumpAQMS Sea Salt and Lightning memo (Morris, Emery, Johnson and Adelman, 2012).

#### *Fugitive Dust Transport Factors*

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

For the 3SAQS 2011 modeling platform we will use the dust transport factors collected for the WestJumpAQMS. WestJumpAQMS implemented fugitive dust correction factors that are derived from the Biogenic Emission Landuse Database version 3 (BELD3; Vukovich and Pierce, 2002). Following the approach of Pouliot et al.(2010) we adjusted the fugitive and road dust emissions as a post-processing step after the emissions data were output from SMOKE. We used transport factors gridded to each of the 3SAQS modeling domains to reduce the dust emissions (Figure 6-1). The values of the transport factors associated with each BELD3 land cover category are available in Pouliot et al. As seen in Figure 6-1, the dust transport factors are close to 1.0 (red) over desert barren land indicating that very little dust is

deposited locally, whereas in the forested Rocky Mountain region (blue) the transport factors are around 0.05 indicating the 95% of the fugitive dust emissions in these areas are deposited locally and not transported downwind.



**Figure 6-1. Fugitive and road dust vegetation scavenging factors gridded to the 3SAQS modeling domains**

### 6.1.3 2011 Oil and Gas Emissions

The base case 2011 emissions were projected from the WestJumpAQMS O&G 2008 emissions or were directly obtained from the state agencies. Future year O&G inventories for the states of Colorado, Wyoming, New Mexico and Utah were primarily based off the 2011 3SAQS Phase 1 oil and gas inventory data and projected to 2020. The base case and future emission inventories were developed for the following basins:

- Piceance
- Denver-Julesburg
- South San Juan
- North San Juan
- Uintah
- Southwest Wyoming
- Powder River
- Wind River
- Big Horn
- Paradox
- Raton

For the Denver-Julesburg, Piceance, North San Juan, South San Juan and Uintah basins in Utah, Colorado and northern New Mexico, the WestJumpAQMS 2008 O&G area source emissions were projected to 2011 using appropriate surrogates whereas the permitted data for the calendar year 2011 were obtained from the state agencies including the Colorado Department of Public Health and Environment (CDPHE), the Utah Department of Environmental Quality (UTDEQ), the New Mexico Environment Department (NMED), and the U.S. Environmental Protection Agency (EPA) for tribal lands.

For all Wyoming basins, including the Wind River, Southwest Wyoming, Powder River and Big Horn basins, 2011 area and permitted O&G emissions were directly provided by the Wyoming Department of Environmental Quality (WYDEQ) for only Wyoming counties. Area and permitted source emissions for 2011

were projected from the 2008 WestJumpAQMS inventory for counties outside Wyoming but within the basin boundary. For the Big Horn Basin, emissions outside Wyoming counties were excluded from the inventory due to lack of information on activity in Montana counties for this basin. It should be noted that for the Paradox and Raton basins, only permitted emissions were included in the inventories as insufficient data was available to estimate area source emissions for these two basins.

For those basins where 2011 emissions were projected from the WestJumpAQMS emission inventory, well count and production activity from a commercially available database of oil and gas data maintained by IHS Corporation, also referred to as the “PI Dwight’s” database, were used. This database contains production statistics that are of significantly higher quality than the primary data in individual state O&G Commission databases. Two types of data were queried from the Enerdeq database: production data and well data. Production data includes information relevant to producing wells in the basin while well data includes information relevant to drilling activity (“spuds”) and completions in the basin.

Processing of the IHS data for the 2011 projections followed the same methodology as used in the WRAP [Phase III](#) study. Summaries of production statistics were 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 were summarized at the county and basin level, for tribal and non-tribal land separately as applicable to each basin.

The 2011 production statistics from the IHS database were used to project the WestJumpAQMS baseline 2008 O&G inventories. The projections were developed as scaling factors that represented the ratio of the value of a specific activity parameter in 2011 to the value in 2008. The scaling factors were developed at the county and tribal levels for all applicable basins. Scaling factors were then matched to all source categories using the same cross-referencing analysis as conducted as part of the WestJumpAQMS study. The 2011 to 2008 scaling factors were used to adjust the activity data for the oil and gas emissions.

When activity specific scaling factors were estimated to be less than one (1), indicating a reduction in an activity parameter from 2008 to 2011, all emissions factors and activity data were assumed to be identical in 2011 as in 2008 and the 2008 emissions were reduced and no emission controls assessment was needed (i.e., when activity was reduced between 2011 and 2008, we assumed that the same equipment was used in the field, it was just producing less and had lower emissions). In this case, the 2011 emissions were developed assuming the direct application of the scaling factor with no additional controls.

Where scaling factors were estimated to be greater than one (1), it was assumed that some growth in activity has occurred in the 2008-2011 time period and that new equipment may have been deployed in the field. A control analysis was conducted specific to each basin and utilizing the control measures identified as part of the WRAP Phase III midterm O&G projections work. For the 3SAQS Phase I 2011 O&G emission inventories, emission controls were applied to survey-based sources projected from 2008, but not to the 2011 “permitted” emissions provided by state agencies. It should be noted that, since all 2011 O&G data for Wyoming were obtained from the Wyoming DEQ, no additional controls were applied to any of Wyoming Basins. The list of controls applied to each basin for 2011 is summarized in Table 6-2 below.

**Table 6-2. List of Additional Controls Applied to 2011 Area Sources Emissions.**

Basin	Source Category	Regulation	Enforcing Agency	Effective Date	Implementation in 2011 Emissions Projection
Denver-Julesburg	Drill Rigs and Workover Rigs	Nonroad engine Tier standards (1-4)	US EPA	Phase in from 1996 - 2014	Assumed fleet wide emissions control based on EPA NONROAD model default estimates
	Pneumatic Controller	Regulation 7	CDPHE	Feb 1, 2009	Assumed that all pneumatic controllers in 8 hours non-attainment area are low-bleed devices
Piceance and North San Juan	Drill Rigs and Workover Rigs	Nonroad engine Tier standards (1-4)	US EPA	Phase in from 1996 - 2014	Assumed fleet wide emissions control based on EPA NONROAD model default estimates
Uintah	Drill Rigs/Workover Rigs	Nonroad engine Tier standards (1-4)	US EPA	Phase in from 1996 - 2014	Assumed fleet wide emissions control based on EPA NONROAD model default estimates
	All New Nonroad Engines	New Source Performance Standards (NSPS)	US EPA	Phase in beginning 2006	Control factors were analyzed based on added horsepower meeting NSPS standards
	All Minor Sources on Tribal Land	New Source Review (NSR) : Under the rule issued, new and modified minor sources and major sources that make minor modifications, located in Indian country, must obtain a permit prior to commencing construction	US EPA	New Minor Source Permit March 2, 2016  For all true minor sources that begin operation before September 2, 2014 : Require to obtain a minor NSR permit 6 months after EPA publishes a general permit. No general permits have been finalized as of July 2014	Not applied
South San Juan	Drill Rigs, Workover Rigs	Nonroad engine Tier standards (1-4)	US EPA	Phase in from 1996 - 2014	Assumed fleet wide emissions control based on EPA NONROAD model default estimates
	Well Head Compressor Engines	EPA NSPS and Farmington RMP within Farmington RMP and EPA NSPS outside Farmington RMP	US EPA	Phase in from 2005 to 2011	Emissions reduction due to NSPS and Farmington RMP Condition of Approval (CA)
Wyoming Basins (Southwest Wyoming, Powder River, Wind River and Big Horn)	No additional control				
Paradox and Raton	Not applicable				

#### 6.1.4 Ancillary Emissions Data

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

- **Spatial data.** All anthropogenic non-point inventory data, except on-road mobile sources, are estimated at the county level. Gridded hourly on-road mobile source emissions were estimated using the SMOKE-MOVES processor with MOVES emissions factor lookup table and hourly gridded meteorology from the 2011 WRF meteorological model. Data files called spatial surrogates are used to map the county-level emission inventories to the model grid cells. Spatial surrogates are generated from Geographic Information System (GIS) Shapefiles using software that calculates the fractions of county-level different geospatial attributes in a model grid cell. For example, a Shapefile of the housing distribution in Los Angeles County is combined with a description of a modeling grid to calculate the percentage of L.A. County housing assigned to each grid cell. This information is then used to allocate county-level emission inventory sources that are associated with housing (e.g.) to the modeling grids.

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

- **Temporal data.** Air quality modeling systems, such as CMAQ and CAMx, require hourly emissions input data. With the exception of a few source types (e.g. Continuous Emissions Monitoring data, biogenic emissions, windblown dust and some fire inventories), most inventory data include annual or daily emission estimates. Temporal profiles are used to compute hourly emissions from the annual or daily inventory estimates. The SMOKE model, which is being used to process emission for the 3SAQS, uses three types of temporal profiles:
  1. **Monthly profiles:** Convert annual inventory to monthly emissions accounting for seasonal and other effects.
  2. **Daily profiles:** Convert monthly emissions to daily emissions accounting for day-of-week and other effects.
  3. **Hourly profiles:** Convert daily emissions to hourly emissions accounting for the diurnal variation in emissions (e.g., work schedules and commute times).

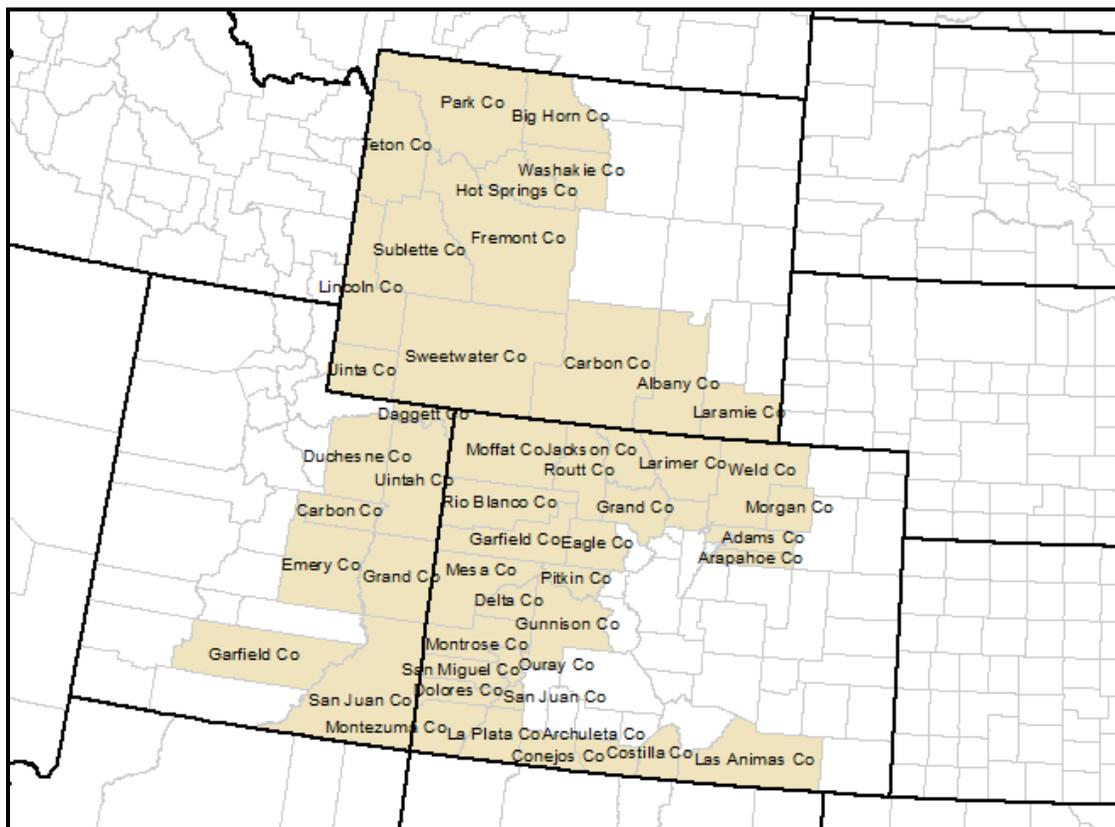
Temporal profiles are assigned to inventory sources using cross-referencing data that match the profiles and inventory sources using country/state/county (FIPS) and source classification codes (SCCs).

- **Chemical speciation data.** Emissions inventories have limited chemical composition information. The emissions inventories for the 3SAQS include 6 criteria pollutants: carbon monoxide (CO), nitrogen oxides (NO<sub>x</sub>), volatile organic compounds (VOC), ammonia (NH<sub>3</sub>), sulfur dioxide (SO<sub>2</sub>), particulate matter with a mean diameter < 10 micrometers (PM<sub>10</sub>), and particulate matter with a mean diameter < 2.5 micrometers (PM<sub>2.5</sub>). Chemical speciation profiles are used to describe the chemical compositions of the effluent from particular emissions sources. The exact specification of the source-specific emissions species is determined by the chemistry mechanism selected for the AQM simulation. Speciation profiles convert the inventory pollutants to more detailed source-specific species in terms required by the AQM chemistry mechanism. For example, there is a speciation profile that converts the inventory pollutant NO<sub>x</sub> to the AQM input species NO, NO<sub>2</sub>, and HONO. Speciation profiles are required to convert inventory NO<sub>x</sub>, VOC, SO<sub>2</sub>, and PM<sub>2.5</sub> into AQM species. For the 3SAQS SMOKE emissions modeling the CB6r2

chemical mechanism will be utilized and VOC will be speciated using source specific speciation profiles developed using the [SPECIATE 4.3](#) database. Note that CB6r2 chemistry also models local excess methane (ECH4) above background concentrations that will also be specified in the emission inputs using the SPECIATE 4.3 speciation profiles. Note that the 3SAQS methane emissions will not be a complete emissions inventory since emissions for all methane sources are not available.

