




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

Final Modeling Plan

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Contents

1.0 INTRODUCTION 1
1.1 Background 2
1.2 Organization of the Modeling Plan 3
2.0 MODEL SELECTION 4
2.1 Overview of Selected Models 4
2.2 Model Interaction 6
3.0 EPISODE SELECTION 7
4.0 DOMAIN SELECTION 8
4.1 Impact Assessment Domains (IAD) 9
4.2 Detailed Source Apportionment Domains (DSAD) 15
4.2 vertical domain structure 22
5.0 METEOROLOGICAL MODELING 23
5.1 Model Selection and Application 23
5.2 Horizontal Domain Definition 23
5.3 Vertical Domain Definition 23
5.4 Topographic Inputs 23
5.5 Vegetation Type and Land Use Inputs 24
5.6 Atmospheric Data Inputs 26
5.7 Water Temperature Inputs 26
5.8 FDDA Data Assimilation 26
5.9 WRF Physics Options 26
5.10 Application Methodology 27
5.11 Evaluation Approach 27
5.12 reporting 27
6.0 EMISSIONS 28
6.1 emission data sources 28
6.2 on-road mobile sources 31
6.3 area and non-road mobile sources 31
6.4 2008 OIL and gas emissions update 31
6.5 Fire Emissions 33
6.6 Ammonia Emissions 34

6.7 Ocean Going Vessels 34
6.8 Biogenic Emissions 34
6.9 Spatial Allocation 34
6.10 Chemical speciation 34
6.11 Quality Assurance and Quality Control 34
6.12 Reporting 35
7.0 PHOTOCHEMICAL MODELING 36
7.1 CAMx and cmaq Science and Input Configurations 36
7.2 2008 Base case modeling and MODEL PERFORMANCE EVALUATION 39
7.3 source apportionment modeling 40
8.0 WEBSITE AND REPORTING 41
8.1 interactive website 41
8.2 Reports 41
9.0 REFERENCES 42

TABLES

Table 5-1. 37 Vertical layer definition for WRF simulations (left most columns), and approach for reducing to 25 vertical layers for CAMx/CMAQ by collapsing multiple WRF layers (right columns). 25
Table 6-1. Summary of sources of emissions and emission models to be used in generating PGM emissions inputs for the WestJumpAQMS study. 30
Table 7-1. CAMx (Version 5.3 or newer) and CMAQ (Version 4.7.1 or newer) model configuration. 38

FIGURES

Figure 4-1. 36-km CONUS, 12-km WESTUS and 4-km IMWD Processing Domain That Meteorological and Emission PGM Inputs Will Be Developed For. 9
Figure 4-2. 4-km Imwd Processing Domain and Four 4-km Impact Assessment Domains (IAD) For Which Stand-Alone 4-Km Photochemical Modeling Databases Will Be Developed For 2008. 11
Figure 4-3. Four Corners 4-km IAD Domain That Includes The San Juan Basin. 12
Figure 4-4. Utah-Colorado 4-km IAD Domain That Includes The Uinta, Piceance and Denver-Julesburg Basins. 13
Figure 4-5. Wyoming 4-Km IAD Domain That Includes The Uinta, Southwest Wyoming And Powder River Basins. 14

Figure 4-6. Montana-North Dakota 4-km IAD Domain That Includes The Williston Basin. 15

Figure 4-7. Relationship Between The Six 4-km DSAD Domains And The 4-km IMWD Processing Domain. 16

Figure 4-8. Southeastern New Mexico 4-km DSAD Domain That Includes The Permian Basin. 17

Figure 4-9. Four Corners 4-km DSAD Domain That Includes The North And South San Juan Basins. 18

Figure 4-10. Uinta-Piceance Basins 4-km DSAD Domain. 19

Figure 4-11. Denver-Julesburg Basin 4-km DSAD Domain. 20

Figure 4-12. Wyoming 4-km DSAD Domain. 21

Figure 4-13. Montana-North Dakota 4-km DSAD Domain. 21

Figure 5-1. Wrf 36/12/4-km Grid Structure For The Westjumpaqms Meteorological Modeling. 24

1.0 INTRODUCTION

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

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

The goals of the WestJumpAQMS include the following:

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

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

1.1 BACKGROUND

In 1997, EPA promulgated the first 8-hour Ozone National Ambient Air Quality Standard (NAAQS) with a threshold of 0.08 ppm (85 ppb). On March 12, 2008, EPA promulgated a more stringent 0.075 ppm (75 ppb) 8-hour Ozone NAAQS. In January 2010, EPA announced that they were considering lowering the 8-hour Ozone NAAQS to within a range of 0.060 ppm to 0.070 ppm. In August 2011, the EPA announced that the 8-hour ozone NAAQS would remain at the March 2008 0.075 ppm level. An initial implementation Memorandum was released by EPA on September 22, 2011 (McCarthy, 2011) that identified 52 potential areas that would be violating the 0.075 ppm 8-hour Ozone NAAQS based on 2008-2010 observations, including many in the western U.S., with EPA expected to finalize the Ozone nonattainment area designations by mid-2012. EPA has also initiated the next round of Ozone NAAQS review with the new Ozone NAAQS currently scheduled to be proposed in March 2013 and finalized in March 2014.

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

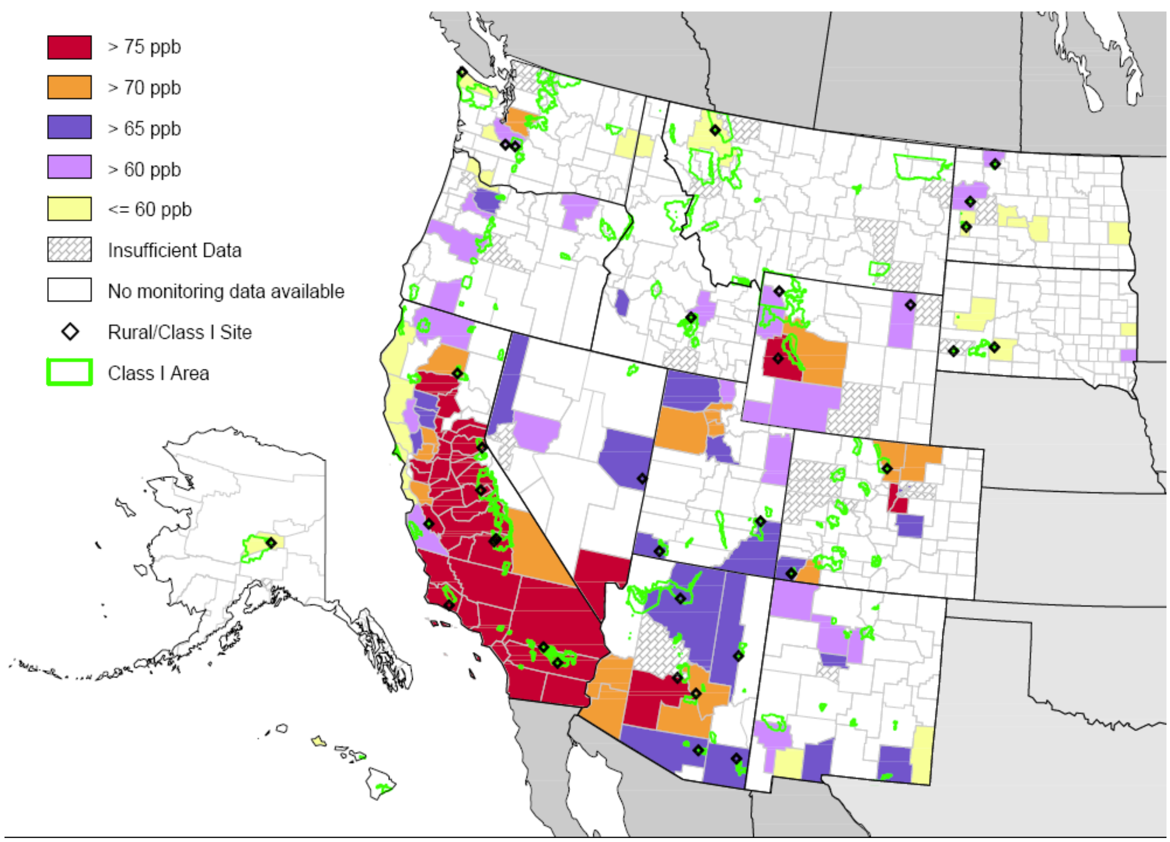

Figure 1-1. 3-year average (2008-2010) fourth highest 8-hour ozone Design Value for selected counties with color scheme indicating whether the Design Value exceeds (red) or is below the

March 2008 ozone NAAQS (EPA AQS Federal Reference Method [FRM] data from the monitoring site with the highest ozone in each county).

1.2 ORGANIZATION OF THE MODELING PLAN

This document represents a Modeling Plan for the WestJumpAQMS. This Modeling Plan is an informal document used to communicate the procedures and objectives of the WestJumpAQMS to the various study stakeholders so that feedback can be obtained and the study can be designed to serve the needs of the stakeholders. This is in contrast with a Modeling Protocol that has specific contents and structure (EPA, 2007) and represents a more formal document. The WestJumpAQMS will have a draft Modeling Protocol developed in Phase 2 of this project, and a final Modeling Protocol in Phase 3. This Modeling Plan has the following sections:

1. Introduction: Presents a summary the background, purpose and objectives of the study.
2. Model Selection: Introduces the models selected for the study.
3. Episode Selection: Discusses the modeling period for the study.
4. Domain Selection: Presents the proposed modeling domains and grid structure for the modeling study.
5. Meteorology: Discusses the strategy for performing WRF meteorological modeling.
6. Emissions: Source of emissions, emissions models and emissions modeling methodology is discussed.
7. Photochemical Modeling: The approach for the photochemical source apportionment modeling is presented.
8. Reporting/Website: How results will be reported and the development of a website for distributing information is presented.
9. References: References cited in the document.

2.0 MODEL SELECTION

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

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

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

2.1 OVERVIEW OF SELECTED MODELS

The following models were selected for use in the WestJumpAQMS study.

WRF[1]: The non-hydrostatic version of the Advanced Research version of the Weather Research Forecast (WRF-ARW[2]) model (Skamarock et al. 2008; Michalakes et al. 2001) 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 meters to thousands of kilometers.

SMOKE[3]: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is an emissions modeling system that generates hourly gridded speciated emission inputs of mobile, non-road, area, point, fire and biogenic emission sources for photochemical grid models (Coats, 1995; Houyoux et al., 2000). As with most 'emissions models', SMOKE is principally an *emission processing system* and not a true *emissions modeling system* in which emissions estimates are simulated from 'first principles'. This means that, with the exception of mobile and biogenic sources, its purpose is to provide an efficient, modern tool for converting an existing base emissions inventory data into the hourly gridded and speciated emission files required by an air quality simulation model. For mobile sources, SMOKE can simulates emissions rates based on input mobile-source activity data, emission factors and outputs from transportation travel-demand models.

1 http://www.wrf-model.org/index.php
2 All references to WRF in this document refer to the WRF-ARW
3 http://www.smoke-model.org/version2.7/

MOVES[4]: The MOtor Vehicle Emission Simulator model (MOVES) is a multi-scale emissions modeling system that generates emission inventories or emission rate lookup tables for on-road mobile sources. MOVES is capable of creating inventories or lookup tables at the national, state, county, or project scales. MOVES was designed by EPA's Office of Transportation and Air Quality (OTAQ) and their latest release version as of August 2010 is MOVES2010a. MOVES is principally an emissions modeling system where emissions estimates are simulated from 'first principles' taking into account the effects of fleet age deterioration, ambient temperature and humidity, activity patterns, fuel properties, and inspection and maintenance programs on emissions from all types of motor vehicles. MOVES outputs can be input to emissions processing systems such as SMOKE.

MEGAN[5]: 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 (Wiedinmyer, Sakulyanontvittaya and Guenther, 2007[6]). 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).

