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March 17, 2015

U.S. Environmental Protection Agency
EPA Docket Center (EPA/DC)
Docket # EPA–HQ–OAR–2008–0699
1200 Pennsylvania Avenue, NW
Mail Code: 288221T
Washington, DC 20460

RE: Docket # EPA–HQ–OAR–2008–0699, Proposed Ozone National Ambient Air Quality Standard

The State of New Mexico provides the attached technical comments on the proposed primary and secondary ozone National Ambient Air Quality Standards (NAAQS). New Mexico supports the use of a health-science based approach to establishing the level of the standard, but has many concerns about the lack of viable options for western states to address natural background, rural transport and international transport issues. The improvement in air quality in the west will depend on how well the states and EPA understand the science, and that understanding needs to improve. We discuss our concerns regarding these implementation constraints in more detail in the attached technical comments.

Thank you for the opportunity to comment on EPA's proposed primary and secondary ozone NAAQS. If you have any questions regarding these comments, please contact Rita Bates of my staff at (505) 476-4304.

Sincerely,

Richard L. Goodyear, P.E.
Chief, Air Quality Bureau

New Mexico's Comments Regarding the
Proposed 2015 Ozone National Ambient Air Quality Standards

The Level of the Ozone Standards

New Mexico recognizes the United States Environmental Protection Agency's (EPA) statutory responsibility to research and propose revisions to the primary and secondary ozone National Ambient Air Quality Standards (NAAQS) to provide requisite protection of public health and welfare with an adequate margin of safety. However, the successful implementation of the ozone standard – at any level – will require EPA to develop an understanding of the unique constraints that affect the western region of the U.S. from attaining or maintaining the current or a revised ozone NAAQS. These constraints include natural background, transported ozone within rural areas, and international transport. It is essential that EPA fully research and address these constraints. The currently available EPA tools do not and cannot effectively address these issues and in most cases require states to expend additional resources on efforts that provide little or no improvement in air quality. New Mexico urges EPA to develop and implement policies, strategies and planning tools that provide the means to address nonattainment violations of the ozone standard in ways that account for and address these constraints.

EPA has proposed setting a corresponding primary and secondary ozone NAAQS. New Mexico supports EPA in setting the secondary standard to be the same as the primary. New Mexico does not support the adoption of a distinct secondary standard using the W126 metric. The promulgation of a distinct secondary standard using the W126 metric would be problematic for the following reasons:

1. The W126 metric is based on the three (3) consecutive month period within the ozone season with the maximum index value and does not account for situations where the three highest months do not coincide with the period of greatest plant sensitivity;
2. The W126 metric is extremely difficult to calculate and to avoid the probability of errors, EPA would need to modify AQS to enable states to determine attainment status;
3. EPA would need to establish criteria for flagging exceptional events under a W126 metric; and
4. States could face the additional significant burden of developing exceptional events demonstrations for a secondary standard.

Ozone Transport

The transport of air pollutants, particularly ozone, in the western U.S. is becoming an increasingly important issue that must be addressed on a regional scale. New Mexico is aware that lowering the current standard may assist in reducing the amount of ozone transport throughout the west, but for the purposes of SIP development, regional modeling from the EPA is needed to aid western states in determining local contributions for the development and adoption of control measures.

New Mexico encourages EPA to provide funding and technical assistance to the regional planning organizations (RPOs) to develop the tools needed for states to better understand regional influences that are affecting air quality. RPOs have amassed data and tools for visibility analyses that can be used for ozone analyses. The Western Regional Air Partnership (WRAP)

unfortunately does not currently have the financial or staffing resources needed to develop an Ozone Transport Commission (OTC)-like analysis for transport and natural background in the west. It is important that the roles of transport and natural background ozone in the west are evaluated carefully as the levels of the NAAQS are reduced. While studies such as the OTC's work in the east led to specific conclusions regarding upwind power plants, the diversity of ozone precursor sources in the west will require at least a similar western study with equivalent or greater support from EPA.

Interpretation of Rural Transport Area

New Mexico contains four metropolitan statistical areas that are separated from each other by mostly rural land. CAA Section 182(h) provides for a rural transport area classification that limits mandatory control strategies for rural areas that are primarily affected by transported emissions. However, large areas of New Mexico do not qualify for this classification because rural transport areas cannot include counties that are in a Metropolitan Statistical Area (MSA) or adjacent to an MSA. The use of this provision is limited for western states like New Mexico due to large county sizes that result in MSAs that are considerably larger than in the eastern portion of the U.S. In addition, significant portions of counties within a specific MSA may be rural in character owing to low population densities. These factors, along with the exclusion of large counties adjacent to the MSA, prevent areas that meet the intent of the rural transport area classification from qualifying.

It would benefit New Mexico for EPA to apply Section 182(h) in a manner that recognizes local conditions in the state. For example, it may be appropriate to deviate from county boundaries in designating a nonattainment area, in order to separate an MSA from a Rural Transport Areas. The current use of the provision excludes many areas within New Mexico that should be designated as rural transport areas. This ultimately leads to these rural areas being required to adhere to the same nonattainment requirement as those areas that are affected by local controllable sources. Allowing states to make a demonstration that rural areas near an MSA should be considered a rural transport area will more accurately reflect the realistic strategies those communities can take to reduce ozone precursors.