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

The base set of ancillary data for 3SAQS will be taken directly from the EPA 2008v2 modeling platform. These were the same data used for the WestJumpAQMS and are detailed in WestJumpAQMS Final Emissions Modeling Parameters Technical Memo (Adelman, Loomis and Morris, 2013). The 3SAQS is developing a comprehensive 2011 PGM air quality modeling platform for the 36/12/4 km domain depicted in Figure 4-1 with refined and comprehensive emissions and meteorological inputs for the Three-State 4 km domain that includes the entirety of the states of Colorado, Utah and Wyoming. For the 3SAQS, we made targeted improvements to the ancillary files for counties in the 3-state study region (Figure 6-2). We focused the improvements on the assignments of spatial/chemical/temporal profiles to inventory sources and on developing profiles that best represent the emissions patterns in the 3-state study region.



**Figure 6-2. List of counties in the three-state study region where targeted emission improvements were made.**

By targeting the largest emitters (top 90% of annual NO<sub>x</sub> and VOC emitters) in the three state region, we maximized the improvement effort by limiting the number of sources to those with the largest impact on air quality. The results of this effort were presented to the states of Utah, Colorado, and Wyoming in a series of 3SAQS workshops during January 2013. The improvements that we made for the targeted CO/UT/WY counties include the following:

#### *Utah*

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

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

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

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

- Created a state-specific, year 2011 monthly temporal profile for residential natural gas heating fuel use with Energy Information Administration data (Figure 6-3);

- Developed confined animal feeding operation (CAFO) spatial surrogates for livestock sources. Figure 6-4 shows the locations of the CAFOs provided by UT. We converted these data to a point Shapefile and then generated UT livestock surrogates for cattle, poultry, and swine for 3SAQS;

- Used point locations of rest areas and truck stops to allocation MOVES extended idling emissions to the modeling grid.

#### *Colorado*

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

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

- Created CAFO spatial surrogates from data provided by CDPHE for livestock ammonia sources;

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

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

- Created a state-specific, year 2011 monthly temporal profile for residential natural gas heating fuel use with Energy Information Administration data (Figure 6-3);

- Developed 2008 vehicle miles traveled (VMT)-based spatial surrogates for on-road mobile sources. Figure 6-4 compares the U.S. Census year 2010 TIGER line roadway data with link-based VMT data from CO.;

- Used point locations of rest areas and truck stops to allocation MOVES extended idling emissions to the modeling grid.

#### *Wyoming*

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

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

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

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

Created a state-specific, year 2011 monthly temporal profile for residential natural gas heating fuel use with Energy Information Administration data (Figure 6-3);

Developed confined animal feeding operation (CAFO) spatial surrogates for livestock sources. Figure 6-5 shows the locations of the CAFOs provided by WY. We converted these data to a point Shapefile and then generated WY livestock surrogates for cattle and swine for 3SAQS;

Used point locations of rest areas and truck stops to allocation MOVES extended idling emissions to the modeling grid.

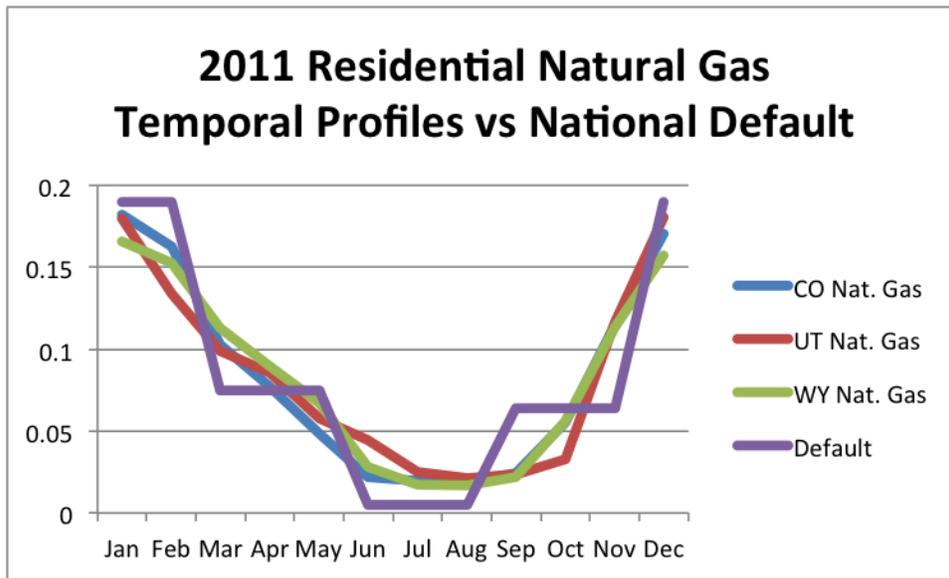


Figure 6-3. 3SAQS 2011 residential natural gas consumption monthly temporal profiles

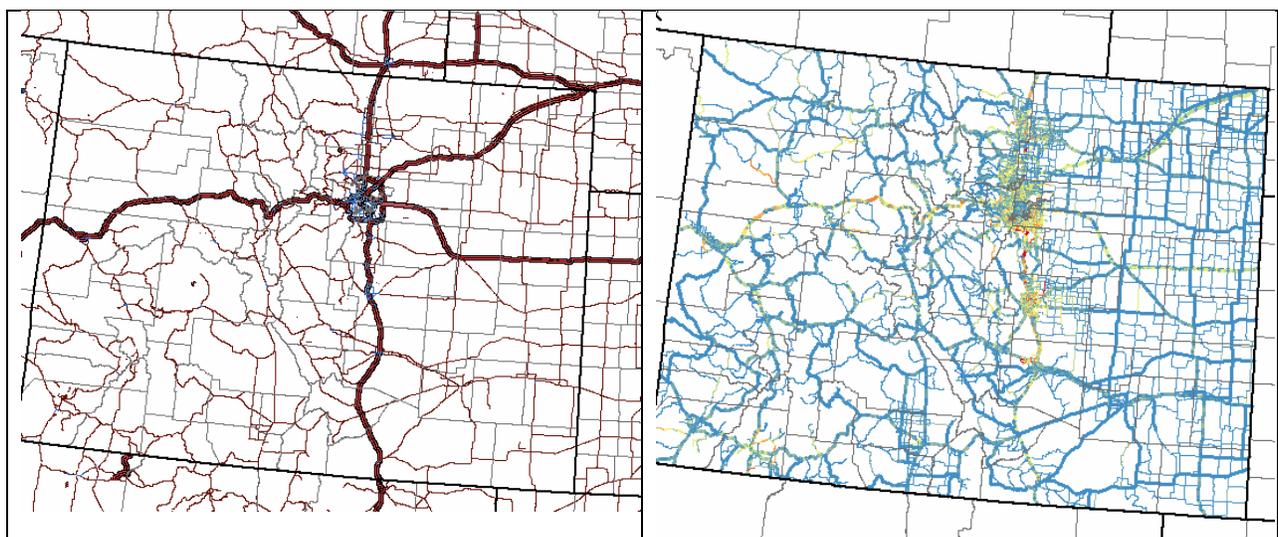
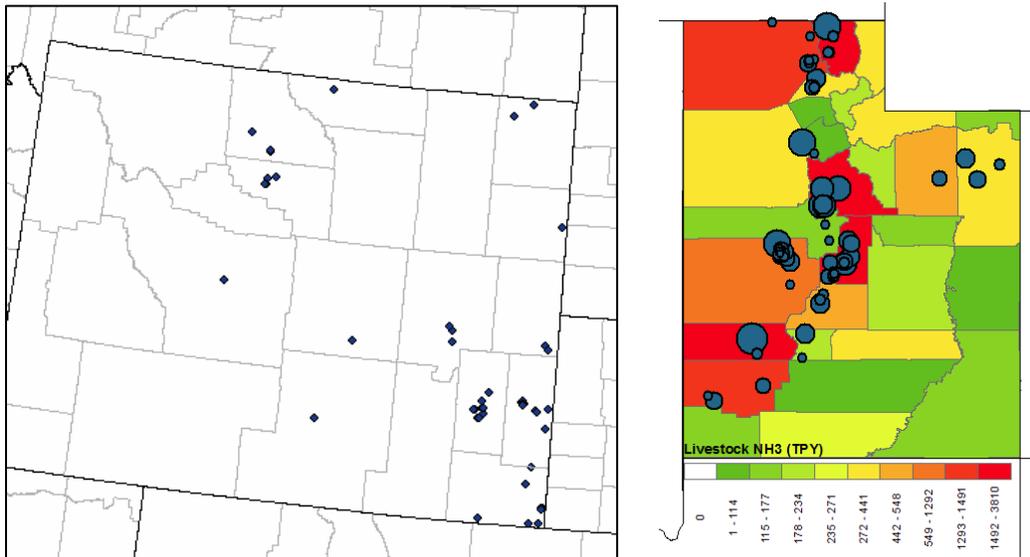


Figure 6-4. Colorado roadway spatial data improvement plots. Left: TIGER 2010 Shapefile of urban/rural primary/secondary roads. Right: CO 2008 VMT-based roadways



**Figure 6-5. Wyoming and Utah CAFO locations. Colorado CAFO locations developed from the NPS RoMANS study are also being used in the 3SAQS**

## 6.2 Future Year 2020 Emissions

We will prepare a future year modeling platform with inventories projected to 2020 using information on emissions growth and controls between the year 2011 and 2020. The inventory data for the 3SAQS 2020 emissions modeling platform will come primarily from the three sources:

- NEI11 (2011v6 modeling platform) 2018 projected inventories for non-oil and gas anthropogenic emission sources.
- 3SAQS 2011 projected to 2020 oil and gas inventory emissions.
- 3SAQS natural emissions, including biogenic and fires, remain at 2011 levels.

### 6.2.1 Non-Oil and Gas Future-Year Emissions Data

For all of the inventory sectors except oil and gas, biogenics, windblown dust, seasalt, and lightning, 2018 inventory and ancillary emissions data will be taken directly from the EPA 2011v6 modeling platform and used in the 3SAQS 2020 emissions scenario. Developed by EPA for use in an expected upcoming ozone transport rule, the 2018 inventory represent the best estimate of future year emissions based off of the 2011 inventory available. The result of using the 2018 inventory from the 2011v6 modeling platform is that the 2020 future year emissions will not be the same for the 3SAQS 2008 and 2011 modeling platforms. This is order for the 2020 future emissions to be consistent with the base case emission in the 2008 and 2011 modeling platforms.

A summary of the 2011v6 modeling platform 2018 inventory is provided below and additional details are available from EPA (2014).

- CEM Point: Unit-specific estimates from EPA's Integrated Planning Model ([IPM](#)), version 5.13 with CAIR and Final MATS.

- Non-CEM Point: Projection factors and percent reduction to reflect Cross-State Air Pollution Rule (CSAPR) comments and emission reductions due to national and local rules, control programs, plant closures, consent decrees and settlements. Projection approaches for corn ethanol and biodiesel plants, refineries and upstream impacts from the Energy Independence and Security Act of 2007 (EISA). Terminal area forecast (TAF) data aggregated to the national level were used for aircraft to account for projected changes in landing/takeoff activity.
- Point and nonpoint oil and gas sectors: For the non-WRAP oil and gas sources, regional projection factors by product type using Annual Energy Outlook (AEO) 2013 projections to year 2018. Cobenefits of stationary engines CAP-cobenefit reductions (RICE NESHAP) and New Source Performance Standards (NSPS) VOC controls reflected for select source categories.
- Nonpoint/Area: Agricultural sector projection factors for livestock estimates based on expected changes in animal population from 2005 Department of Agriculture data, updated based on personal communication with EPA experts in July 2012; fertilizer application NH<sub>3</sub> emissions projections include upstream impacts EISA. Fugitive dust projection factors for dust categories related to livestock estimates based on expected changes in animal population and upstream impacts from EISA. Other nonpoint source projection factors that implement Cross State Air Pollution Rule comments and reflect emission reductions due to control programs. Residential wood combustion projections are based on projection factors that reflect assumed growth of wood burning appliances based on sales data, equipment replacement rates and change outs. These changes include growth in lower-emitting stoves and a reduction in higher emitting stoves. PFC projection factors reflect impact of the final Mobile Source Air Toxics (MSAT 2) rule. Upstream impacts from EISA, including post-2007 cellulosic ethanol plants are also reflected.
- Off-road Mobile: Other than for California and Texas, this sector uses data from a run of NMIM that utilized NONROAD2008a, using future-year equipment population estimates and control programs to the year 2018 inputs that were either state-supplied as part of the 2011NEIv1 processing or using national level inputs. Controls from the final locomotive-marine and small spark ignition OTAQ rules are included. California and Texas-specific data were provided by CARB and TCEQ.
- Aircraft/locomotive/marine: For all states except California, projection factors for Class 1 and Class 2 commercial marine and locomotives, which reflect final locomotive-marine controls and RFS2 adjustments. California projected year-2017 inventory data were provided by CARB.
- Offshore shipping: Base-year 2011 emissions grown and controlled to 2018, incorporating controls based on Emissions Control Area (ECA) and International Marine Organization (IMO) global NO<sub>x</sub> and SO<sub>2</sub> controls.
- On-road Mobile, not including refueling: MOVES2010b (extended idle mode) and MOVESTier3NPRM-based emissions factors for year 2018 were developed using the same representative counties, state-supplied data, meteorology, and procedures that were used to produce 2011 emission factors. California and Texas-specific data were provided by CARB and TCEQ. This sector includes all non-refueling on-road mobile emissions (exhaust, extended idle, evaporative, evaporative permeation, brake wear and tire wear modes).
- On-road Refueling: Uses the same projection and processing approach as the on-road sector, except for California and Texas where EPA projected using MOVES2010b and did not include CARB or TCEQ data.
- Canada Sources: Held constant and 2006 levels

- Mexico Sources: Projections from 1999 to 2018

We will not make any changes to the ancillary emissions data (spatial/temporal/chemical) for the 2020 future year emissions. These data will be held constant at the 2011 values when preparing the 2020 emissions for CAMx.