CAMx[7]: 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, 2010). CAMx is a publicly available open-source computer modeling system for the integrated assessment of gaseous and particulate air pollution. Built on today's understanding that air quality issues are complex, interrelated, and reach beyond the urban scale, CAMx is designed to (a) simulate air quality over many geographic scales, (b) treat a wide variety of inert and chemically active pollutants including ozone, inorganic and organic $PM_{2.5}$ and PM_{10} and mercury and toxics, (c) provide source-receptor, sensitivity, and process analyses and (d) be computationally efficient and easy to use. The U.S. EPA has approved the use of CAMx for numerous Ozone and PM State Implementation Plans throughout the U.S, and has used this model to evaluate regional mitigation strategies including those for recent regional rules (e.g., CSAPR, CATR, CAIR, NO_X SIP Call, etc.). Of particular importance for the WestJumpAQMS study is the available of Ozone and Particulate Source Apportionment Technology (OSAT/PSAT) that will be used to perform source apportionment modeling across the western states.

CMAQ[8]: 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

4 http://www.epa.gov/otaq/models/moves/index.htm
5 http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm
6 http://acd.ucar.edu/~guenther/MEGAN/MEGANguideFORTRAN204.pdf
7 http://www.camx.com/
8 http://www.cmaq-model.org/

motions, (b) an emission models for man-made and natural emissions that are injected into the atmosphere, and (c) a chemistry-transport modeling system for simulation of the chemical transformation and fate.

2.2 MODEL INTERACTION

Both the CAMx and CMAQ PGMs will be applied in the WestJumpAQMS project. Because an important aspect of the study will be Ozone and PM source apportionment modeling, the CAMx model will be the primary lead model because of its more advanced source apportionment implementation (Arunachalam, 2009). However, model inputs will also be developed for the CMAQ model. The most current versions of these two PGMs are CAMx Version 5.4 (October 2011) and CMAQ Version 4.7.1 (June 2010). Major updates to both PGMs (CAMx Version 6.0 and CMAQ Version 5.0) are expected, with CMAQ Version 5 scheduled to be released in January 2012. Depending on timing and initial indications of the robustness of the updates; the WestJumpAQMS may switch to newer versions of CAMx and CMAQ.

The WRF meteorological model Version 3.3 (April 2011) will be applied for the selected modeling episode and grid structure. The WRF output will be processed using the MM5CAMx and the Meteorology-Chemistry Interface Processor (MCIP) to generate meteorological inputs for the, respectively, CAMx and CMAQ models.

Day-specific hourly SO_2 and NO_X emissions for large (typically > 25 MWe) Electrical Generating Units (EGUs) will be obtained from the EPA Clean Air Markets Division's (CAMD) Continuous Emissions Monitoring Systems (CEMS) data. Emissions for other point sources will be acquired from the most appropriate sources as described in Chapter 5. The MOVES2010 on-road mobile source emissions model will be applied to generate county-level emissions for each county in the U.S. Oil and gas emissions will be based on the latest WRAP Phase III oil and gas emissions inventory[9] for the Rocky Mountain States. Anthropogenic emissions for area, non-road and other source categories will be acquired from the most appropriate sources as described in Chapter 5. Biogenic emissions will be generated using an enhanced version of the MEGAN biogenic emissions modeling system from an ongoing WRAP study to improve biogenic emissions modeling in the western U.S.[10] WRAP is also engaged in a study to generate improved fire emissions for the U.S.[11], which will likely be used in the WestJumpAQMS study as a sensitivity analysis. Otherwise alternative interim fire emission inventories will be used in the initial PGM simulations, such as those from the Fire Inventory from NCAR (FINN[12]).

With the exception of biogenic emissions, where MEGAN generates PGM-ready gridded hourly speciated inputs, each major source sector will be processed separately by SMOKE to generate pre-merged PGM-ready emissions inputs. This will allow for the ease of specifying alternative source apportionment source categories in later stages of the study. The SMOKE processed pre-merged emissions for all source categories and MEGAN biogenic emissions will be merged together to generate the PGM-ready emission inputs. The SMOKE and MEGAN modeling will be performed to generate emissions in the CAMx model format and the CAMX2CMAQ processor will be used to generate CMAQ emission inputs.

9 http://www.wrapair2.org/PhaseIII.aspx
10 http://www.wrapair2.org/pdf/WGA_Task1_TechnicalAnalysisReport_ImprovedBiogenicEmissionInventories.pdf
11 http://www.wrapair2.org/pdf/JSFP_DEASCO3_TechnicalProposal_November19_2010.pdf
12 http://bai.acd.ucar.edu/Data/fire/

3.0 EPISODE SELECTION

The 2008 calendar year was selected for the WestJumpAQMS modeling for the following reasons:

- Simulating an entire year allows the evaluation of the seasonal behavior of pollutants.
- Annual simulations also allow the assessment of annual AQ/AQRV issues such as sulfur and nitrogen depositions, annual average NAAQS and annual average evaluation using NADP, CASTNet and other observation networks.
- Of the most recent four-year period (2008-2011), 2008 had the highest ozone concentrations in the inter-mountain west, fairly typical meteorological conditions and more typical emissions:
  - The meteorological conditions of 2009 in the western U.S. were not conducive to ozone formation, which combined with the depressed emissions due to the recession resulted in the lowest ozone concentration in recent history.
  - The 2010 meteorological conditions were more typical, but emissions and oil and gas development was still depressed due to lingering effects of the recession.
- 2008 is one of the triennial National Emissions Inventory (NEI) years so will have a unified and quality assured 2008 emissions inventory for all states.
- 2008 is being used for other studies including several BLM Environmental Impact Statements (EISs) and Resource Management Plans (RMPs) as well as the Denver ozone SIP modeling being conducted by the Denver Regional Air Quality Council (RAQC) and the Colorado Department of Public Health and Environment (CDPHE)..

The decision to model for an entire calendar year rather than just for the summer ozone season is due to a need to address $PM_{2.5}$ and visibility issues as well as the recent events in Wyoming and Utah that found elevated ozone concentrations in the winter. Although the modeling will not be tailored to simulate the winter ozone events, the regional transport signal may prove useful to provide boundary conditions for such a tailored winter assessment, although the winter events are thought to be highly localized phenomena.

4.0 DOMAIN SELECTION

A 36/12/4-km nested grid structure will be used for the WestJumpAQMS meteorological, emissions and air quality modeling using a 3:1 grid-nesting ratio typically used for MM5/WRF meteorological modeling:

- The 36-km continental U.S. (CONUS) domain will be the same as used by the RPOs (e.g., WRAP) and most other recent modeling studies (e.g., Denver Ozone SIP).
- The 12-km western U.S. (WESTUS) domain will be larger than used in WRAP and contain all of the WRAP and adjacent states as well as extending into Canada and Mexico.
- There will be several types of 4-km domains utilized in the WestJumpAQMS study:
    - A large 4-km Inter-Mountain West Domain (IMWD) will cover all of the areas of primary interest with one 4-km grid and will be the domain for 4-km meteorological modeling and emissions processing.
    - Detailed Source Apportionment Domains (DSAD) 4-km domains will be defined so that fully linked 36/12/4 km ozone and PM source apportionment modeling can be performed to examine the upwind transport of pollutants from throughout the 36/12/4 km CONUS region into the 4-km DSAD domains, as well as downwind transport of emissions from the DSAD and other regions on downwind Ozone and PM concentrations. Because the DSAD 4-km domains are run with the 36-km and 12-km domains using two-way interactive grid nesting, they cannot overlap and the boundaries need to be aligned with the 36-km parent grid cells.
    - Impact Assessment Domains (IAD) are larger 4-km domains for which stand-alone 4-km photochemical modeling databases will be developed using boundary conditions (BCs) from the 36/12 km modeling. The IADs are defined for performing air impact assessments of sources within the IAD 4-km domain on receptors within the IAD 4-km domain.

Figure 4-1 displays the 36-km CONUS, 12-km western U.S. WESTUS and 4-km IMWD processing domain and the definition of their extent. The SMOKE and MEGAN emissions modeling will be conducted on the 36/12/4-km domain grid structure shown in Figure 4-1.

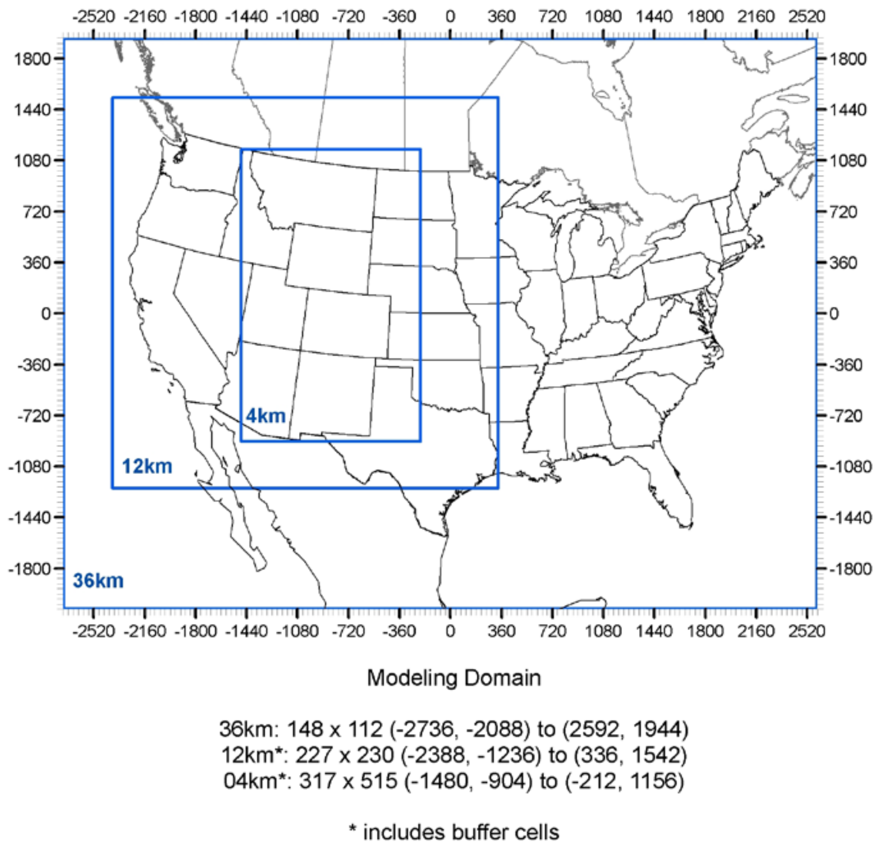

Figure 4-1. 36-km CONUS, 12-km WESTUS and 4-km IMWD processing domain used for developing PGM emission inputs.

4.1 IMPACT ASSESSMENT DOMAINS (IAD)

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

- The San Juan, NM IAD includes the North and South San Juan Basins and nearby Class I areas in the Four Corners region (Figure 4-3) and can be used to assess the AQ/AQRV impacts due to O&G developments in the San Juan Basin.
    - o 173 x 191 4 km resolution with SW and NE corners of (-1336, -724) and (-644,40).