### 6.2.2 O&G Future-Year Emissions Data

The 2011 baseline O&G inventories were projected to 2020 based on controls analysis and activity growth and decline. The activity projections were developed from a linear fitting of trend-lines based on an analysis of historic production statistics in the IHS database through 2012. IHS production history of well counts, spud counts, and production by type (gas, condensate, oil) were mined for developing the trend-lines. The historic trend-lines were forecasted to 2020. For forecasts that indicated a decline in production, we continued the decline toward 2020 without allowing the productions to drop to zero. For forecasts that indicated an increase, we continued the increase toward 2020. For forecasts that indicated relatively flat trends, we assumed the emissions remains constant at 2011 levels. The trend-lines developed for each basin was used to develop scaling factors (2020 activity/2011 activity) which were applied to 2011 emissions to generate uncontrolled 2020 inventories for each basin.

For each basin in Colorado, Utah, Wyoming and New Mexico, controls were applied based on both state and federal regulatory requirements. If redundant controls were found in a comparison of the state and federal rules by year and source category, the more stringent control was applied to the inventory. The impacts of some controls required a year-to-year controls analysis, while others were applied directly to the projected 2020 inventory. The control analysis included all source categories subject to regulations that are currently promulgated, but not controls that are under consideration. We have used a “no turnover” assumption in developing the control scenarios, which speculate that existing equipment in use in the basins are unlikely to be replaced with newer technologies before 2020. It was also assumed that the existing equipment is subject only to regulations that existed at the time of installation. Due to time and resource constraints, for the 3SAQS Phase I 2020 O&G projections, controls were only applied to survey (area) sources. For 2011 O&G emissions provided by the three states and EPA, no additional controls were applied when making 2018 projections as agreed to by the 3SAQS technical committee. For the 3SAQS Phase 2 2018 O&G emissions, additional control analysis for O&G sources that states and EPA provided 2011 emissions for will be considered. Due to lack of equipment specific data for all Wyoming basins, the control factors were developed for only drilling and workover rigs.

We applied the control data for each basin to the 2020 uncontrolled forecasted O&G inventories to develop the future year inventories for use in the 3SAQS. Table 6-3 summarizes all controls applied to 2020 emissions by basin. The control analysis indicated that for a given source category the state specific controls are either equivalent to federal regulation requirement or are less stringent. Table 6-4 lists state specific oil and gas regulations by source category<sup>2</sup>.

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<sup>2</sup> Analysis of States' and EPA Oil & Gas Air Emissions Control Requirements for Selected Basins in the Western United States , November,2013. <http://www.wrapair2.org/Analysis.aspx>

**Table 6-3. List of Controls Applied to 2020 Area Sources Emissions**

Basin	Source Category	Regulation	Enforcing Agency	Effective Date	Implementation in 2020 Emissions Projection
Denver-Julesburg, Wind River, Powder River, Southwest Wyoming and Big Horn	Drill Rigs and Workover Rigs	Nonroad engine Tier standards (1-4)	US EPA	Phase in from 1996 - 2014	Assumed fleet wide emissions control based on EPA NONROAD model default estimates
Piceance	Drill Rigs and Workover Rigs	Nonroad engine Tier standards (1-4)	US EPA	Phase in from 1996 - 2014	Assumed fleet wide emissions control based on EPA NONROAD model default estimates
	Well Completions	New Performance Standard Subpart OOOO	US EPA	Phase in from 2015	Assumed all gas well completions from 2015 make use of Reduced emissions completions (REC) technology with a 95% efficiency
North San Juan	Drill Rigs/Workover Rigs	Nonroad engine Tier standards (1-4)	US EPA	Phase in from 1996 - 2014	Assumed fleet wide emissions control based on EPA NONROAD model default estimates
	All New Nonroad Engines	New Source Performance Standard. (NSPS)	US EPA	Phase in beginning 2006	Total Gas production declined from 2011 to 2020. Hence, this regulation is not be applicable
Uintah	Drill Rigs/Workover Rigs	Nonroad engine Tier standards (1-4)	US EPA	Phase in from 1996 - 2014	Assumed fleet wide emissions control based on EPA NONROAD model default estimates
	All New Nonroad Engines	New Source Performance Standard. (NSPS)	US EPA	Phase in beginning 2006	Controls were applied to base year emissions. No further control required in future
	Pneumatic Controllers	New Performance Standard Subpart OOOO	US EPA	Phase in beginning October, 15 ,2013	Assumed gas well emissions controlled per subpart OOOO requirement
	Well Completions	New Performance Standard Subpart OOOO	US EPA	Phase in from 2015	Assumed all gas well completions from 2015 make use of Reduced emissions completions (REC) technology with a 95% efficiency
	Condensate Tanks	New Performance Standard Subpart OOOO	US EPA	Phase in from 2012	Assumed that 42% of new production added after 2011 will be controlled via flare with a 95% control efficiency
	Oil Tanks	New Performance Standard Subpart OOOO	US EPA	Phase in from 2012	Assumed that 75% of new production added after 2011 will be controlled via flare with a 95% control efficiency
South San Juan	Drill Rigs/Workover Rigs	Nonroad engine Tier standards (1-4)	US EPA	Phase in from 1996 - 2014	Assumed fleet wide emissions control based on EPA NONROAD model default estimates
	Well Head Compressor Engines	EPA NSPS and Farmington RMP within Farmington RMP and EPA NSPS outside Farmington RMP	US EPA	Phase in from 2005 to 2011	The control analysis shows <1% control for all pollutants. Conservatively assumed no further control for this category
	Pneumatic Controllers	New Performance Standard Subpart OOOO	US EPA	Phase in beginning October, 15 ,2013	Assumed gas well emissions controlled per subpart OOOO requirement
	Well Completions	New Performance Standard Subpart OOOO	US EPA	Phase in from 2015	Assumed all gas well completions from 2015 make use of Reduced emissions completions (REC) technology with a 95% efficiency
	Condensate Tanks	New Performance Standard Subpart OOOO	US EPA	Phase in from 2012	Assumed that 7% of new production added after October 2015 will be controlled via flare with a 95% control efficiency
	Oil Tanks	New Performance	US EPA	Phase in	Assumed that 26% of new production added after

Basin	Source Category	Regulation	Enforcing Agency	Effective Date	Implementation in 2020 Emissions Projection
		Standard Subpart 0000		from 2012	October 2015 will be controlled via flare with a 95% control efficiency
Paradox and Raton	Not applicable				

No changes were made to the spatial patterns or chemical profiles of the O&G emissions for the 2020 projections from what was used in the 2011 emissions modeling. The basin-specific spatial surrogates and VOC speciation profiles for 2011 will be applied to the 2020 inventories to estimate 2020 model-ready emissions.

### 6.3 Emissions Processing

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

#### 6.3.1 SMOKE Processing

The procedures for processing the emissions for generating CAMx emission inputs using SMOKE are described below. Similar procedures will be used for CMAQ only using the formats used by CMAQ.

- Import (Smkinven) – read raw inventory files  
 Calculate coarse mode primary particulate matter (PMC) emissions, where SMKINVEN\_FORMULA:  
 $PMC = PM_{10} - PM_{2.5}$   
 For the hourly CEM inventories, set to read hourly data, where HOUR\_SPECIFIC\_YN = Y  
 Do NOT normalize weekly emissions by weekdays only, where WKDAY\_NORMALIZE = N
  - Do NOT process hazardous air pollutant emissions, where SMK\_PROCESS\_HAPS = N
- Grid (Grdmat) – read and match spatial surrogates to inventory sources and assign the emissions to PGM grid cells  
 For all sources other than agriculture, use population as the fallback surrogate, where  
 $SMK\_DEFAULT\_SRGID = 100$   
 For livestock and fertilizer, use rural land area as the fallback surrogate, where  
 $SMK\_DEFAULT\_SRGID = 400$ 
  - Process all sources on a normal sphere with radius 6,370,000 m, where IOAPI\_ISPH = 20
- Speciation (Spcmat) – read and match VOC and PM chemical profiles to inventory sources and calculate emissions in terms of PGM species
  - Convert inventory VOC to total organic gases (TOG) for consistency with the NEI SPECIATE speciation profiles, where POLLUTANT\_CONVERSION = Y
- Temporal (Temporal) – read and match monthly/week/hourly temporal profiles to inventory sources and estimate hourly emissions

Renormalize the temporal profiles, where RENORM\_TPROF = Y

Do NOT force all temporal profiles to be flat, where UNIFORM\_TPROF\_YN = N

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

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

Use a configuration file to select elevated sources, where SMK\_ELEV\_METHOD = 1

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

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

Combine gridding, temporal, and speciation intermediates to create PGM-ready emissions, where MRG\_GRDOUT\_YN = MRG\_TEMPORAL\_YN = MRG\_SPCMAT\_YN = Y

Output an elevated file that includes the emissions for elevated sources, where SMK\_ASCIIIELEV\_YN = Y

○ Output emissions in CAMx units, where MRG\_GRDOUT\_UNIT = moles/hr

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

Process MOVES emissions, where SMK\_EF\_MODEL = MOVES

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

○ Extend a 10 degree temperature buffer on either side of the emissions factor look up tables, where TEMP\_BUFFER\_BIN = 10

- Final merge (Mrggrid) - Merge the low-level sector emissions to a single file per day
- Create CAMx-ready binary files (Smk2emis) – convert netCDF SMOKE outputs to UAM-formatted data for CAMx
- Merge elevated source (Mrgelev) – combine elevated files to a single file per day and convert to UAM-formatted data for CAMx

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

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

- Single day per year (aveday\_yr)
- Single day per month (aveday\_mon)
- Typical Monday, Weekday, Saturday, Sunday per year (mwdss\_yr)
- Typical Monday, Weekday, Saturday, Sunday per month (mwdss\_mon)
- Emissions estimated for each model simulation day (daily)
- Emissions estimated for each model simulation day with temporal profiles generated with average daily meteorology (daily met)
- Emissions estimated for each model simulation day with temporal profiles generated with hourly meteorology (hourly met)

Table 6-4 defines the emissions categories that we will define for the 3SAQS project. The “Temporal” column in Table 6-4 refers to the temporal configuration that will be used for each category.