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

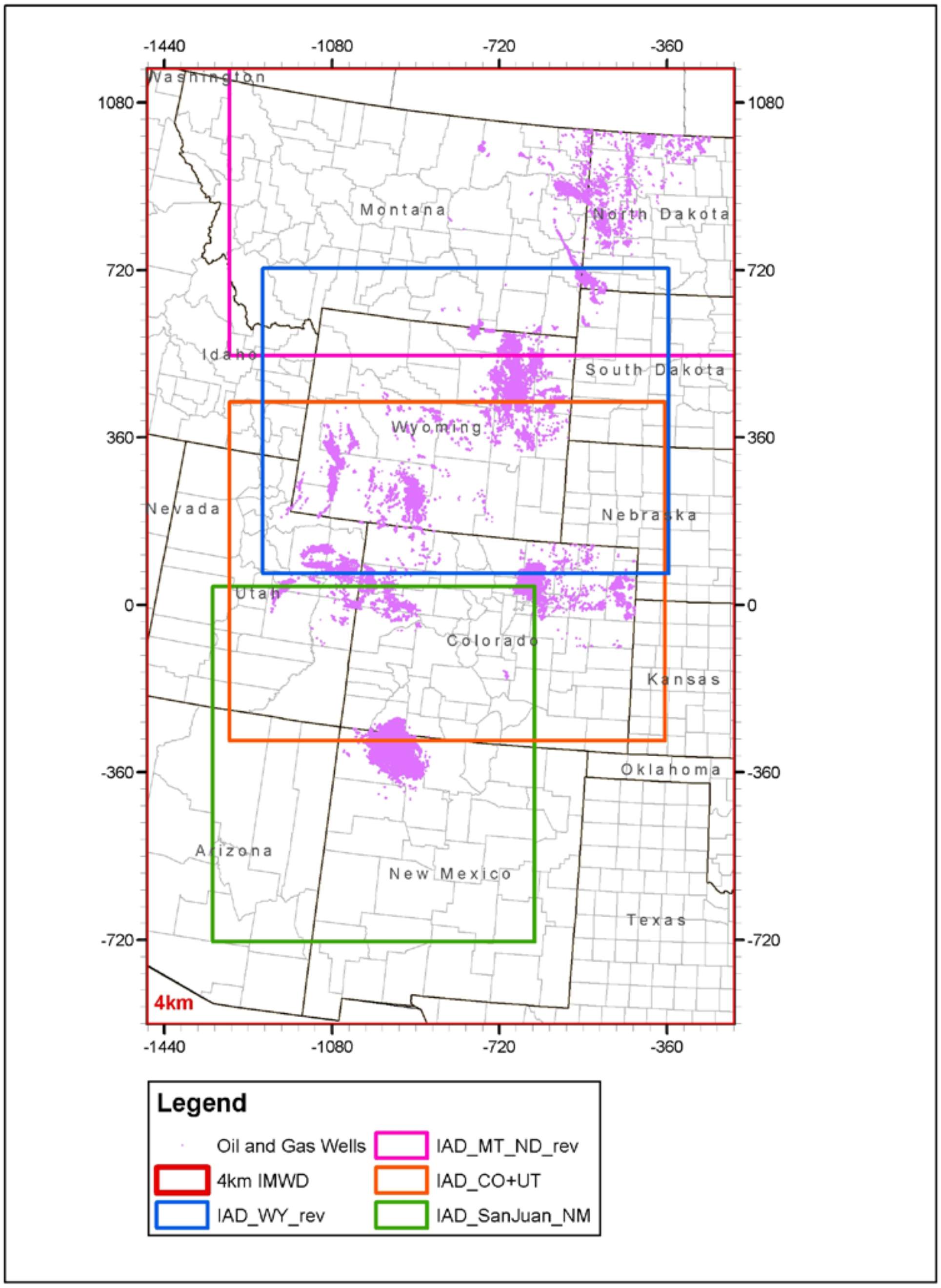

Figure 4-2. 4-km IMWD processing domain and four 4-km Impact Assessment Domains (IAD) for which stand-alone 4-km photochemical modeling databases will be developed for 2008.

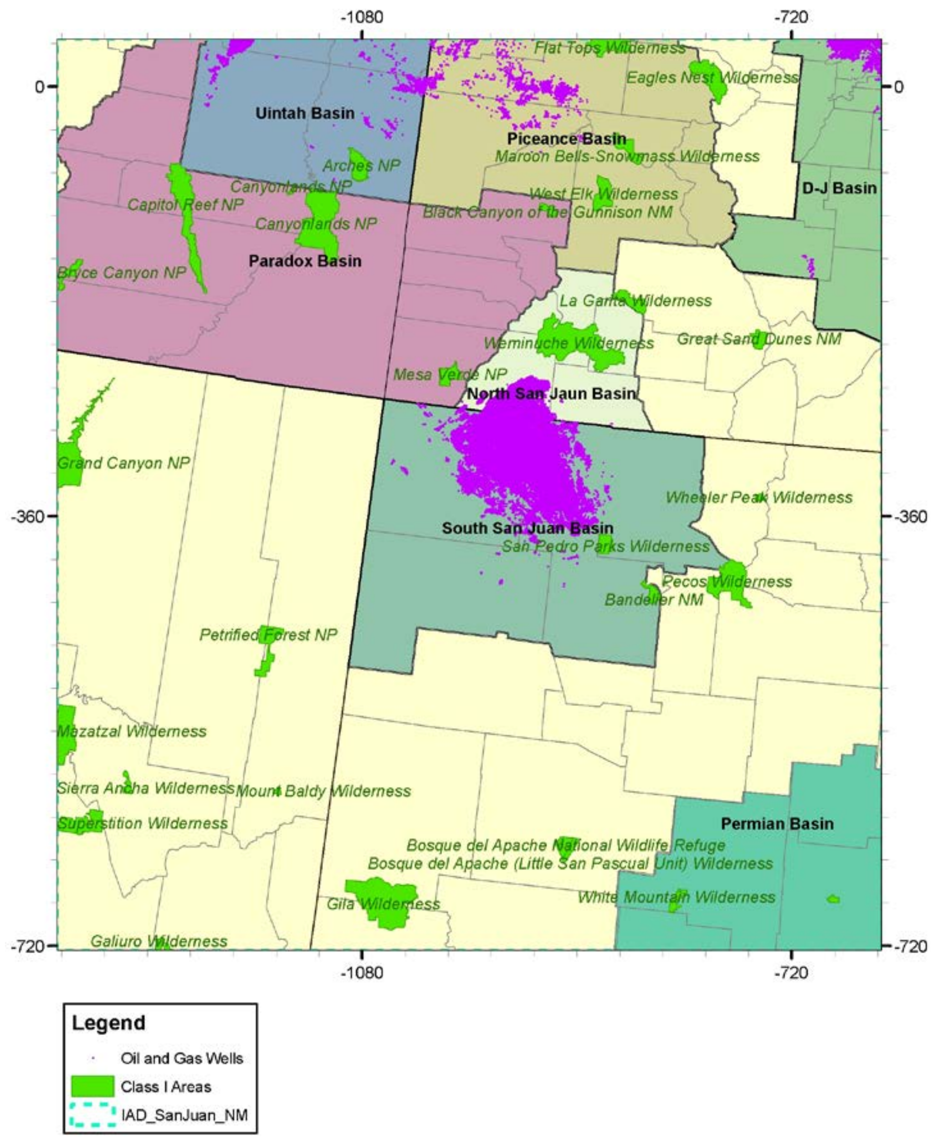

Figure 4-3. Four Corners 4-km IAD domain that includes the San Juan Basin.

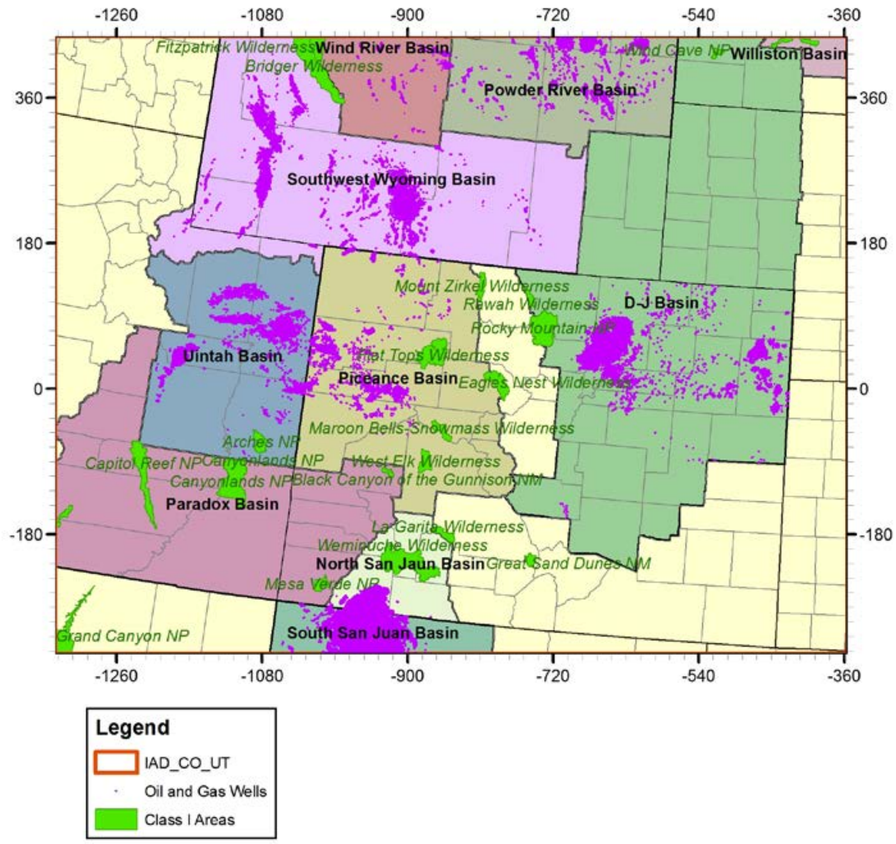

Figure 4-4. Utah-Colorado 4-km IAD domain that includes the Uinta, Piceance and Denver-Julesburg Basins.

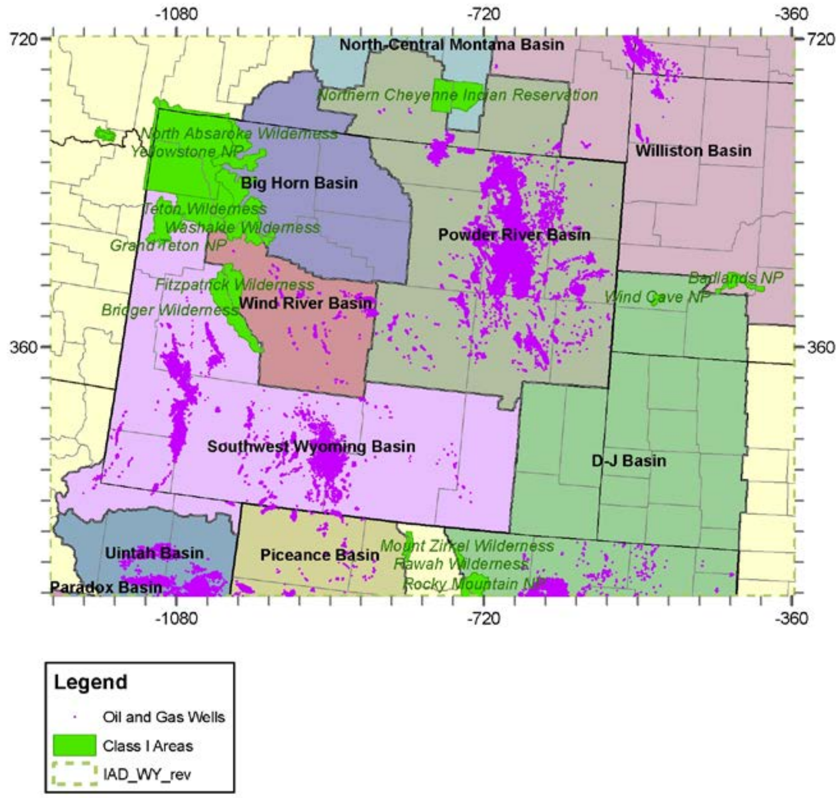

Figure 4-5. Wyoming 4-km IAD domain that includes the Uinta, Southwest Wyoming and Powder River Basins.