**Table 6-4. 3SAQS 2011-based emissions processing categories.**

Emissions Processing Category (Abbr)	Inventory Year	Inventory Source	Temporal	Processing Comments
Nonpoint/Area (nonpt)	2011	NEI2011v6	mwdss_mon	Remove oil & gas, agricultural NH <sub>3</sub> , and dust, and includes commercial marine and rail
Livestock NH <sub>3</sub> (lv)	2011	NEI2011v6	mwdss_mon	Met-based temporal profiles;
Fertilizer NH <sub>3</sub> (ft)	2011	NEI2011v6	mwdss_mon	
Fugitive and Road Dust (fd)	2011	NEI2011v6	mwdss_mon	Includes paved and unpaved road dust; apply transport factors but not met factors
Residential Wood Combustion (rwc)	2011	NEI2011v6	mwdss_mon	Met-based temporal profiles
Area Oil & Gas (arog)	2011	IPAMS	aveday_mon	Oil and gas sources for the 3SAQS basins; basin specific speciation profiles and spatial surrogates
US Area Oil & Gas (usarog)	2011	NEI2011v6	aveday_mon	Oil and gas sources outside of the 3SAQS basins
Nonroad mobile (nr)	2011	NEI2011v6	mwdss_mon	NMIM commercial marine and rail moved to alm
Aircraft/locomotive/maring (alm)	2011	NEI2011v6	mwdss_mon	Includes monthly and annual inventories
MOVES RPD (rpd)	2011	NEI2011v6/ MOVES20110414a	hourly met	Daily emissions factor lookup tables
MOVES RPD Refueling (rpd_rfl)	2011	NEI2011v6/ MOVES20110414a	hourly_met	Daily emissions factor lookup tables
MOVES RPD for CA and TX (RPD_CATX)	2011	NEI2011v6/ MOVES20110414a	hourly_met	MOVES temporal and spatial distribution with magnitudes from CARB and TCEQ
MOVES RPP (rpp)	2011	NEI2011v6/ MOVES20110414a	hourly met	Daily emissions factor lookup tables
MOVES RPP for CA and TX (RPP_CATX)	2011	NEI2011v6/ MOVES20110414a	hourly_met	MOVES temporal and spatial distribution with magnitudes from CARB and TCEQ
MOVES RPV (rpv)	2011	NEI2011v6/ MOVES20110414a	hourly met	Daily emissions factor lookup tables
MOVES RPV Refueling (rpv_rfl)	2011	NEI2011v6/ MOVES20110414a	hourly_met	Daily emissions factor lookup tables
MOVES RPV for CA and TX (RPV_CATX)	2011	NEI2011v6/ MOVES20110414a	hourly_met	MOVES temporal and spatial distribution with magnitudes from CARB and TCEQ

Emissions Processing Category (Abbr)	Inventory Year	Inventory Source	Temporal	Processing Comments
CEM Point (ptcem)	2011	NEI2011v6/CAMD	daily	Anomalies removed from 2008 CAMD data
Non-CEM Point (ptncem)	2011	NEI2011v6	mwdss_mon	Removed oil & gas sources and transferred to ptog sector; includes point aircraft and ports
Point Oil & Gas (ptog)	2011	IPAMS	mwdss_mon	Point oil and gas sources for the 3SAQS basins
US Point Oil & Gas (usptog)	2011	NEI2011v6	aveday_mon	Oil and gas sources outside of the 3SAQS basins
Point Fires (ptfire)	2011	PMDETAIL	daily	Pre-computed plume rise, processing outside of SMOKE. Separately process for WF, Rx and AGfires.
Commercial Marine (ptseca)	2011	NEI2011v6	aveday_mon	
Canada Area (canar)	Canada 2006	Canada NPRI	mwdss_mon	
Mexico Area (mexar)	Mexico 2012	Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2008
Canada/Mexico Point (nuspt)	Can2006/Mex2012	Canada NPRI Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2008
Canada Mobile (canmb)	Can2006	Canada NPRI	mwdss_mon	
Mexico Mobile (mexmb)	Mex2012	Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2008
Lightning NOx (Inox)	N/A	ENVIRON	hourly met	Gridded monthly NLCD lightning flash counts converted to hourly, gridded NO emissions with WRF convective rainfall
Sea salt (ss)	N/A	ENVIRON	hourly met	Surfzone and open ocean PM emissions
Windblown Dust (wbd)	N/A	WRAP WBD Model	hourly met	
MEGAN Biogenic (bg)	N/A	MEGAN2.1	hourly met	Use new versions of MEGAN V2.10 updated by WRAP for the western U.S.

### **6.3.2 MEGAN Biogenic Modeling**

For the 3SAQS, we will use the MEGAN biogenic emissions model version 2.10. Details on the model inputs, software, and configuration are available in the [Improved Biogenic Emission Inventories Across the West Final Report](#) (Sakulyanontvittaya, Yarwood and Guenther, 2012). MEGAN was applied using the 3SAQS 2011 36/12/4 km WRF meteorological model output using the same databases and approach as used in the WestJumpAQMS MEGAN application for 2008 (Sakulyanontvittaya, et al., 2012). MEGAN was selected over BEIS due to the recent WRAP study to improve the model inputs to be more representative of plant types in the western U.S.

### **6.3.3 Windblown Dust Processing**

For the 3SAQS, we will use the WRAP windblown dust (WBD) emissions model. The WRAP WBD model will be applied using the 3SAQS 2011 WRF model output and the same approach and data as used by WestJumpAQMS. Details on the model inputs, software, and configuration are available in the WestJumpAQMS Final Dust Emissions Technical Memo (Adelman, Morris and Loomis, 2013).

### **6.3.4 Seasalt and Lightning Emissions Processing**

For the 3SAQS, we will use the seasalt and lightning emissions processors developed by ENVIRON and the 3SAQS 2011 WRF data. Details on the model inputs, software, and configuration are available in the WestJumpAQMS final Seasalt and Lightning Emissions Technical Memo (Morris, Emery, Johnson and Adelman, 2012).

### **6.3.5 Methane Emissions Sources**

Special treatment will be given to methane emissions sources in the 3SAQS 2011 modeling platform. The CB6r2 photochemical mechanism in CAMv6.10 includes an active methane emissions species (ECH4) that contributes to the ozone chemistry. The species is input to the model on top of the background, steady state methane. For the first 3SAQS 2011 CAMx simulation (3SAQS\_CAMx\_Base11a), a single methane emission species emitted from all sources of methane in the NEI that does not distinguish between the different emissions sources will be input to CAMx. Adelman (2014) described a series of recommendations to improve the NEI methane inventory for 3SAQS. Only the correction to the wastewater treatment speciation profile will be implemented in 3SAQS\_CAMx\_Base11a; the additional inventory recommendations will be considered for future 3SAQS simulations.

## **6.4 Quality Assurance and Quality Control**

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

- Single day per year (aveday\_yr)
- Single day per month (aveday\_mon)
- Typical Monday, Weekday, Saturday, Sunday per year (mwdss\_yr)
- Typical Monday, Weekday, Saturday, Sunday per month (mwdss\_mon)

- Emissions estimated for each model simulation day (daily)
- Emissions estimated for each model simulation day with temporal profiles generated with average daily meteorology (daily met)
- Emissions estimated for each model simulation day with temporal profiles generated with hourly meteorology (hourly met)

## 7.0 PHOTOCHEMICAL MODELING

The 3SAQS project will conduct photochemical modeling using the CAMx and CMAQ photochemical grid models (PGMs).

PGM model simulations will be conducted for two emission scenarios:

- 2011 base case modeling that is used in the model performance evaluation and to define baseline air quality conditions.
- 2020 future year modeling for estimating the change to air quality under future year emissions conditions

The 3SAQS photochemical modeling will provide the framework for 2011-based NEPA EIS and other modeling for the three state region. This Chapter describes the model configurations for the CAMx and CMAQ 2011 and 2020 base case simulations, whereas Chapter 8 describes the model performance evaluation procedures for the 2011 simulation.

### 7.1 CAMx AND CMAQ Science and Input Configurations

Tables 7-1 and 7-2 summarize the, respectively, CAMx and CMAQ science configurations and options to be used for the 2011 base case simulations. CAMx Version 6.10 (released April 2014) and CMAQ Version 5.0.2 (released May 2014) will be used. CAMx V6.10 includes several recent updates that will be used in the 3SAQS such as the new CB6r2 chemical mechanism. CMAQ V5.0.2 does not include the CB6r2 chemistry so CB05 will be used. The models will be configured to predict both ozone and PM species as well as nitrogen and sulfur deposition.

We will use the PPM advection solver for horizontal transport (Colella and Woodward, 1984) along with the spatially varying (Smagorinsky) horizontal diffusion approach. CAMx will use K-theory for vertical diffusion using the CMAQ-like vertical diffusivities from WRF-CAMx, whereas CMAQ will use vertical diffusion coefficients from the MCIP processor. The CB6r2 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 as well as active methane chemistry. Additional CAMx and CMAQ inputs will be as follows:

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

**Initial/Boundary Conditions:** The boundary conditions (BCs) for the 36 km CONUS domain simulation will initially be based on the [MOZART](#) global chemistry model (GCM). Existing programs will be used to interpolate from the MOZART horizontal and vertical coordinate system to the CAMx LCP coordinate system and vertical layer structure and to map the MOZART chemical species to the chemical mechanisms being used by CAMx. The use of an alternative source for the BCs (e.g., GEOS-Chem GCM) will be the subject of sensitivity tests if available. However, at the time of the 2011 input development only MOZART GCM output data were available.

**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 be based on the Total Ozone Mapping Spectrometer (TOMS) data measured using the satellite-based Ozone Monitoring Instrument ([OMI](#)). 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<sup>3</sup>. For CAMx, the [TUV](#) 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.

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, 2010) will be used on the 36 km CONUS domain before adding the 12 and 4 km nested domains for the last two days of 2010 before the start of the 2011 calendar year (January 1, 2011).

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<sup>3</sup> Note that for the initial CAMx 2011 simulations the model is being configured for more typical warm season ozone conditions. To simulate winter ozone events, the model needs to be configured with higher resolution, with more refined WRF meteorological modeling and likely updated emission inventories and potentially chemistry, which will be done after the initial CAMx simulations.

**Table 7-1. CAMx (Version 6.10) model configurations for 3SAQS.**

Science Options	Configuration	Details
Model Codes	CAMx V6.10 – April 2014 Release	
Horizontal Grid Mesh	36/12/4 km	Added the 4km domain to the 3SAQS 2011 simulation
36 km grid	148 x 112 cells	36 km CONUS domain
12 km grid	227 x 230 cells	12 km WESTUS domain
4 km grid	281 x 299 cells	
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	
Initial Conditions	10 day spin-up on 36 km grid	Clean initial conditions
Boundary Conditions	36 km from global chemistry model	Initially use MOZART GCM data that is available for 2011. Investigate use of alternative GCM output for BCs as a sensitivity test if available.
Emissions		
Baseline Emissions Processing	SMOKE, MOVES and MEGAN	
Sub-grid-scale Plumes		
Chemistry		
Gas Phase Chemistry	CB6r2	Active methane chemistry and ECH4 tracer species
Meteorological Processor	WRFCAMx	Compatible with CAMx V6.10
Horizontal Diffusion	Spatially varying	K-theory with Kh grid size dependence
Vertical Diffusion	CMAQ-like in WRF2CAMx	
Diffusivity Lower Limit	Kz_min = 0.1 to 1.0 m <sup>2</sup> /s or 2.0 m <sup>2</sup> /s	Lane use dependent
Deposition Schemes		
Dry Deposition	Zhang dry deposition scheme (CAMx)	Zhang 2003
Wet Deposition	CAMx-specific formulation	rain/snow/graupel/virga
Numerics		
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) -- Fast Solver	
Vertical Advection Scheme	Implicit scheme w/ vertical velocity update (CAMx)	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	
Integration Time Step	Wind speed dependent	~0.1-1 min (4 km), 1-5 min (1 -km), 5-15 min (36 km)

**Table 7-2. CMAQ (Version5.0.2) model configurations for 3SAQS.**

Science Options	Configuration	Details/comments
Model Codes	CMAQ V5.0.2 – May 2014 Release	
Horizontal Grid Mesh	36/12/4 km	
36 km grid	148 x 112 cells	36 km CONUS domain
12 km grid	227 x 230 cells	12 km WESTUS domain
4 km grid	281 x 299 cells	4 km 3SAQS domain
Vertical Grid Mesh	25 vertical layers, defined by WRF	Layer 1 thickness ~24- m. Model top at ~19-km above MSL
Grid Interaction	36/12/4 km one-way nesting for CMAQ	CMAQ does not support two-way grid nesting
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 2011.
Emissions		
Baseline Emissions Processing	SMOKE, MOVES and MEGAN	
Sub-grid-scale Plumes		
Chemistry		
Gas Phase Chemistry	CB05 in CMAQ	CMAQ does not support CB6
Meteorological Processor	MCIPv4.2	
Horizontal Diffusion	Spatially varying	K-theory with Kh grid size dependence
Vertical Diffusion	ACM2	
Diffusivity Lower Limit	$Kz_{min} = 0.1$ to $1.0 \text{ m}^2/\text{s}$ or $2.0 \text{ m}^2/\text{s}$	Dependent on dominant land-use type (urban vs. rural)
Deposition Schemes		
Dry Deposition	Models-3 Scheme	
Wet Deposition		
Numerics		
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) -- Fast Solver	
Vertical Advection Scheme	Hybrid of Piecewise Parabolic Method and WRF omega calculation	
Horizontal Advection Scheme	Piecewise Parabolic Method	
Integration Time Step		

## 8.0 MODEL PERFORMANCE EVALUATION

This chapter describes the general model performance evaluation procedures that are designed to estimate the reliability of the CAMx/CMAQ models for simulating air quality, visibility and deposition in the western U.S. for the 2011 modeling period. An initial model performance evaluation would be conducted for ozone and fine particulate matter (PM<sub>2.5</sub>) and if the ozone and PM<sub>2.5</sub> model performance seems reasonable, a more detailed model performance evaluation would be conducted that also includes ozone/PM<sub>2.5</sub> 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. In addition, sensitivity simulations will be conducted for the winter ozone episodes and the model evaluated using the special winter field study data.