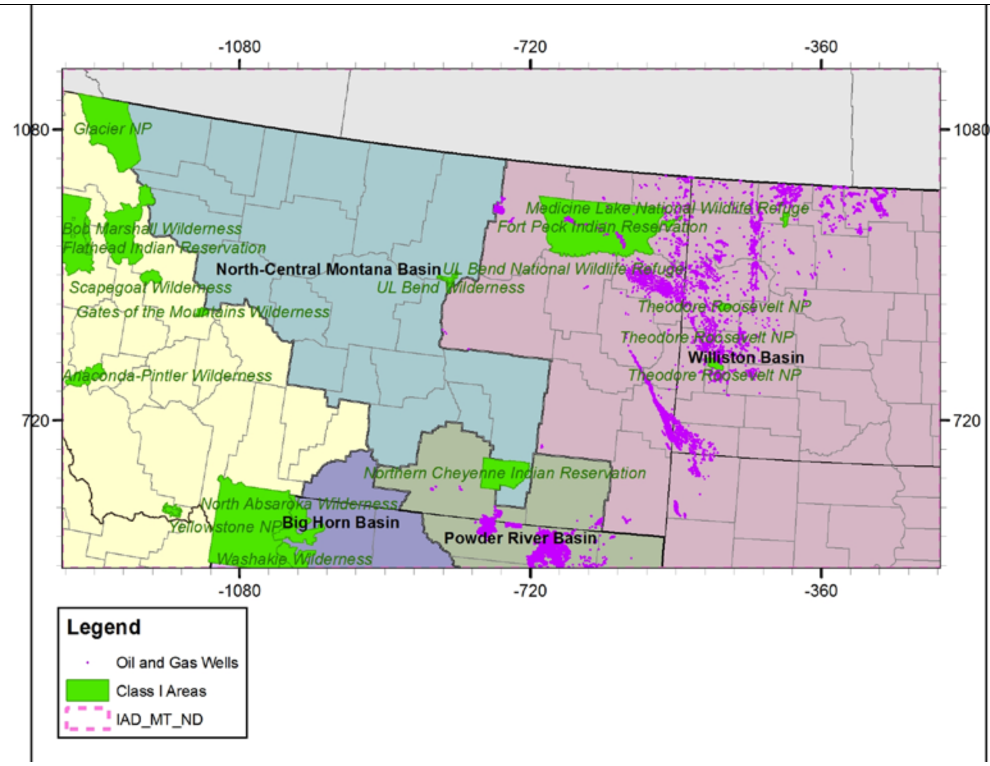

Figure 4-6. Montana-North Dakota 4-km IAD domain that includes the Williston basin.

4.2 DETAILED SOURCE APPORTIONMENT DOMAINS (DSAD)

The DSAD 4-km domains are designed to nest within the 12-km WESTUS domain and be used with two-way grid nesting to assess transport into and out of the DSAD domains. Consequently, they must be compliant with the CAMx two-way grid nesting rules (e.g., boundaries must align with the parent 36-km grid cells) and they cannot overlap. The DSAD domains were defined to include all of the major oil and gas development areas in the Rocky Mountain region. Figure 4-7 displays the six 4-km DSADs and their relationship with the 4-km IMWD processing domain with Figures 4-8 through 4-13 displaying each individual DSAD.

- Southeast New Mexico (NM_SE) DSAD (Figure 4-8).
  - 137 x 83 4 km resolution with SW and NE corners of (-1084, -904) and (-536, -572).
- Four Corners DSAD (Figure 4-9).
  - 101 x 92 4 km resolution with SW and NE corners of (-1192, -508) and (-788, -140).
- Uinta-Piceance Basins DSAD (Figure 4-10).
  - 119 x 110 4 km resolution with SW and NE corners of (-1264, -112) and (-788, 328).
- D-J Basin/Denver DSAD (Figure 4-11).
  - 92 x 110 4 km resolution with SW and NE corners of (-760, -112) and (-392, 328).
- Powder River Basin DSAD (Figure 4-12).
  - 173 x 92 4 km resolution with SW and NE corners of (-1192, 356) and (-500, 724).

- Montana-North Dakota DSAD (Figure 4-13).
  - o 182 x 83 4 km resolution with SW and NE corners of (-940, 752) and (-212, 1084).

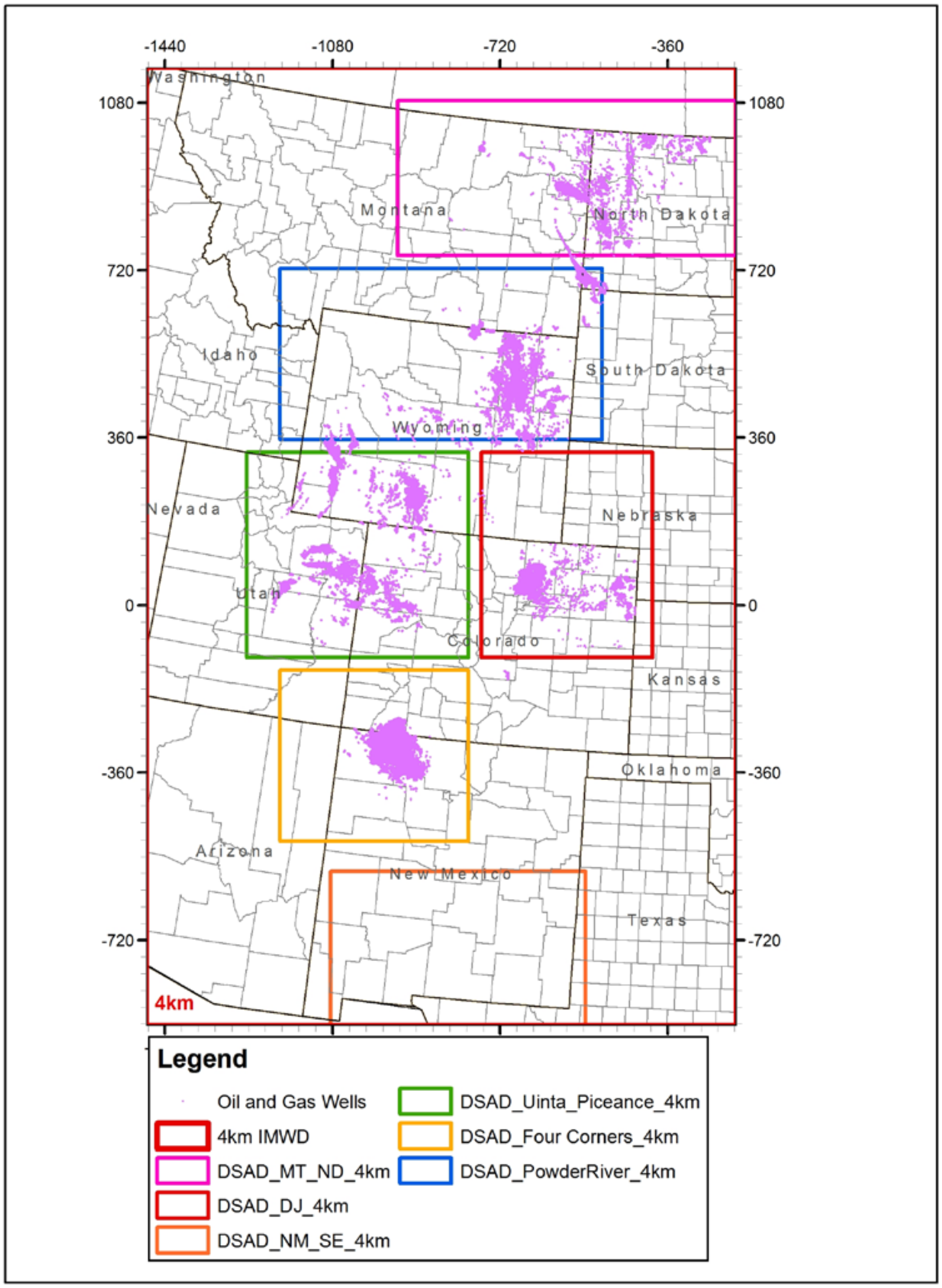

Figure 4-7. Relationship between the six 4-km proposed DSAD domains and the 4-km IMWD processing domains.

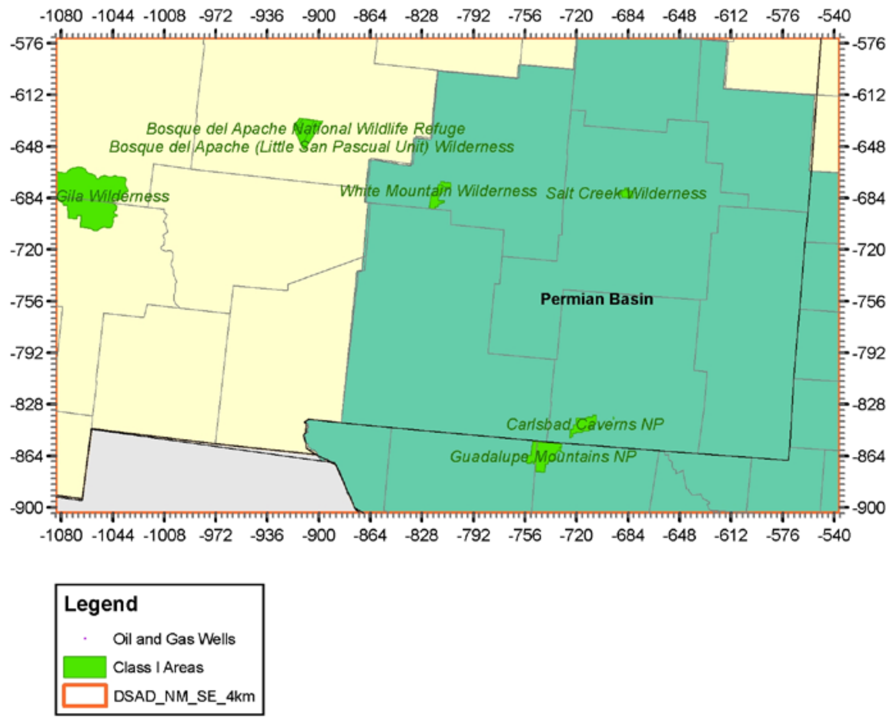

Figure 4-8. Proposed Southeastern New Mexico 4-km DSAD domain that includes the Permian basin.

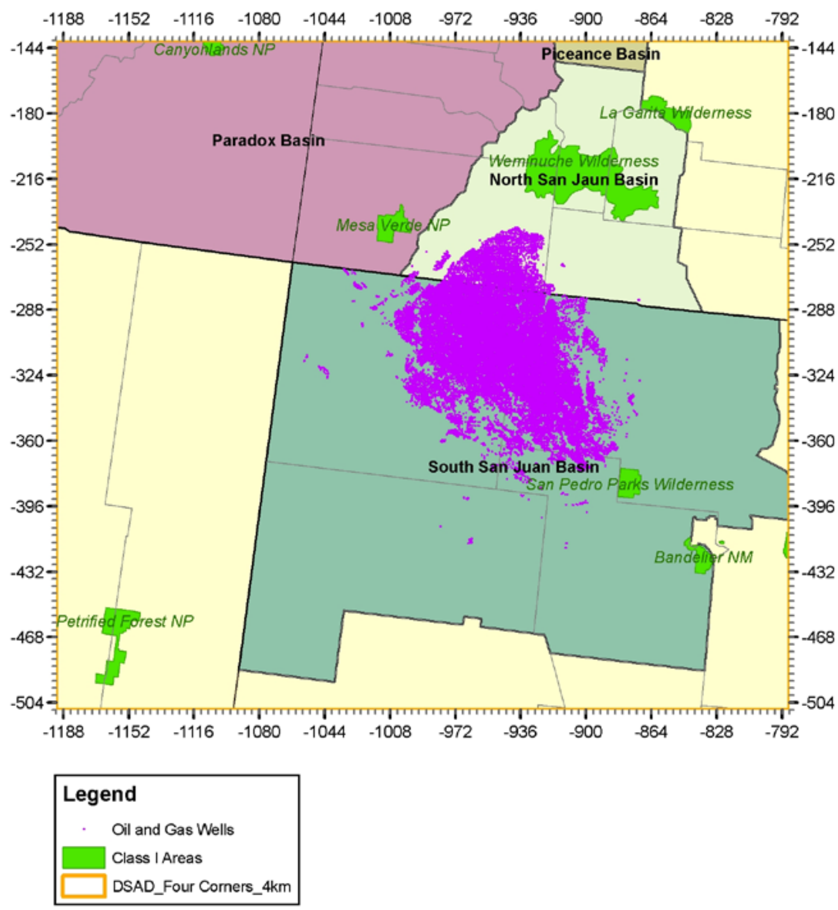

Figure 4-9. Proposed Four Corners 4-km DSAD domain that includes the North and South San Juan basins.

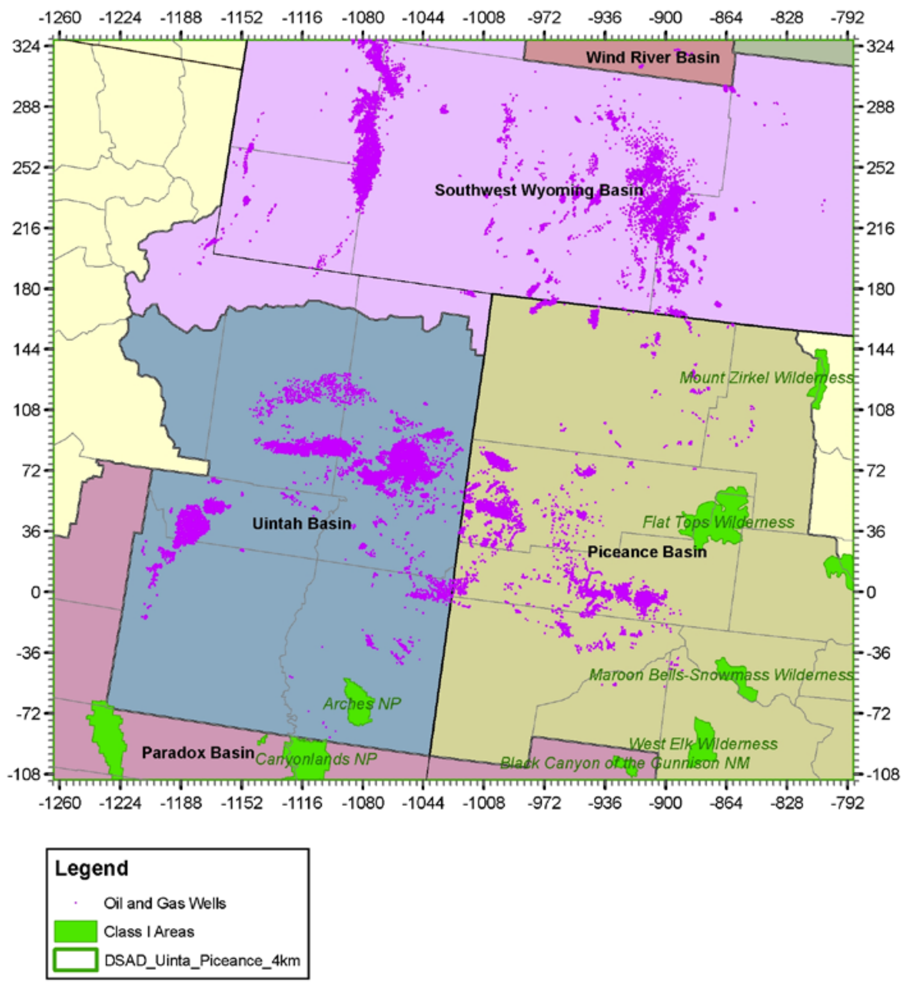

Figure 4-10. Proposed Uinta-Piceance Basins 4-km DSAD domain.

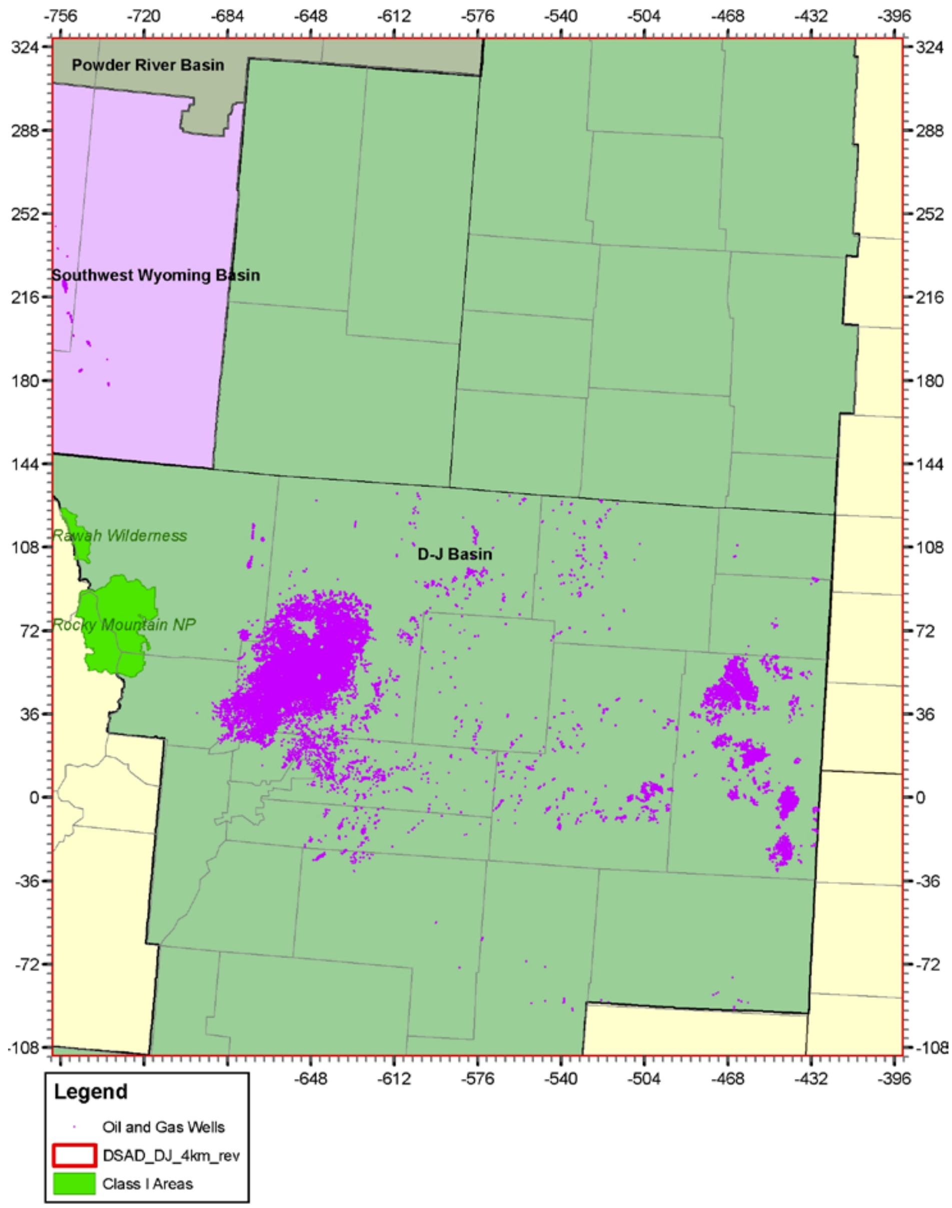

Figure 4-11. Proposed Denver-Julesburg Basin 4-km DSAD domain.

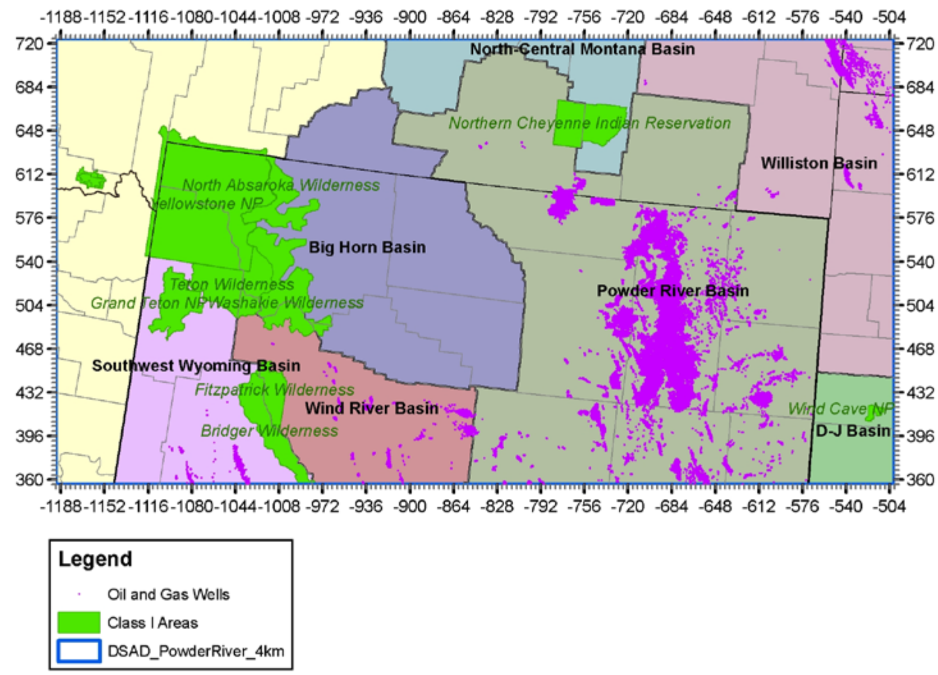

Figure 4-12. Proposed Wyoming 4-km DSAD domain.

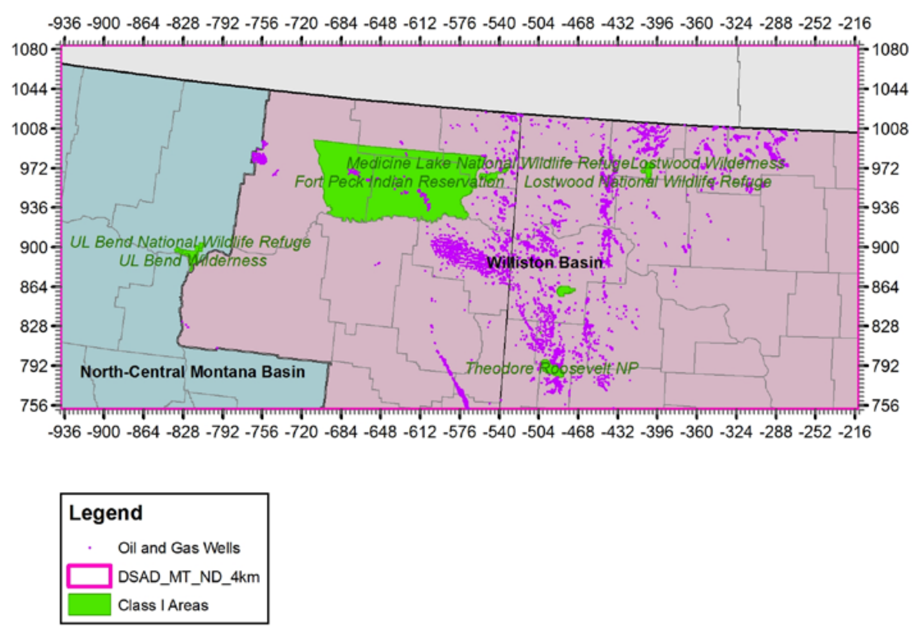

Figure 4-13. Proposed Montana-North Dakota 4-km DSAD domain.