### 8.1 Overview of Model Performance Evaluation

Using the inputs and model configurations described in this Modeling Protocol, an initial CAMx base case simulation will be conducted for the 36/12/4 km domains and the 2011 calendar period. The initial 2011 base case ozone, total PM<sub>2.5</sub> mass and speciated PM<sub>2.5</sub> concentrations would be evaluated against concurrent measured ambient concentrations using graphical displays of model performance and statistical model performance measures that would be compared against established model performance goals and criteria. The CAMx performance evaluation will follow the procedures recommended in EPA's photochemical modeling guidance documents (e.g., EPA, 1991; 2007). Note that EPA is currently updating their modeling guidance, but the basic features on how to evaluate a photochemical grid model are expected to be similar.

After an initial overview of the model performance evaluation focusing on ozone and PM<sub>2.5</sub> is performed, a more detailed model performance evaluation will be conducted that also includes ozone/PM<sub>2.5</sub> precursor species (e.g., NO, NO<sub>2</sub>, NO<sub>x</sub> and SO<sub>2</sub>), related species (e.g., HNO<sub>3</sub>), visibility and deposition. The more detailed evaluation will also include more subregional evaluations and evaluations for specific episode periods of interest.

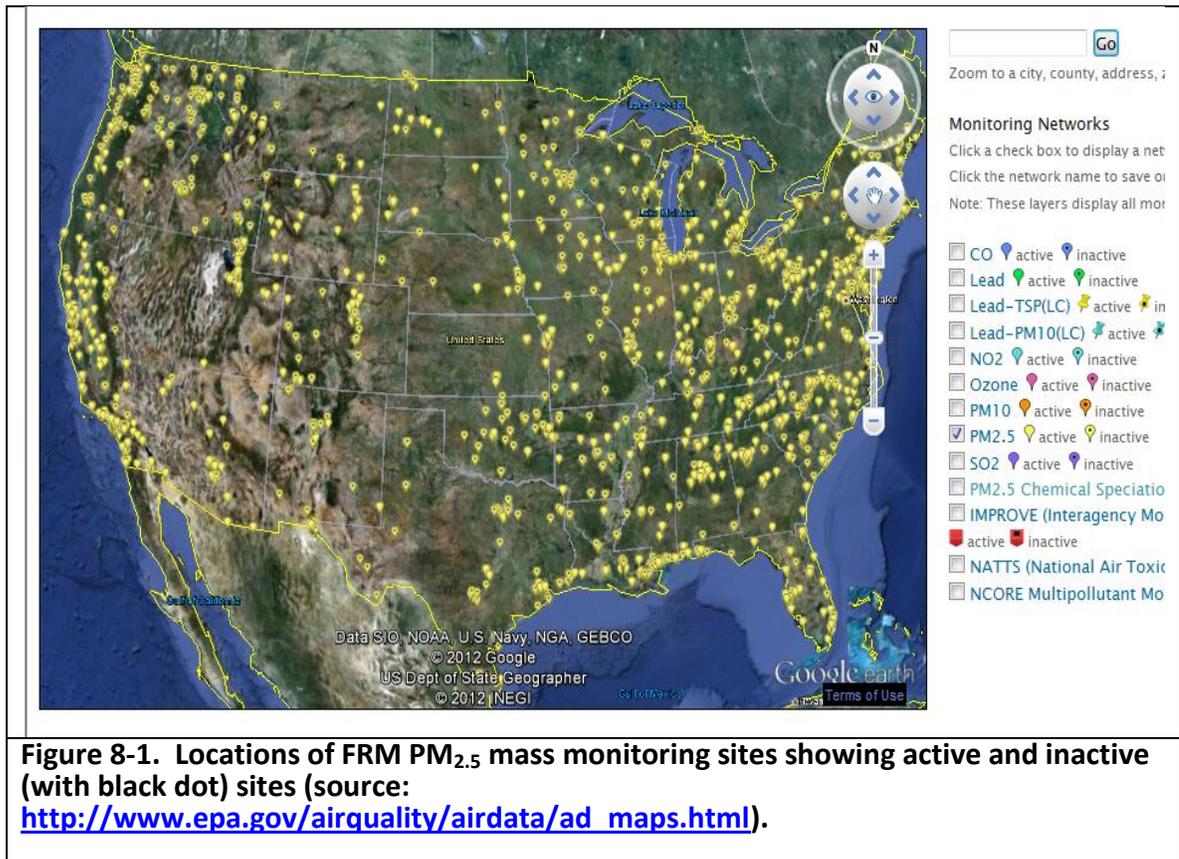
2011 CMAQ modeling and model performance evaluation will start in October 2014 and be performed under the 3SAQS 2015 SOW.

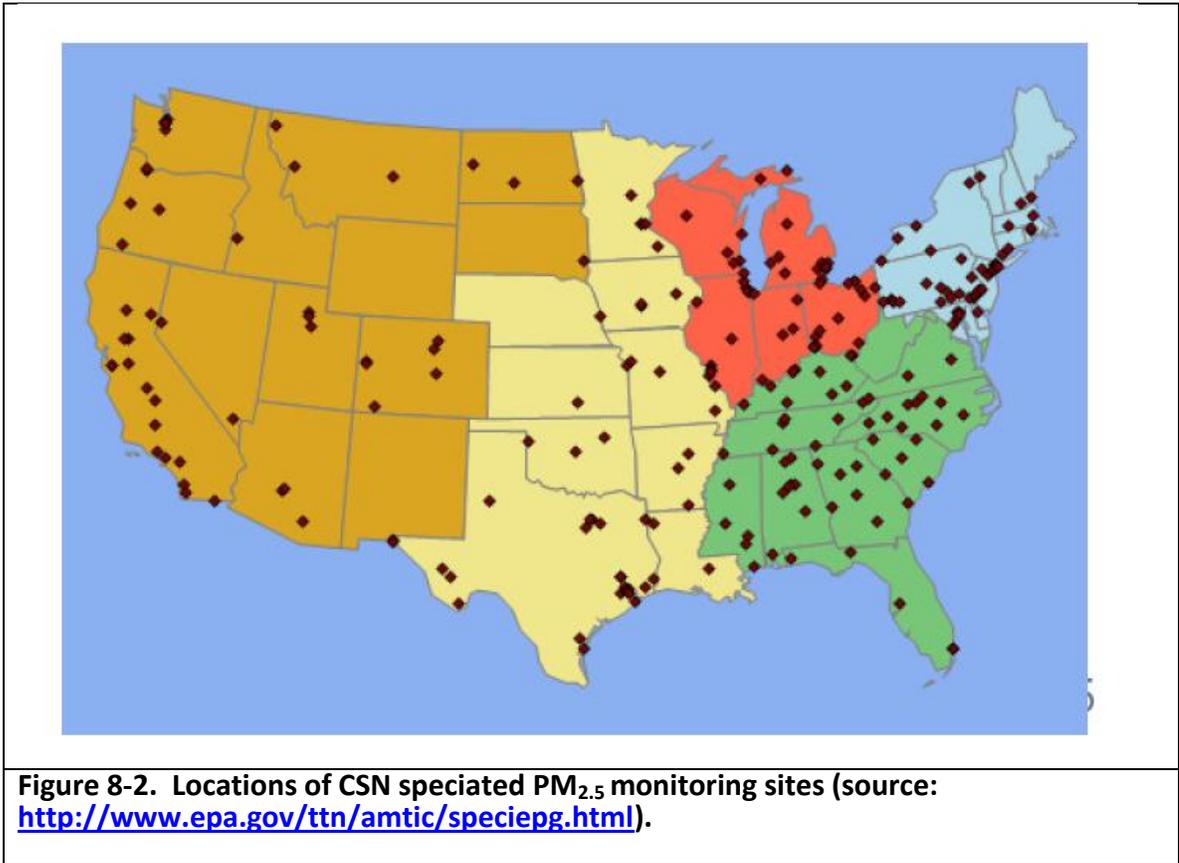
### 8.2 Available Aerometric Data for the model Evaluation

The following routine air quality measurement data networks operating in in 2011 will be used in the 3SAQS model performance evaluation:

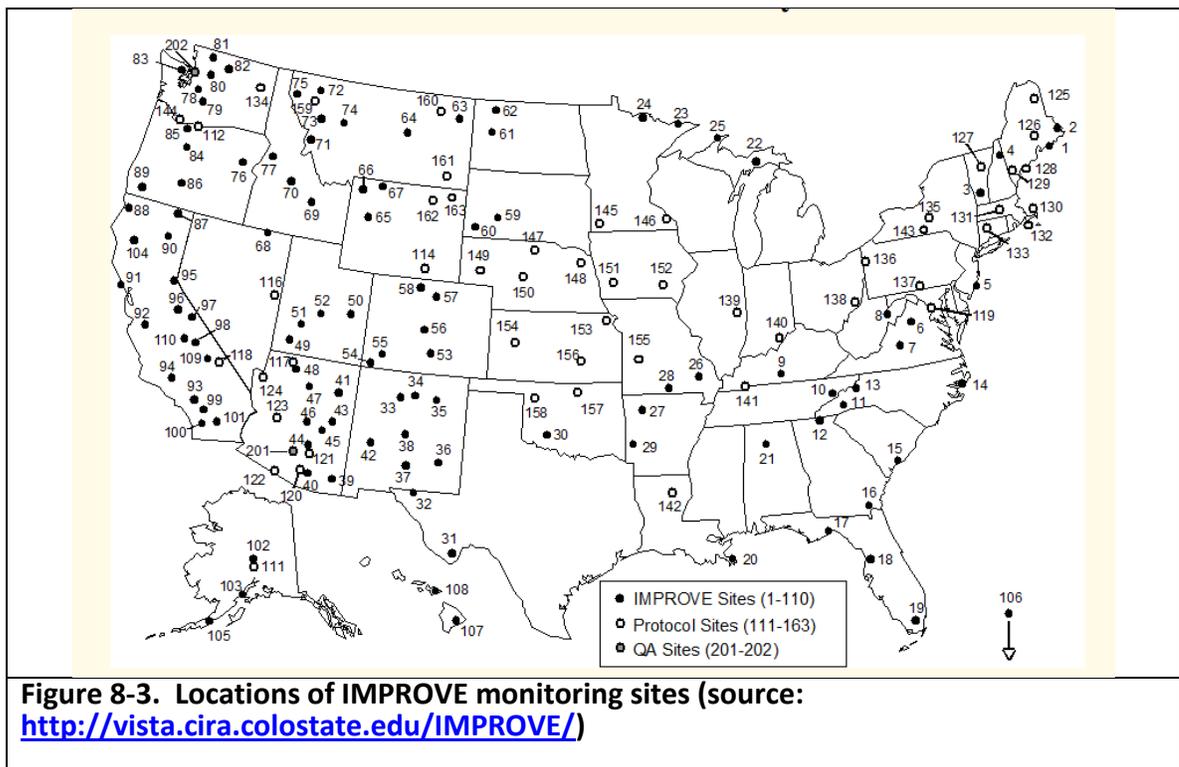
EPA AQS Surface Air Quality Data: Data files containing hourly-averaged concentration measurements at a wide variety of state and EPA monitoring networks are available in the Air Quality System ([AQS](#)) database throughout the U.S. The AQS consists of many sites that tend to be mainly located in and 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<sub>2</sub>, NO<sub>x</sub> and CO concentration and there are thousands of sites across the U.S. The Federal Reference Method (FRM) network measures 24-hour total PM<sub>2.5</sub> 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<sub>2.5</sub> concentrations

including SO<sub>4</sub>, NO<sub>3</sub>, NH<sub>4</sub>, 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 networks, respectively, the AIRS hourly network is not shown because the large number of sites makes the map unreadable.