4.2 VERTICAL DOMAIN STRUCTURE

The CAMx/CMAQ vertical domain structure will depend on the definition of the WRF vertical layers structure. WRF will be run with 37 vertical layers from the surface up to 50 mb (~19-km AGL). As discussed in Section 5.3 and shown in Table 5-1, the WRF layer structure will be collapsed to 25 vertical layers for the CAMx/CMAQ modeling.

5.0 METEOROLOGICAL MODELING

The WRF meteorological model was applied for the 2008 calendar year using a 36/12/4-km domain structure. The WRF modeling results for the 2008 annual period were evaluated against surface meteorological observations of wind speed, wind direction, temperature and humidity and the WRF model performance was compared against meteorological modeling benchmarks and with past regional meteorological model performance evaluations[13]. The WRF precipitation fields were compared against analysis fields that were based on observations.

5.1 MODEL SELECTION AND APPLICATION

As discussed in Chapter 2, the WestJumpAQMS project is using the current publicly available version of WRF (version 3.3). The WRF preprocessor programs including GEOGRID, UNGRIB, and METGRID were used to develop model inputs.

5.2 HORIZONTAL DOMAIN DEFINITION

The WRF computational grid was designed so that it can generate CAMx/CMAQ meteorological inputs for the 36-km CONUS, 12-km WESTUS and 4-km IMWD processing as well as all of the IAD and DSAD 4-km domains depicted in Figures 4-1 through 4-14 in Chapter 4. The WRF modeling domain needs to be defined slightly larger than the CAMx/CMAQ PGM modeling domains to eliminate any 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 modeling domain used in the WestJumpAQMS project. The outer 36-km domain (D01) has 165 x 129 grid cells, selected to be consistent with existing Regional Planning Organization (RPO) and EPA modeling CONUS domain. The projection is Lambert Conformal with the "national RPO" grid projection pole of 40^o, -97^o with true latitudes of 33^o and 45^o. The 12 km has 256 x 253 grid cells with offsets from the 36 km grid of 15 columns and 26 rows. The 4-km domain was defined to be slightly bigger than the 4-km IMWD processing domain discussed in Chapter 4. The three nests were run together with continuous updating without feedback from the 12-km to 36-km or from the 4-km to 12-kmn domains.

5.3 VERTICAL DOMAIN DEFINITION

The WRF modeling was based on 37 vertical layers with an approximately 12 meter deep surface layer. The vertical domain is presented in both sigma and height coordinates in Table 5-1. Also shown in Table 5-1 is the mapping of the WRF 37 vertical layer structure to the 25 vertical layers that will be employed by the CAMx/CMAQ PGMs.

5.4 TOPOGRAPHIC INPUTS

Topographic information for the WRF was developed using the standard WRF terrain databases available from the National Center for Atmospheric Research (NCAR)[14.] The 36 km CONUS domain was based on the 10 min. (~18 km) global data. The 12 km WESTUS domain was based on the 2 min. (~4 km) data. The 4 km IMWD was based on the 30 sec. (~900 m) data.

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13 Western Regional Air Partnership (WRAP) West-wide Jump Start Air Quality Modeling Study (WestJumpAQMS) – WRF Application/Evaluation, Prepared by Environ, Alpine and UNC, Draft dated January 23, 2012.
14 http://dss.ucar.edu/

5.5 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.

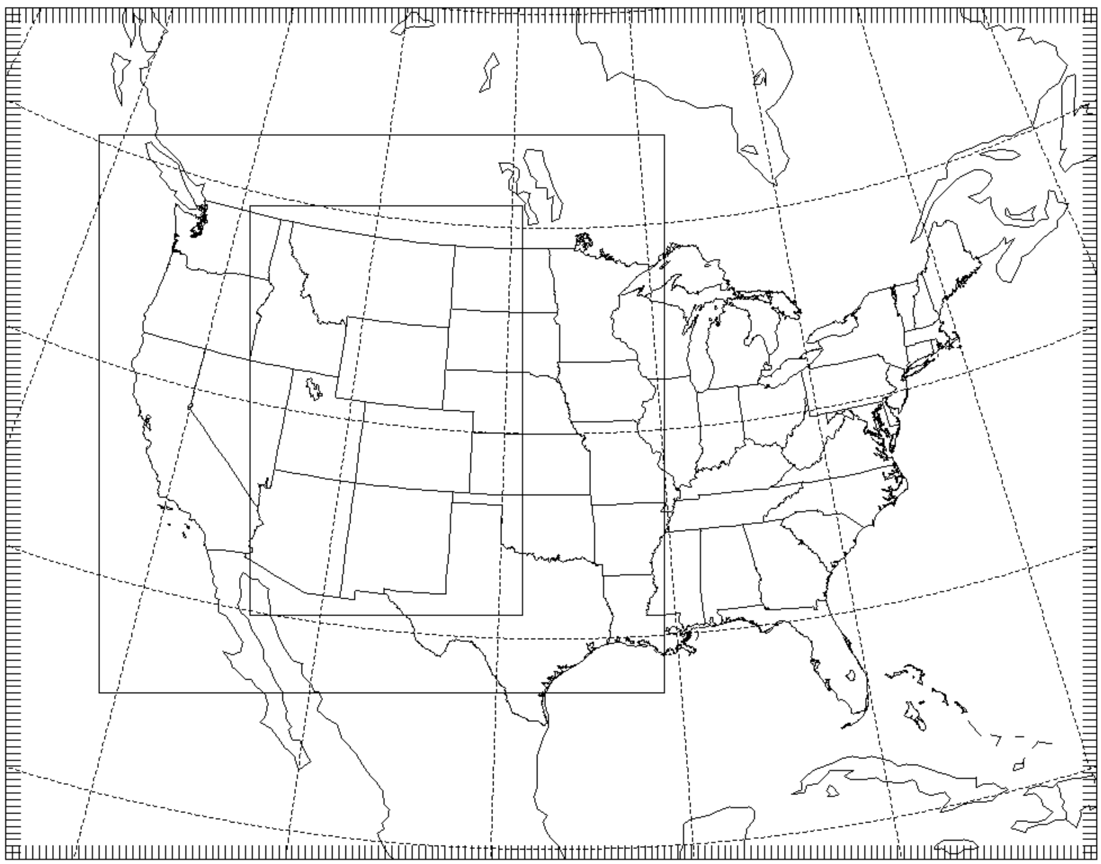

Figure 5-1. WRF 36/12/4-km grid structure for the WestJumpAQMS meteorological modeling.

Table 5-1. 37 Vertical layer definition for WRF simulations (left most columns), and approach for reducing to 25 vertical layers for CAMx/CMAQ by collapsing multiple WRF layers (right columns).

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

5.6 ATMOSPHERIC DATA INPUTS

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

5.7 WATER TEMPERATURE INPUTS

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

5.8 FDDA DATA ASSIMILATION

The WRF simulation used analysis based nudging for the 36/12 km domains and observation nudging in the 4 km domain. For winds and temperature, analysis nudging coefficients of $5x10^{-4}$ and $3.0x10^{-4}$ were used on the 36 km and 12 km grids, respectively. For mixing ratio, analysis nudging coefficients of $1.0x10^{-5}$ were used for both the 36 km and 12 km grids. The nudging used both surface and aloft nudging with nudging for temperature and mixing ratio excluded in the boundary layer. Observation nudging was performed on the 4 km grid domain using the Meteorological Assimilation Data Ingest System (MADIS)[15] observation archive. The MADIS archive includes the National Climatic Data Center (NCDC)[16] observations and the National Data Buoy Center (NDBC) Coastal-Marine Automated Network C-MAN[17] stations. The observational nudging coefficients for winds, temperatures and mixing ratios were $1.0x10^{-4}$, $1.0x10^{-4}$, and $1.0x10^{-5}$, respectively and the radius of influence was set to 50 km.

5.9 WRF PHYSICS OPTIONS

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

- WSM 3-class simple ice scheme (mp_physics=3)
- RRTMG long wave radiation (ra_lw_physics=4)
- RRTMG short wave radiation (rw_sw_physics=4)
- Monin-Obukhov surface layer (sf_sfclay_physics=1)
- Unified NOAH land-surface model (sf_surface_physics=2)

15 Meteorological Assimilation Data Ingest System. http://madis.noaa.gov/
16 National Climatic Data Center. http://lwf.ncdc.noaa.gov/oa/ncdc.html
17 National Data Buoy Center. http://www.ndbc.noaa.gov/cman.php

- Kain-Fritsch cumulus parameterization in the 36/12 km domains and no cumulus parameterization (cu_physics=0) in the 4 km domain
- YSU planetary boundary layer (bl_pbl_physics=7)

5.10 APPLICATION METHODOLOGY

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

5.11 EVALUATION APPROACH

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

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

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

We will also evaluate the WRF cloud predictions using satellite data.

5.12 REPORTING

The evaluation of an annual WRF simulation using a multi-level subregional evaluation generates numerous displays. Not all displays are of interest to everyone and different stakeholders may be interested in the WRF model performance in different locations. To accommodate these varying interests, the WRF evaluation products will be loaded on the project website that will allow the user to access results for particular regions of interest. The project website is discussed in Chapter 8.

6.0 EMISSIONS

Emissions modeling will be performed for the 36-km CONUS, 12-km WESTUS and 4-km IMWD processing domains. Separate streams of emissions modeling will be conducted for each major source category to assist in the quality assurance and quality control (QA/QC) process and for ease of performing source apportionment modeling in later stages of the study. These major source categories would likely consist of the following:

- Electrical Generating Unit (EGU) point sources.
- Non-EGU point sources.
- Upstream Oil and Gas development sources.
- Off-Shore Shipping sources.
- On-Road Mobile sources.
- Non-Road Mobile sources.
- Other Area sources.
- Ammonia emissions.
- Biogenics.
- Fires.
- Sea Salt.
- Lightning.

6.1 EMISSION DATA SOURCES

We have reviewed available emissions data for appropriateness for use in the WestJumpAQMS 2008 modeling. The 2008 National Emissions Inventory (NEI) will be the starting point for anthropogenic U.S. emissions. The 2008 NEI will be augmented, updated and replaced by other more appropriate emissions as available. Our latest information is that Version 2.0 of the 2008 NEI should be available in February 2012 which we intend to use for the WestJumpAQMS study. Table 6-1 summarizes the emissions models and source of emissions that would be based on the 2008 NEI with the following enhancements:

- Major point source SO_2 and NO_X emissions will be based off of Continuous Emissions Monitor (CEM) data that are available online from the EPA Clean Air Markets Division (CAMD). These data are hour-specific for SO_2, NO_x, and heat input. The temporal variability of other pollutant emissions (e.g., PM) from the CEM sources will be simulated using the hourly CEM heat input data to allocate the annual emissions to each hour.
- The states may have updates to the 2008 NEI non-EGU point and area sources inventory for some sources that may be more appropriate for use. We will review those with WRAP region states and limit state updates to those in the western U.S. WRAP region.
- As part of the Phase I of the WestJumpAQMS project, the WRAP-IPAMS Phase III oil and gas emissions inventories will be projected to 2008 for all Phase III basins available and a "Phase III-light" oil and gas emissions inventory will be developed for the New Mexico portion of the Permian Basin.
- On-road mobile source emissions will be based on the latest versions of the MOVES (currently MOVES2010a) model with county-specific VMT for the 2008 baseline modeling year.
- The sources of ammonia emissions will be analyzed, including state and EPA estimates, the Carnegie Mellon ammonia model, and the WRAP ammonia model. We will select the best estimate of these emissions that we can obtain under the WestJumpAQMS project resources. We will coordinate the selection of these data with the NPS RoMANS2 study.