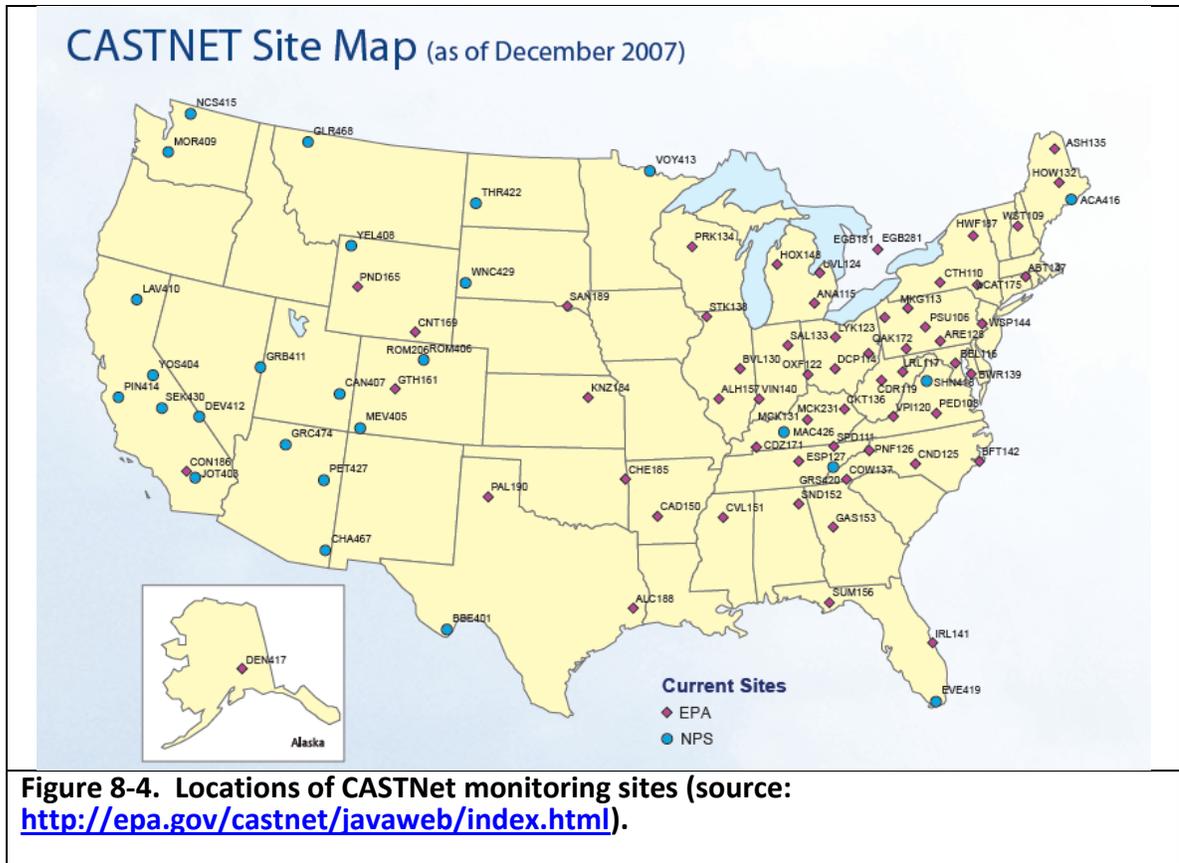




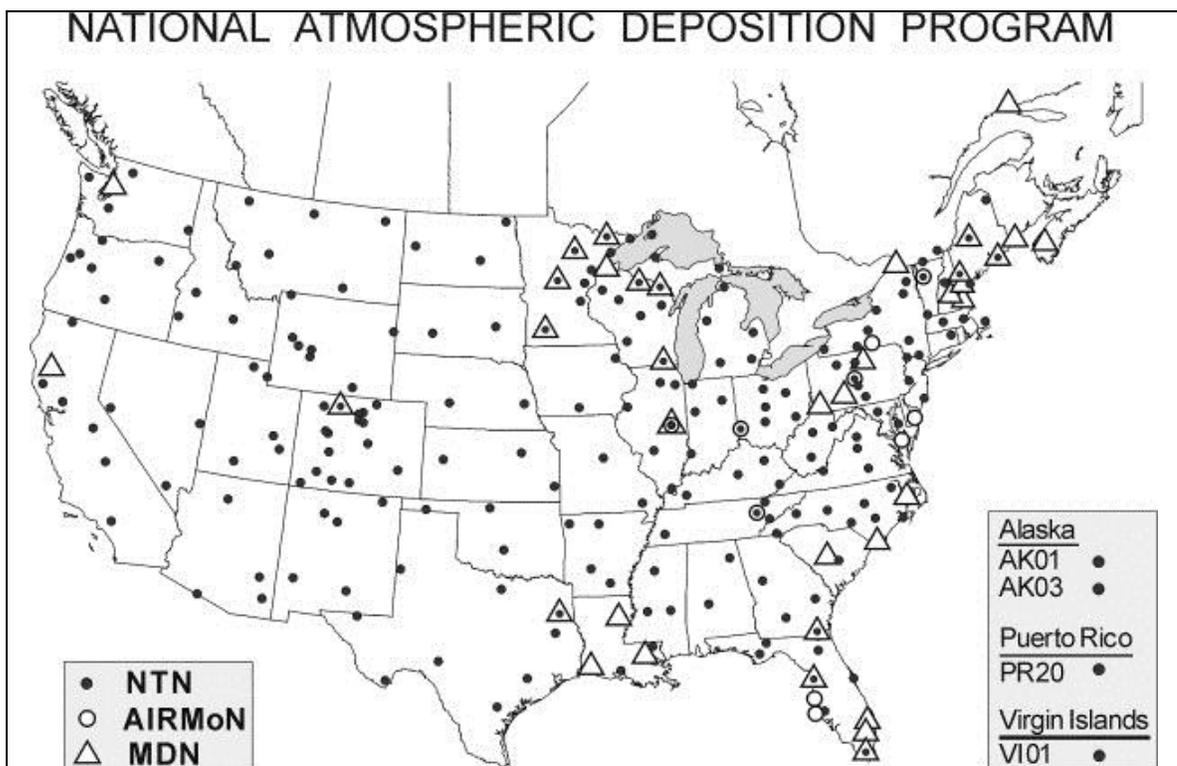
**IMPROVE Monitoring Network:** The Interagency Monitoring of Protected Visual Environments (IMPROVE) network collects 24-hour average PM<sub>2.5</sub> and PM<sub>10</sub> mass and speciated PM<sub>2.5</sub> concentrations (with the exception of ammonium) using a 1:3 day sampling frequency. IMPROVE monitoring 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.



**CASTNet Monitoring Network:** The Clean Air Status and Trends Network (**CASTNet**) operates approximately 80 monitoring sites in mainly rural areas across the U.S. CASTNet sites typically collected hourly ozone, temperature, wind speed and direction, sigma theta, solar radiation, relative humidity, precipitation and surface wetness. CASTNet also collects weekly (Tuesday to Tuesday) samples of speciated PM<sub>2.5</sub> sulfate, nitrate, ammonium and other relevant ions and weekly gaseous SO<sub>2</sub> and nitric acid (HNO<sub>3</sub>). Figure 8-4 displays the locations of the ~80 CASTNet sites across the U.S.



**NADP Network:** The National Acid Deposition Program ([NADP](#)) collects weekly samples of  $\text{SO}_4$ ,  $\text{NO}_3$  and  $\text{NH}_4$  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](#) throughout the world that measure the vertical structure of ozone concentrations throughout the troposphere and into the lower stratosphere. Ozonesonde monitoring sites within the 3SAQS modeling domain include: (1) Trinidad Head on the coast in northern California; (2) Boulder, Colorado; and (3) at the University of Alabama at Huntsville.

**Ammonia Monitoring Network (AMoN):** The [AMoN](#) collects gaseous ammonia measurements and currently operates ~50 sites across the U.S. It started in the fall of 2007 and was added to the NADP network in October 2010. There are currently 9 AMoN sites in the Three-State region. Unfortunately only one was operating throughout 2011, although 5 others started up in 2011. The models will be evaluated using all available ammonia measurements.

There is special study air quality or related monitoring sites that were operating during 2011 (e.g., Upper Green River Winter Ozone Study). However, since the 3SAQS is performing a regional air quality assessment of the western U.S., the initial focus of the model performance evaluation will be on the regional networks described above. However, sensitivity modeling and model performance evaluation will be conducted using the winter ozone study data under the 3SAQS 2015 SOW.

### 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)  $\leq \pm 20\%$
- Mean Normalized Bias (MNB)  $\leq \pm 15\%$
- Mean Normalized Gross Error (MNGE)  $\leq 35\%$

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

The MNB/MNGE uses hourly predicted and observed ozone concentrations paired by time and location and is defined as the difference between the predicted and the observed hourly ozone divided by the observed hourly ozone concentrations averaged over all predicted/observed pairs (see Table 8-2) within a given region and for a given time period (e.g., by day, month or modeling period). The MNGE is defined similarly only it uses the absolute value of the difference between the predicted and observed hourly ozone concentrations so is an unsigned metric. As the MNB/MNGE performance metrics divide by the observed hourly ozone concentration, the metric is calculated just using the predicted and observed hourly ozone pairs for which the observed hourly ozone concentration is above a threshold concentration. As recommended by EPA, a 60 ppb observed ozone cut-off threshold will be used when calculating ozone model performance statistics. Alternative cut-off thresholds will also be considered including using no threshold.

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<sub>2.5</sub> species definitions are defined by the measurement technology used to measure them and different measurement technologies can produce very different PM<sub>2.5</sub> concentrations. Given this, several researchers have developed PM model performance goals and criteria that are less stringent than the ozone goals as shown in Table 8-1 (Boylan, 2004; Morris et al., 2009a,b). However, unlike the 1991 ozone model performance goals that use the MNB and MNGE performance metrics, for PM species the Fractional Bias (FB) and Fractional Error (FE) are utilized with no observed concentration threshold screening. The FB/FE differ from the MNB/MNGE in that the difference in the predicted and observed concentrations are divide by the average of the predicted and observed values, rather than just the observed value as in the MNB/MNGE. This results in the FB being bounded by -200% to +200% and the FE being bounded by 0% to +200%. There are additional statistical performance metrics that

evaluate correlation, scatter as well as bias and error and a full suite of model performance metrics will be calculated for all species as given in Table 8-2.

**Table 8-1. PM model performance goals and criteria.**

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

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

More recently, EPA compiled and interpreted the model performance from 69 PGM modeling studies in the peer-reviewed literature between 2006 and March 2012 and developed recommendations on what should be reported in a model performance evaluation (Simon, Baker and Phillips, 2012). Although these recommendations are not official EPA guidance, they are useful and will be used in the 3SAQS model performance evaluation:

- PGM MPE studies should at a minimum report the Mean Bias (MB) and Error (ME or RMSE), and Normalized Mean Bias (NMB) and Error (NME) and/or Fractional Bias (FB) and Error (FE). Both the MNB and FB are symmetric around zero with the FB bounded by -200% to +200%.
- Use of the Mean Normalized Bias (MNB) and Gross Error (MNGE) is not encouraged because they are skewed toward low observed concentrations and can be misinterpreted due to the lack of symmetry around zero.

Given this recommendation the MNB/MNGE will just be calculated for ozone using an appropriate observed ozone cut-off concentration (3SAQS will use 60 ppb).

- The model evaluation statistics should be calculated for the highest resolution temporal resolution available and for important regulatory averaging times (e.g., daily maximum 8-hour ozone).
- It is important to report processing steps in the model evaluation and how the predicted and observed data were paired and whether data are spatially/temporally averaged before the statistics are calculated.

- Predicted values should be taken from the grid cell that contains the monitoring site, although bilinear interpolation to the monitoring site point can be used for higher resolution modeling (< 12 km).
- PM<sub>2.5</sub> should also be evaluated separately for each major component species (e.g., SO<sub>4</sub>, NO<sub>3</sub>, NH<sub>4</sub>, EC, OA and OPM<sub>2.5</sub>).
- Evaluation should be performed for subsets of the data including, high observed concentrations (e.g., ozone > 60 ppb), by subregions and by season or month.
- Evaluation should include more than just ozone and PM<sub>2.5</sub>, such as SO<sub>2</sub>, NO<sub>2</sub> and CO.
- Spatial displays should be used in the model evaluation to evaluate model predictions away from the monitoring sites. Time series of predicted and observed concentrations at a monitoring site should also be used.
- It is necessary to understand measurement artifacts in order to make meaningful interpretation of the model performance evaluation.

We will incorporate the recommendations of Simon, Baker and Philips (2012) into the 3SAQS model performance evaluation. The 3SAQS evaluation products will include qualitative and quantitative evaluation for the following model output species:

- Maximum daily 1-hour and maximum daily 8-hour average (MDA8) ozone, including MDA8 with a 60 ppb threshold
- Carbon monoxide, nitrogen dioxide, NO<sub>x</sub>, volatile organic compounds (VOCs) and ammonia
- Total PM<sub>2.5</sub>, elemental carbon, organic carbon, sulfate, nitrate, ammonium, and visibility metrics
- Total sulfur and total nitrogen wet and dry deposition
- Vertical ozone comparisons to ozonesonde and available aircraft observation data

**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)	$\frac{\left[ \sum_{i=1}^N (P_i - \bar{P})(O_i - \bar{O}) \right]^2}{\sum_{i=1}^N (P_i - \bar{P})^2 \sum_{i=1}^N (O_i - \bar{O})^2}$	$P_i$ = prediction at time and location $i$ ; $O_i$ = observation at time and location $i$ ; $\bar{P}$ = arithmetic average of $P_i$ , $i=1,2,\dots, N$ ; $\bar{O}$ = arithmetic average of $O_i$ , $i=1,2,\dots, N$
Normalized Mean Error (NME)	$\frac{\sum_{i=1}^N  P_i - O_i }{\sum_{i=1}^N O_i}$	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  \frac{P_i - O_i}{P_i + O_i} \right $	Reported as % and bounded by 0% to 200%
Mean Absolute Gross Error (MAGE)	$\frac{1}{N} \sum_{i=1}^N  P_i - O_i $	Reported as concentration (e.g., $\mu\text{g}/\text{m}^3$ )
Mean Normalized Gross Error (MNGE)	$\frac{1}{N} \sum_{i=1}^N \frac{ P_i - O_i }{O_i}$	Reported as %
Mean Bias (MB)	$\frac{1}{N} \sum_{i=1}^N (P_i - O_i)$	Reported as concentration (e.g., $\mu\text{g}/\text{m}^3$ )
Mean Normalized Bias (MNB)	$\frac{1}{N} \sum_{i=1}^N \frac{(P_i - O_i)}{O_i}$	Reported as %
Mean Fractionalized Bias (Fractional Bias, FB)	$\frac{2}{N} \sum_{i=1}^N \left( \frac{P_i - O_i}{P_i + O_i} \right)$	Reported as %, bounded by -200% to +200%
Normalized Mean Bias (NMB)	$\frac{\sum_{i=1}^N (P_i - O_i)}{\sum_{i=1}^N O_i}$	Reported as %
Bias Factor (BF)	$\frac{1}{N} \sum_{i=1}^N \left( \frac{P_i}{O_i} \right)$	Reported as BF:1 or 1: BF or in fractional notation (BF/1 or 1/BF).

## 8.4 Subregional Evaluation of Model Performance

The evaluation of the CAMx 36/12/4 km base case simulations will focus on a monthly, quarterly and annual model performance at monitors in Colorado, Utah, and Wyoming. We will also examine a few high ozone episodes for more detailed analysis and determine how well the model performs on ozone exceedance days and locations.

## 8.5 Example Model Performance Displays

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

### 8.5.1 Model Evaluation Tools

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

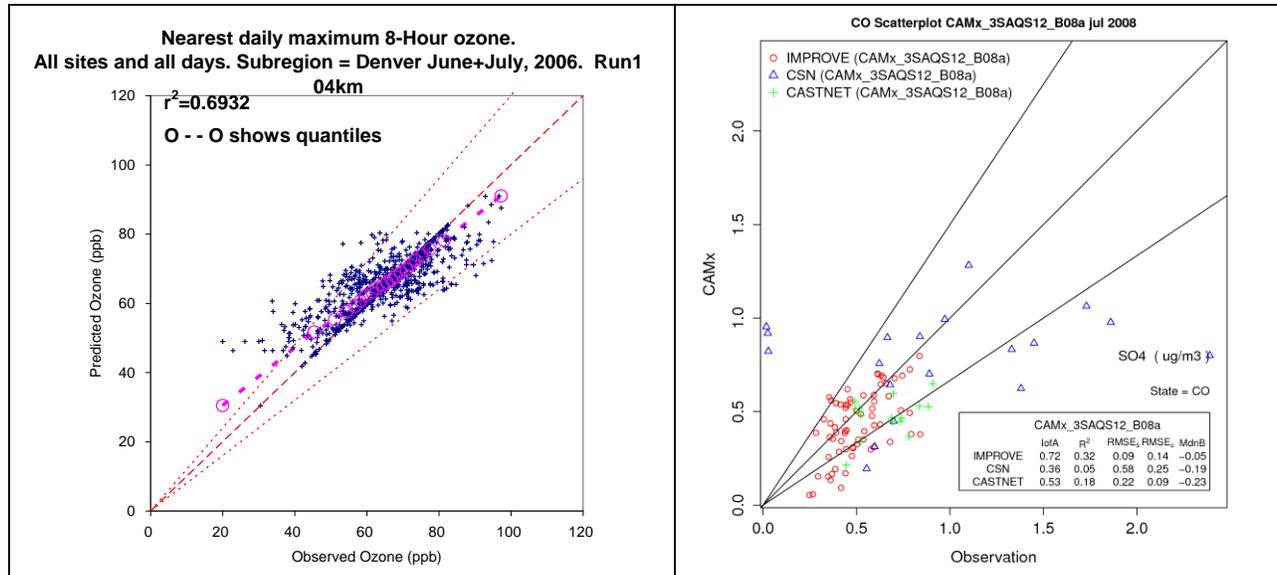
- **PAVE and VERDI:** The Package for Analysis and Visualization ([PAVE](#)) and Visualization Environment for Rich Data Interpretation ([VERDI](#)) are visualization tools specifically designed to visualize photochemical grid model output. They can run on both a Linux and Windows environment, so can be used while the photochemical grid model is running or has recently been completed. Both tools are primarily used for spatial maps where modeled tile plots can be displayed with superimposed observations. VERDI can also generate scatter and time series plots. Although VERDI has replaced PAVE, which is no longer supported, because the modeling community has scripts already set up for PAVE, PAVE is easier to use and VERDI does not have some of the functionality of PAVE, PAVE is still a useful and viable model evaluation tool.
- **Excel:** The Microsoft Excel spreadsheet software tool is used extensively to generate various model performance displays (e.g., scatter, time series and soccer plots) under Windows. 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](#)) 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. AMET will be used extensively for the 3SAQS 2011 model performance evaluation.

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

### 8.5.2 Scatter Plots

Figure 8-6 displays example scatter plots using the Excel and AMET. An example Excel scatterplot is given in the 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  $\pm 20\%$  of each other; in the past EPA had a performance goal that the predicted daily

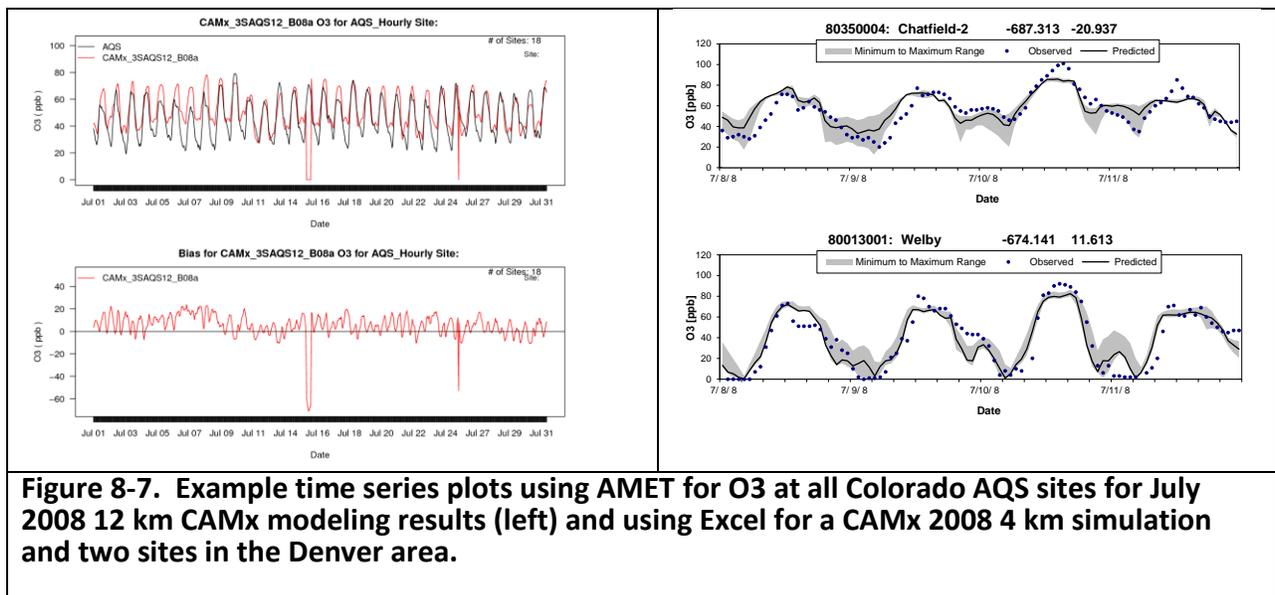
maximum 8-hour ozone concentration near a monitor be within  $\pm 20\%$  of the observed value most of the time. The example scatterplot in the right panel of Figure 8-6 was generated using AMET and shows CMAQ monthly average sulfate performance for July 2008 for all sites in Colorado. The AMET scatterplot can also display statistical performance measures and in this case uses separate symbols for  $\text{SO}_4$  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 CSN networks.



**Figure 8-6. Example model performance evaluation scatterplots for predicted and observed daily maximum 8-hour ozone concentrations using Excel (left) and July 2008 monthly averaged predicted and observed sulfate at all Colorado sites using AMET (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 hourly time series comparison for 1-hour average O<sub>3</sub> concentrations at all AQS sites in Colorado for July 2008 using AMET. The AMET timeseries displays the model to observations in the top panel and the model bias for each hour in the bottom panel. 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 AMET for O<sub>3</sub> at all Colorado AQS sites for July 2008 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.

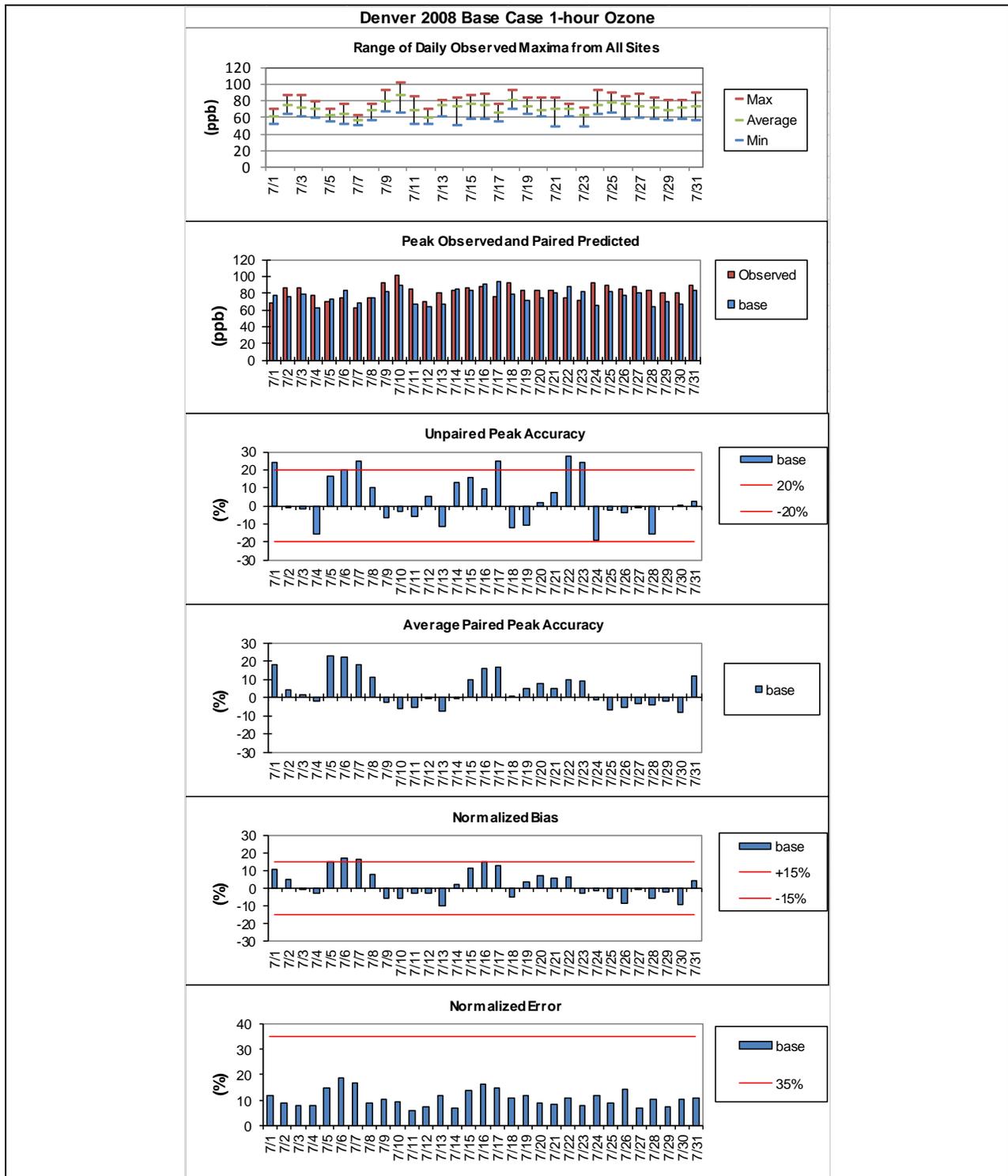
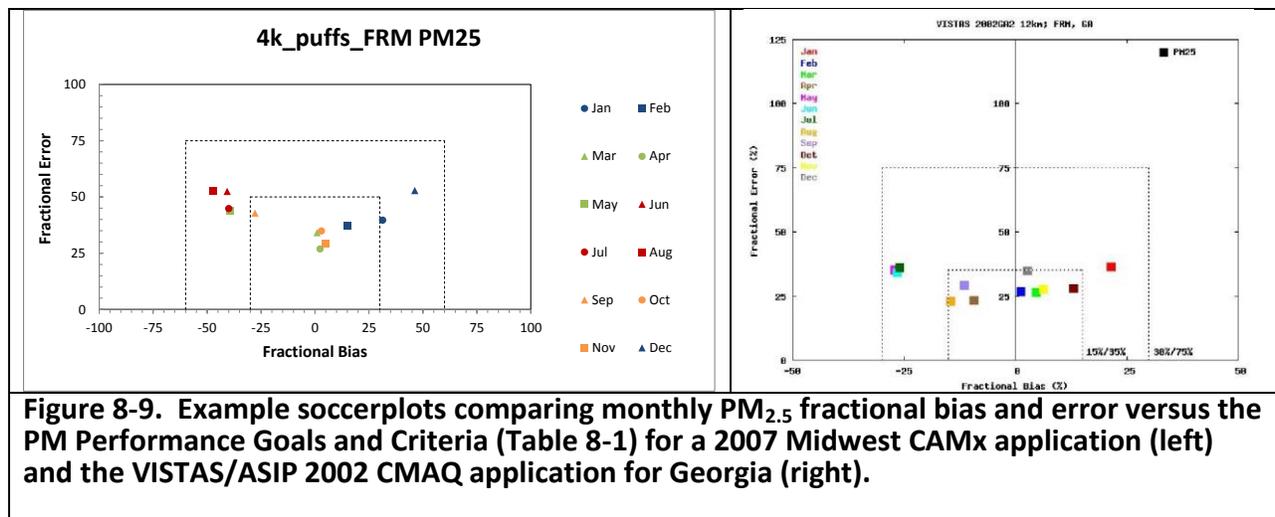


Figure 8-8. Example of hourly ozone model performance statistics comparing the UPA, MNB and MNGE statistics with EPA's 1991 ozone performance goals (red lines).