- Methods for generating windblown dust (WBD) emissions will be investigated, including potentially using the WRAP WBD model[18] with day-specific hourly meteorology.
- The source of emissions from fires (wildfires, prescribed burns and agricultural burning) will be investigated and the best available database selected. Fire emission results from the DEASCO3[19] study for the Joint Fire Sciences Program (JFSP) will likely be the most comprehensive fire emissions inventory available for 2008, however they may not be available at the time of the initial WestJumpAQMS PGM modeling. An interim 2008 fire emissions inventory based on the Fire Inventory from NCAR (FINN[20]) will be used while the comprehensive DEASCO3 inventory is being developed.
- Biogenic emissions will be generated using an enhanced version of the Model of Emissions of Gases and Aerosols in Nature (MEGAN[21]) that is being updated by WRAP.
- Emissions from ocean going vessels will be based on the latest emissions inventory developed by EPA. This includes data recently released by EPA that include vertically resolved shipping lane emissions that distinguish between in-shore, near-shore, and commercial shipping lane sources for all waters surrounding North America.
- Mexico emissions will use 2008 projections from the 1999 Mexico national emissions inventory.
- The Environment Canada 2006 (or newer) National Pollutant Release Inventory (NPRI) will be used for Canada.
- New spatial surrogates for the emissions will be developed using the latest 2010 Census data that are now available and will include population and housing statistics for 2010 and interpolations for the years between 2000 and 2010.

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18 http://www.wrapair.org/forums/dejf/fderosion.html
19 https://www.firescience.gov/projects/11-1-6-6/proposal/11-1-6-6_11-1-6_attachment_1_primary.pdf
20 http://bai.acd.ucar.edu/Data/fire/
21 http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm

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

Emissions Component	Configuration	Details
Model Code	SMOKE Version 2.7	http://www.smoke-model.org/index.cfm
Oil and Gas Emissions	WRAP Phase III plus Permian Basin update	WestJumpAQMS study 2008 updates to WRAP Phase III O&G emissions.
Area Source Emissions	2008 NEI Version 1.5	Western state updates, then SMOKE processing of http://www.epa.gov/ttn/chief/net/2008inventory.html
On-Road Mobile Sources	MOVES2010a	County specific emissions run for representative days during the modeling episode.
Point Sources	2008 hourly day-specific for CEM sources 2008 NEI Version 1.5 for other	Use 2008 day-specific hourly CEM for actual and processed CEM for Typical 2008 emissions from major stationary sources with CEMS http://www.epa.gov/ttn/chief/net/2008inventory.html
Off-Road Mobile Sources	2008 NEI Version 1.5	Based on EPA NONROAD model http://www.epa.gov/ttn/chief/net/2008inventory.html
Wind Blown Dust Emissions	WRAP Wind Blown Dust (WBD)	WRAP WBD Model with 2008 WRF meteorology
Ammonia Emissions	Tentatively CMU Ammonia Model	Evaluate various options including NEI, State, WRAP and CMU ammonia models and latest results from NPS ROMANS
Biogenic Sources	MEGAN	Enhanced version of MEGAN Version 2.1 from WRAP Biogenics study http://www.wrapair2.org/emissions.aspx
Fires	FINN placeholder and then 2008 DEASCO3 fire inventory	Fire Inventory from NCAR (FINN) used as placeholder until 2008 DEASCO3 fire inventory is available: http://www.wrapair2.org/pdf/JSFP_DEASCO3_TechnicalProposal_November19_2010.pdf
Temporal Adjustments	Seasonal, day, hour	Based on latest collected information
Chemical Speciation	CB6 Chemical Speciation	Updated rate constants, kinetics and reactions in CB6. Use CB05 in CMAQ since CB6 not supported by CMAQ.
Gridding	Spatial Surrogates based on landuse	Develop new spatial surrogates using 2010 census data
Growth and Controls	TBD	Future attainment year(s) to be determined
Quality Assurance	QA Tools in SMOKE; PAVE, VERDI plots; Summary reports	
Boundary Conditions	MOZART-4/GEOS5	Boundary Conditions (BCs) for 36 km CONUS domain will be based on the MOZART-4/GEOS5 global chemistry model (http://www.acd.ucar.edu/wrf-chem/mozart.shtml). If available, results from GEOS-Chem global chemistry model will be investigated.

6.2 ON-ROAD MOBILE SOURCES

County-level on-road mobile source emissions will generated for each county and month using the MOVES2010a on-road mobile source emissions model, representative temperatures and 2008 county-level Vehicle Miles Travelled (VMT) data. The county-level on-road mobile sources emissions will then be allocated to the 36-km, 12-km and 4-km domains using the SMOKE emissions model and appropriate surrogate distributions. Default SMOKE diurnal variations and day-of-week adjustments will be utilized to allocate the MOVES monthly emissions to account for temporal variations. Default SMOKE CB6 chemical speciation will also be used.

6.3 AREA AND NON-ROAD MOBILE SOURCES

The 2008 NEI area and non-road emissions will be processed using the SMOKE emissions model using new 2010 census spatial surrogates and default temporal and CB6 speciation adjustments.

6.4 2008 OIL AND GAS EMISSIONS UPDATE

The WRAP-IPAMS Phase III 2006 oil and gas (O&G) emissions will be projected to 2008. In addition, 2008 O&G emissions will be developed for the southeast New Mexico portion of the Permian Basin.

6.4.1 2008 Phase III O&G Emissions Update

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

(1) Denver-Julesburg Basin (CO)
(2) Piceance Basin (CO)
(3) Uinta Basin (UT)
(4) North San Juan Basin (CO)
(5) South San Juan Basin (NM)
(6) Wind River Basin (WY)
(7) Powder River Basin (WY)
(8) Greater Green River Basin (WY)
(9) Williston Basin – Pending (MT and ND)

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

Processing of the IHS data for the 2008 projections will follow the same methodology as used in the Phase III study[22]. Summaries of production statistics will be extracted from the HIS database, including well count by well type and location, spud count, production of gas by well type and well location, production of liquid petroleum (oil or condensate) by well type and well location, and production of water by well type and well location. All data will be summarized at the county and basin level, for tribal and non-tribal land separately as applicable to each basin. As no new survey work is anticipated in this

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

study, the IHS database analysis will not include an analysis of company-specific production statistics as done in the development of the Phase III 206 O&G emission inventories. The resulting production statistics data will be summarized at the county, tribal and basin levels for all basins including the Permian Basin.

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

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

The 2008 updated inventories for the Phase III basins will be formatted identically to the baseline 2006 inventories generated for the Phase III study. The 2008 O&G emissions for the Phase III and Permian Basins will also be processed into the IDA format used by the SMOKE emissions modeling system. The IDA O&G emissions will include information for both area and point sources. Area source emissions are released into the lowest layer of the air quality model. Whereas, point source emissions are released into vertical layers depending on the point sources' stack parameters (e.g., height, diameter, temperature and flow rate) and local hourly meteorological conditions. New 2008 spatial surrogate data will also be developed that will be used to spatially allocate the O&G area source emissions to the air quality model grid cells in the SMOKE emissions modeling.

6.4.2 2008 Emission Inventory for the Permian Basin

A study prepared by Applied EnviroSolutions, Inc. (AES) on 2007 O&G emissions in the New Mexico portion of the Permian Basin will be used to develop a comprehensive inventory of the Permian Basin including activities in Texas. The AES study was commissioned for the Bureau of Land Management (BLM) Carlsbad Field Office (CFO), and used a methodology developed by ENVIRON for the Central Regional Air Planning Association (CENRAP)[23]. The preparation of the 2008 inventory for the Permian Basin will expand on the AES study, including both additional emissions estimates in the New Mexico portion of the basin and potentially new emissions estimates for the Texas portion of the basin. The steps in developing the Permian Basin inventory are described below.

For the New Mexico portion of the Permian Basin, additional O&G area source categories may need to be added to the inventory that are not included in the AES study. The AES study only examined emissions from wellhead/lateral compression, heaters, and flaring. Given the prevalence of both O&G

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

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

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

6.5 FIRE EMISSIONS

If available in time, fire emissions will be based on the comprehensive 2008 fire emissions inventory being developed in the DEASCO3[24] project being sponsored by the Joint Fire Science Forum (JFSF). However, the DEASCO3 2008 fire emissions inventory may not be available in time for the initial WestJumpAQMS photochemical model simulations in which case a placeholder 2008 fire emissions inventory based on the Fire Inventory from NCAR (FINN[25]) system will be utilized. The FINN emissions will be processed to generate the hourly gridded emissions using the CB6 chemical species. At a minimum, the DEASCO3 project fire emissions will be modeled using the WestJumpAQMS platform described in this plan and the results

24 http://www.wrapair2.org/pdf/JSFP_DEASCO3_TechnicalProposal_November19_2010.pdf
25 http://bai.acd.ucar.edu/Data/fire/

evaluated as a sensitivity study, comparing the change in fire inventories from FINN to DEASCO3 and the associated effects on elevated Ozone and PM episodes.

6.6 AMMONIA EMISSIONS

We will evaluate various sources of ammonia emissions for use in the WestJumpAQMS project. These include the 2008 NEI, state data, CMU ammonia model, WRAP ammonia model and any new developments from the NPS ROMANS study. The WRAP ammonia model is now rather dated, whereas CMU has made more recent updates to their ammonia model. Note that ammonia emissions are not important for ozone modeling; however they are very important for $PM_{2.5}$, visibility, and deposition modeling. The default approach is to use the CMU model to generate ammonia emission inputs to the air quality models. We will consult with a workgoup of state, federal, and academic experts to assemble the best available inputs to CMU, considering 2008 NEI and state data in the WRAP region.

6.7 OCEAN GOING VESSELS

The latest 2008 emissions inventory for ocean going vessels similar to what was used for the Emissions Control Area (ECA) analysis[26] will be used in the WestJumpAQMS project. The ship emissions will be gridded, speciated and temporally adjusted for input into CAMx/CMAQ.

6.8 BIOGENIC EMISSIONS

WRAP is currently enhancing the MEGAN biogenic emissions model to better simulate biogenic emissions in the western U.S. The WestJumpAQMS project will use the new enhanced version of MEGAN along with the 2008 WRF 36/12/4 –km data to generate hourly gridded speciated biogenic emission inputs.

6.9 SPATIAL ALLOCATION

New spatial allocation surrogates will be developed at 4-km resolution for the CONUS domain using the latest 2010 CENSUS data and disaggregated to 36-km for the CONUS and 12-km for the WESTUS domains.

6.10 CHEMICAL SPECIATION

The new SPECIATE 4.3 chemical speciation database will be used to speciate emissions for the CB6 chemical mechanism using the SMOKE emissions model. We will explicitly document which updated SPECIATE factors are applied to the source categories in the SMOKE model. Note that CMAQ will use the CB05 chemical mechanism, whose species will be obtained by mapping the CB6 species to CB05.

6.11 QUALITY ASSURANCE AND QUALITY CONTROL

The emissions will be processed by major source category in several different "streams", including area sources, on-road mobile sources, non-road mobile sources, biogenic sources, non-CEM point sources, CEM point sources using day-specific hourly emissions (Actual), CEM sources using average emissions (Typical) and, as available, emissions from fires. Separate Quality Assurance (QA) and Quality Control (QC) will be performed for each stream of emissions processing and in each step. SMOKE includes advanced quality assurance features that include error logs when emissions are dropped or added. In addition, we will generate visual displays that include:

26 http://www.epa.gov/otaq/oceanvessels.htm

- Spatial plots of the hourly emissions for each major species (e.g., NO_X, VOC, some speciated VOC, SO2, NH3, PM and CO);
- Vertical average emissions plots for major species and each of the grids;
- Diurnal plots of total emissions by major species and by state; and
- Summary tables of emissions for major species for each grid and by major source category.

This QA information will be examined against the original point and area source data and summarized in an overall QA/QC assessment.