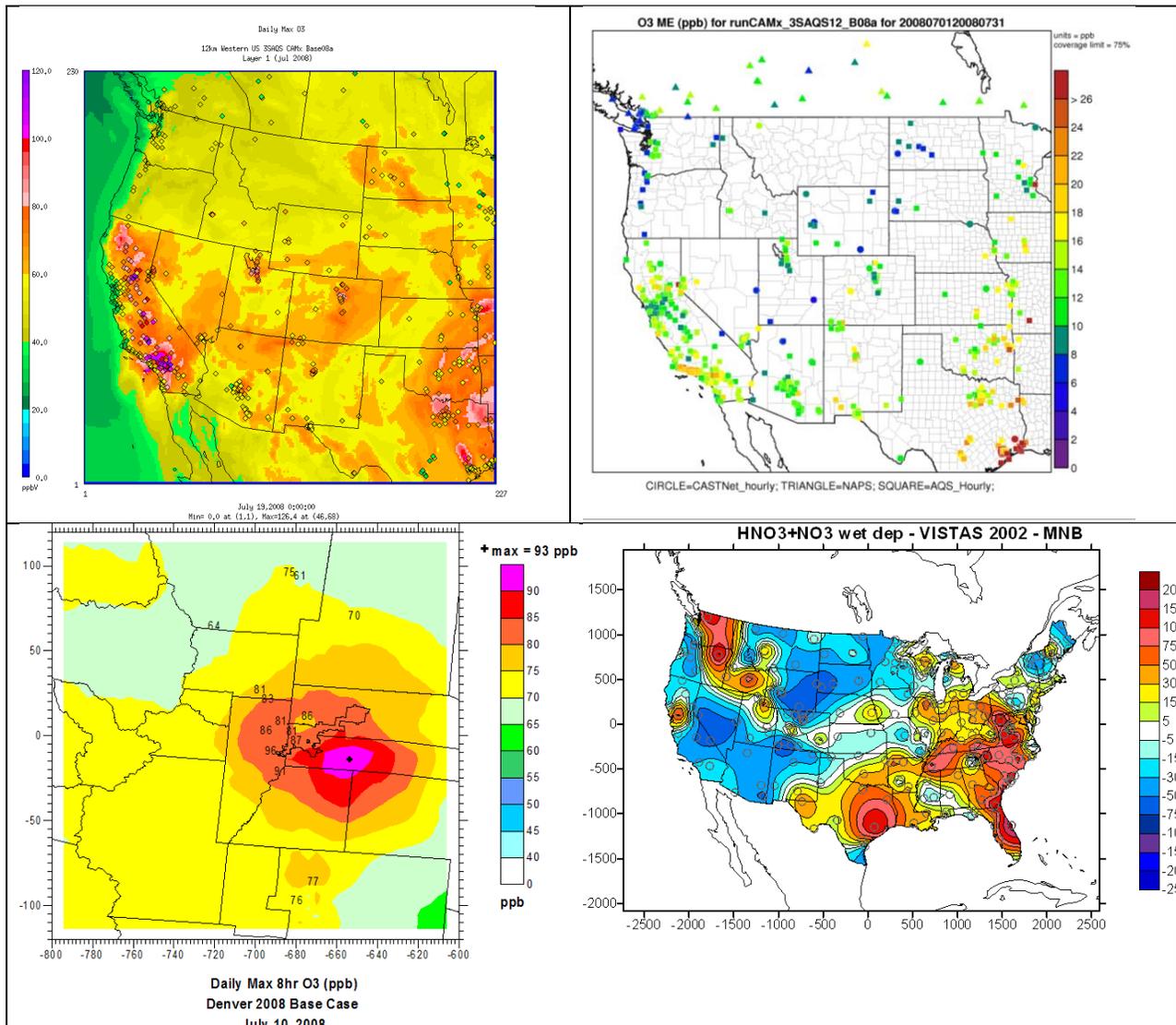
### 8.5.5 SoccerPlots Comparing Model Performance Statistics with Performance Goals

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<sub>2.5</sub> 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<sub>2.5</sub> underestimation bias that fails to achieve the PM Performance Goal, but does achieve the PM Performance Criteria.



### 8.5.6 Spatial Plots of Model Performance

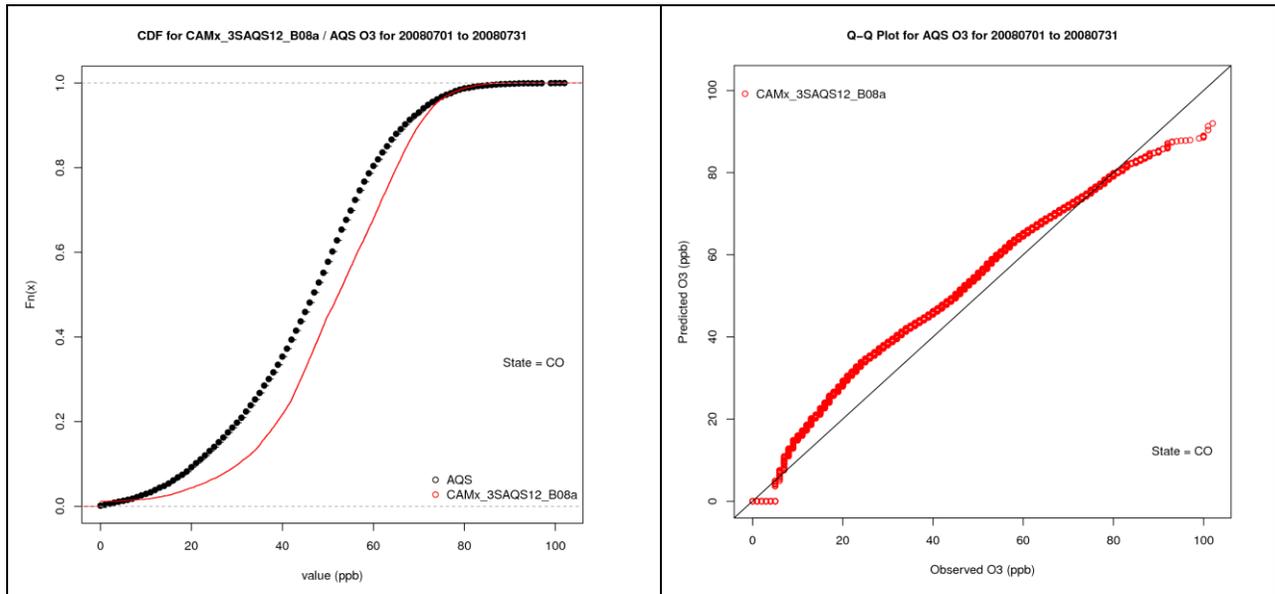
Examples of spatial displays of modeling results are presented in Figure 8-10. The top left panel of Figure 8-10 is from the VISTAS/ASIP 2002 CMAQ modeling (Morris et al., 2009a) and compares the predicted 24-hour average PM<sub>2.5</sub> concentrations on September 5, 2002 (the tile plot) with superimposed observations (the diamond symbols) using the same color scale and 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. 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 3SAQS CAMx 12-km daily max O<sub>3</sub> performance on July 19, 2008 using PAVE (top left); July 2008 monthly mean error for O<sub>3</sub> at different monitors using AMET (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).**

### 8.5.6 Additional Plots of Model Performance

Examples of additional displays of modeling results are presented in Figure 8-11. Both plots in Figure 8-11 are from the 3SAQS 2008 CAMx modeling and compare the predicted 1-hour average O<sub>3</sub> concentrations for all AQS sites in Colorado in July 2008. The left plot is a cumulative density function and organizes the model results and observations by the cumulative fraction of values that are less than a series of concentration bins. The Q-Q plot on the right shows unpaired observation and model results sorted from small to large values. Both of these plots lend perspective on the model performance at different concentration ranges (i.e. under-estimation at high concentrations).



**Figure 8-11. Example plots comparing hourly July 2008 AQS O3 for the 3SAQS 2008 CAMx application. A cumulative density function plot organizes the model and observations by the cumulative fraction of values below different concentration bins (left); a Q-Q plot displays an unpaired numerical sorting of the model results and observations (right).**

## 8.6 Summary of Model Performance

A model performance of the CAMx and CMAQ 36/12/4 km 2011 base case simulations will be conducted for ozone, ozone precursors, methane, PM<sub>2.5</sub> and speciated PM<sub>2.5</sub> concentrations and wet sulfur and nitrogen depositions over the three state region. This will be followed by subregional evaluation of the 12 and 4 km modeling results focusing on subdomains in Colorado, Utah, and Wyoming. Dry deposition will be evaluated as appropriate (note that dry deposition “measurements” are obtained through application of a surface layer model) and we will keep track of the nitrogen species components in the modeled wet and dry deposition.

## 9.0 WEBSITE REPORTING AND SOURCE APPORTIONMENT MODELING

Because of the sheer volume of information that will be generated as part of the meteorological and emissions modeling, and in the model performance evaluation, the results will be made available on the Three-State Data Warehouse (3SDW) project website with summary reports and PowerPoint presentations also generated. We will post data and reports as work is completed. Note that in addition to 3SAQS, WESTAR is also managing the 3SDW that will also be distributing related information.

### 9.1 Interactive Website

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

In addition to the contributions to ozone and PM<sub>2.5</sub> 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.

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

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

[http://www.ie.unc.edu/cempd/projects/data\\_viewer/index.cfm?project=3SAQS](http://www.ie.unc.edu/cempd/projects/data_viewer/index.cfm?project=3SAQS)

### 9.2 Reports

Summary reports and PowerPoint presentations will be prepared at the end of each major task of the 2011 modeling. An important component of the reporting summaries will be examples of where more information can be obtained on the website. The following reports have been or will be prepared under the 3SAQS:

- Technical Scope of Work
- Modeling Plan
- 3SDW Design Document
- 2011 WRF Modeling Protocol
- 2011 WRF Model Performance Evaluation Report
- 2011 Air Quality Modeling Protocol (this document)
- 2011 Base Case Modeling and Model Performance Evaluation Report
- 2020 Base Case and Air Quality Modeling Results Report
- Final Report

### 9.3 Source Apportionment Modeling

Ozone and Particulate Matter (PM) source apportionment modeling will be performed using the 2011 modeling platform and the CAMx PGM. Both geographic (e.g., state) and emission sector source

apportionment modeling will be conducted. A source apportionment design document will be prepared with the 3SAQS cooperators that defines how the source apportionment runs will be conducted and analyzed prior to performing them.

## 10.0 ACRONYMS

3SAQS	Three-State Air Quality Study
3SDW	Three-State Data Warehouse
ACHD	Allegheny County Health Department
ACM	Asymmetric Convective Mixing
AES	Applied Envirosolutions
AMET	Atmospheric Model Evaluation Tool
APCA	Anthropogenic Precursor Culpability Assessment
APU	Auxiliary Power Units
AQ	Air Quality
AQRV	Air Quality Related Value
AQS	Air Quality System
BC	Boundary Condition
BEIS	Biogenic Emissions Information System
BLM	Bureau of Land Management
CAFOS	Concentrated Animal Feeding Operations
CAMD	Clean Air Markets Division
CAMx	Comprehensive Air-quality Model with extensions
CASTNet	Clean Air Status and Trends Network
CAVR	Clean Air Visibility Rule
CB05	Carbon Bond mechanism version 5
CB6r2	Carbon Bond mechanism version 6, revision 2
CD-C	Continental Divide-Creston
CDPHE	Colorado Department of Health and Environment
CEM	Continuous Emissions Monitor
CENRAP	Central Regional Air Planning Association
CMAQ	Community Multiscale Air Quality modeling system
CMU	Carnegie Mellon University
ConCEPT	Consolidated Community Emissions Processing Tool
CONUS	Continental United States
CPC	Center for Prediction of Climate
CSAPR	Cross State Air Pollution Rule
CSN	Chemical Speciation Network
DDM	Decoupled Direct Method
DEASCO3	Deterministic and Empirical Assessment of Smoke's Contribution to Ozone
DMA	Denver Metropolitan Area
DSAD	Detailed Source Apportionment Domain
EAC	Early Action Compact
ECA	Emissions Control Area
EGU	Electrical Generating Units
EIS	Environmental Impact Statement
EM	Emissions Model
EMS	Emissions Modeling System
EPA	Environmental Protection Agency
EPS	Emissions Processing System

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

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

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