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

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

6.12 REPORTING

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

7.0 PHOTOCHEMICAL MODELING

The WestJumpAQMS project will conduct photochemical modeling using both the CAMx and CMAQ photochemical grid models (PGMs). Applying both PGMs provides insight into the capabilities of photochemical modeling for the western U.S. and what features are important. Because a major objective of the study is to address western U.S. ozone source-receptor relationships, CAMx will be the primary model due to its more advanced Ozone and PM source apportionment implementation (Arunachalam, 2009) and ability to perform two-way grid nesting. However, CMAQ will also be run for the 2008 base case scenario and evaluated against ambient air quality measurements; we have found that running both models has provided unique and valuable insight into model performance. Three types of PGM model simulations will be conducted:

- 2008 base case modeling and model performance evaluation, including the use of diagnostic sensitivity tests to improve the base case model performance.
- Ozone source apportionment modeling to characterize Ozone source receptor relationships across the West including the contributions of upwind emissions to elevated Ozone concentrations in the western U.S. as well as estimating the impact of emissions in the western U.S. on downwind elevated Ozone concentrations.
- Parallel Particulate Matter (PM) source apportionment to characterize PM 2.5, visibility and sulfur and nitrogen deposition source-receptor relationships in the western U.S.

The WestJumpAQMS photochemical modeling will also form a framework for future air quality modeling in the western U.S. This potentially includes the development of State implementation Plans (SIPs) and air quality modeling to support the development of Environmental Impact Statements (EIS) and Resource Management Plans (RMP) to address requirements of the National Environmental Policy Act (NEPA)

7.1 CAMX AND CMAQ SCIENCE AND INPUT CONFIGURATIONS

This section describes the model configuration and science options to be used in the WestJumpAQMS CAMx and CMAQ modeling effort. Table 7-1 summarizes the CAMx and CMAQ configuration to be used. The latest version of CAMx, which is currently Version 5.3 (released December 2010), will be used. CAMx Version 6.0 is expected to be released in time for the WestJumpAQMS, but if not available we will use an updated version of CAMX Version 5.3. The update consists of the CB6 chemical mechanism. The model will be configured to predict both Ozone and PM species. The current version of CMAQ is Version 4.7.1 that was released in June 2010. CMAQ Version 5.0 is scheduled to be released in October 2011 and represents a complete reworking of the CMAQ code. If the tests performed by the user community indicate CMAQ Version is robust and working well, it may be adopted for the WestJumpAQMS project.

Many common parameterizations will be selected for both CAMx and CMAQ. The PPM advection solver will be used for horizontal transport along with the spatially varying (Smagorinsky) horizontal diffusion approach. CAMx will initially use K-theory for vertical diffusion using the CMAQ-like vertical diffusivities from WRFCAMx and CMAQ will use the analogous vertical mixing approach. The CB6 gas-phase chemical mechanism is selected because it includes the very latest chemical kinetic rates and represents improvements over the CB05 and SAPRC chemical mechanisms. Additional CAMx inputs will be as follows:

<u>Meteorological Inputs:</u> The WRF-derived meteorological fields will be prepared for CAMx and CMAQ using the, respectively, WRFCAMx and MCIP processors. Several alternative vertical diffusivity options will be generated for CAMx input and evaluated in sensitivity tests.

Initial/Boundary Conditions: The boundary conditions (BCs) for the 36 km CONUS domain simulation would be based on the latest available information. Boundary conditions will be extracted from a global chemistry model, such as MOZART, CAM-Chem and/or GEOS-Chem. Existing programs will be used to interpolate from the MOZART/GEOS-Chem horizontal and vertical coordinate system to the CAMx LCP coordinate system and vertical layer structure and to map the MOZART/GEOS-Chem chemical species to the CB6 chemical mechanism.

Photolysis Rates: The modeling team will prepare the photolysis inputs as well as albedo/haze/ozone/snow inputs for CAMx based on Total Ozone Mapping Spectrometer (TOMS) data. For CAMx the TUV processor will be used. If there are periods of more than a couple of days where daily TOMS data are unavailable, monthly average TOMS data will be used. CAMx will also be configured to use the in-line TUV to adjust for cloud cover. Photolysis rates for the CMAQ model will be base in the JPROC processor.

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

Spin-Up Initialization: A minimum of ten days of model spin up (December 21-31, 2007) will be used on the 36-km continental U.S. configuration before adding the 12 and 4 km nested domains for the last two days before the start of the 2008 calendar year (January 1, 2008).

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

Table 7-1. CAMx (Version 5.4 or newer) and CMAQ (Version 4.7.1 or newer) model configuration.

Science Options	Configuration	Details
Model Codes	Updated CAMx V5.4 – October 2011 Release [CMAQ V4.7.1 – June 2010 Release]	CB6 chemical mechanism update. Newer version if available at time of modeling
Horizontal Grid Mesh	36/12/4 km	
36 km grid	148 x 112 cells	36-km CONUS domain
12 km grid	239 x 206 cells	12-km WESTUS domain
4 km grid	Several DSAD 4-km domains	Also set up 4 km IADs as a one-way nest
Vertical Grid Mesh	25 vertical layers, defined by WRF	Layer 1 thickness ~2- m. Model top at ~19-km AGL
Grid Interaction	36/12/4 km two-way nesting for CAMx	One-way grid nesting for CMAQ
Initial Conditions	10 day spin-up on 36 km grid	Clean initial conditions
Boundary Conditions	36-km from global chemistry model	Evaluate MOZART, CAM-Chem and GEOS-Chem global chemistry models
Emissions		
Baseline Emissions Processing	SMOKE, MOVES and MEGAN	
Sub-grid-scale Plumes	Plume-in-Grid for major NO_X sources in CAMx	CMAQ has no subgrid-scale Plume-in-Grid module
Chemistry		
Gas Phase Chemistry	CB6	If CMAQ V4.7.1 then use CB05 in CMAQ
Meteorological Processor	WRFCAMx and MCIP 3.6]	Compatible with CAMx V5.3 and CMAQ V4.7.1
Horizontal Diffusion	Spatially varying	K-theory with Kh grid size dependence
Vertical Diffusion	Kz (ACM2, CMAQ, TKE methods)	Sensitivity tests to Kz methods
Diffusivity Lower Limit	Kz-min = 0.1 to 1.0 m^2/s or 2.0 m^2/s	Run WRFCAMx with Kz_min = 0.1 m2/s; sensitivity tests for Kz_min
Deposition Schemes		
Dry Deposition	Zhang dry deposition scheme (CAMx) M3Dry Pleim dry deposition (CMAQ)	Zhang 2003
Wet Deposition	CAMx and CMAQ-specific formulation	rain/snow/graupel
Numerics		
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) -- Fast Solver	EBI implemented in both CAMx and CMAQ
Vertical Advection Scheme	Implicit scheme w/ vertical velocity update (CAMx) New vertical velocity scheme (CMAQ)	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	PPM in both CAMx and CMAQ
Integration Time Step	Wind speed dependent	~0.5-1 min (4-km), 1-5 min (12-km), 5-15 min (36-km)

7.2 2008 BASE CASE MODELING AND MODEL PERFORMANCE EVALUATION

This chapter describes the strategy for the 2008 base case modeling and model performance evaluation. The model performance evaluation is designed to establish the reliability of the CAMx and CMAQ for simulating ozone, particulate matter, visibility and deposition in the western U.S.

A CAMx 2008 base case simulation would first be conducted using two-way grid nesting with the 36-km CONUS and 12-km WESTUS domains and a preliminary ozone model performance evaluation conducted for the western U.S. A subregional evaluation would then be conducted (e.g., by state). For selected episode period(s) sensitivity tests would be conducted to determine the optimal model configuration. The types of things to be investigated in the model sensitivity modeling would include the following:

- Use of the 4-km DSAD domains;
- Layer collapsing between the WRF meteorological and PGM air quality models.
- Vertical mixing algorithm and treatment of minimum Kv.
- Use of Plume-in-Grid (PiG) module.
- Use of MOZART versus GEOS-Chem BCs for the 36 km CONUS domain.
- Use of the CMAQ model.

The performance of the CAMx for the sensitivity tests would be analyzed for Ozone, ozone precursors, $PM_{2.5}$ and $PM_{2.5}$ precursors and an optimal model configuration will be identified. The objective in identifying optimum model configurations is to obtain the best performance for the right reasons consistent with sound science and EPA guidance. Sometimes, decisions must be made that trade off better/poorer model performance for one pollutant against another. For example, although the focus of the model evaluation is on Ozone and ozone precursor and product species, we will also evaluate the model for $PM_{2.5}$, PM species (e.g., SO_4, NO_3, NH_4, EC, OA, Soil and CM), deposition and visibility. These factors will be considered and potential issues discussed among the WestJumpAQMS modeling team, WRAP and others. Based on the analysis and comments from WRAP and other interested parties, the modeling team will select the final model configurations.

Once the optimal model configuration has been selected a revised CAMx and CMAQ 2008 base case simulations and model performance evaluation would be conducted. A summary of the model performance evaluation and sensitivity modeling would be documented in a report and PowerPoint presentation. However, because of the amount of monitoring sites in the western U.S. and different interests among the project participants, we would make model evaluation products available on the WestJumpAQMS website so that interested parties can drill down into the results including obtaining model performance results for specific monitoring sites if desired, along with the subregional evaluation by state and by domains (e.g., IAD and DSAD).

The model evaluation would be conducted using the Atmospheric Model Evaluation Tool (AMET[27]). AMET can generate numerous visualizations of model performance. The model performance would use other tools

27 http://www.cmascenter.org/help/model_docs/amet/1.0/AMET_Users_Guide_v1.0.pdf

such as VERDI[28] and Excel macros. Numerous displays of model performance would be generated including time series, scatter plots, spatial maps, etc. These displays would be made available on the project website.

7.3 SOURCE APPORTIONMENT MODELING

Preliminary CAMx 2008 Ozone and PM source apportionment modeling will be conducted on the 36/12-km grids by state using two source categories: anthropogenic and natural emissions. The results will be analyzed in a similar fashion as EPA used in the Cross-State Air Pollution Rule (CSAPR) to determine upwind states contribution to Average and Maximum Ozone and $PM_{2.5}$ Design Values at monitoring sites within the western U.S. as well as further east. Preliminary source apportionment modeling benchmarks would also be performed that included some and all of the DSAD domains so that run times and memory requirements could be assessed.

Based on the preliminary CAMx Ozone and PM source apportionment modeling linkages, we would develop a plan for more detailed source apportionment modeling that would be submitted to WRAP and others for review. The source apportionment modeling plan would discuss three types of source apportionment modeling: (1) assessing the contributions of emissions from upwind states to Ozone and/or PM in the western U.S. (Upwind Transport); (2) assessment of the contributions of western states to downwind areas many may be out of the WRAP region (Downwind Transport); and (3) assessment of the contributions of local sources (Local Contributions). The types of issues that need to be addressed in each of these three types of source apportionment are as follows:

- Ozone and/or PM Source apportionment.
- Boundaries, Processing Time, and Number of non-overlapping 4-km DSAD domains to be used.
- Period of modeling.
- Number and comparability of Source Regions for source apportionment modeling
- Number and relative accuracy of emissions inventories for individual Source Categories to be use for source apportionment modeling
    - For example, biogenic, EGU point, non-EGU point, on-road mobile, non-road mobile, oil and gas, area, etc.

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

The design of the more detailed source apportionment runs would be documented and provided to WRAP and other project participants for review and comment.

28 http://www.verdi-tool.org/

8.0 WEBSITE AND REPORTING

Because of the sheer volume of information that will be generated as part of the meteorological and emissions modeling, in the model performance evaluation and from the source apportionment modeling, the results will be made available on a project website with summary reports and PowerPoint presentations also generated. We will post data and reports as work is completed in each of the 3 phases of the WestJumpAQMS.

8.1 INTERACTIVE WEBSITE

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

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

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

8.2 REPORTS

Summary reports and PowerPoint presentations will be prepared at the end of each major task. An important component of the reporting summaries will be examples of where more information can be obtained on the website.

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