Implications for Rural Areas

EPA's assumptions in its Regulatory Impact Analysis (RIA) about workload for state/local air programs are not realistic for New Mexico. While some states have been addressing state-wide ozone levels for many years, New Mexico will be facing new issues as we determine how to reduce ozone levels in rural areas. It will require a tremendous effort to improve the technical information (inventories, models, etc.); to educate local governments and rural communities about new requirements; and to develop control strategies. In addition, it will require a significant effort to determine which emission sources are affecting regional background ozone levels and the degree to which interstate and international transport and background are contributing to the problem. The eastern U.S. has been grappling with these issues for many years through the OTC, Ozone Transport Assessment Group (OTAG), and other regional analysis efforts. EPA needs to undertake similar efforts for understanding ozone in the western U.S.

Many of the rural areas within New Mexico that will be grappling with nonattainment for the first time have very few, if any, major sources and have very limited abilities to address requirements, such as transportation conformity, that come along with the designation of nonattainment. Limited resources and the absence of local emissions, resulting in limited offset opportunities for these areas, will impede successful attainment of the ozone standard through locally applicable control strategies, resulting in reduced economic development in already economically disadvantaged rural areas.

Classification as rural transport areas would benefit some of these areas, but rural transport areas still need to meet requirements for marginal ozone areas, including a baseline emissions inventory, source emission statements, nonattainment new source review, and transportation and general conformity. This does not provide regulatory relief for many rural areas that are slightly above the standard due to pollution transported from outside the area. These requirements apply over a 20 year period for rural areas with few or no emissions sources and lightly populated areas. This may prevent any new economic development opportunities for these areas which may already be struggling. A rural transport designation would still impose a significant workload and resource constraint on these areas.

Background Ozone Concentrations

EPA has done very little in terms of addressing the issue of chronic high background ozone within the intermountain west. The *Policy Assessment for the Review of the Ozone National Ambient Air Quality Standards* (PA) does provide some insight as to EPA's current understanding of background ozone in the intermountain west, but it appears to gloss over this issue with the proposed ozone standards and provides very limited reassurance to New Mexico that EPA fully understands the limitations that could be placed on this region.

The PA states on page 2-17 that natural background is high in the intermountain west due to stratospheric influences and international transport impact that increases with altitude. The PA on page 2-20 goes on to state that background ozone can be as high 70-80% of the total seasonal mean for ozone in the intermountain west and along the U.S. border. It is clear from these statements that EPA is aware of the background ozone issues within the intermountain west, but is glossing over the real question of how to deal with these issues by proposing a one-size fits all approach that may work for the most of the U.S., but not all areas. EPA also does not address in the PA that background ozone concentrations can be affected by elevation. The higher the elevation, the more likely the background ozone concentration will be high. This is not due to stratospheric intrusions or transport, but is rather a function of proximity to the stratosphere.

The Clean Air Scientific Advisory Committee (CASAC) states in their June 26, 2014 comments on the Second Draft of the Policy Assessment:

> *"The Second Draft PA cites a 2002 court decision (American Trucking Associations, Inc. v. EPA, 283 F.3d at 379) that allows the EPA to consider relative proximity to peak background levels when evaluating alternative standards but it also cites a case where the court said "attainability and technological feasibility are not relevant considerations in the promulgation of the NAAQS" (American Petroleum Institute v. Costle, 665 F. 2d at 1185). The Second Draft PA was silent as to how the EPA intends to navigate between these two legal guidelines when considering background ozone in a policy and standard-setting*

context. This question became an important issue in the CASAC deliberations as we listened to public comments regarding high background levels in the intermountain Western United States."

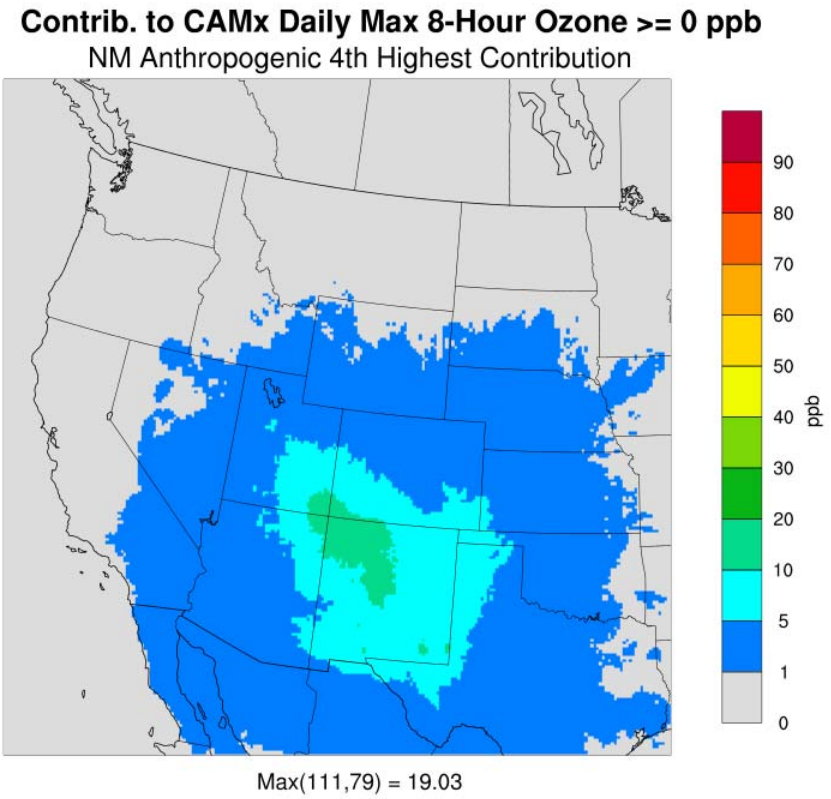
CASAC goes on in their comments to state:

> *"The authors also indicated that the background ozone is higher than average when ozone concentrations exceed 60 ppb, particularly in the intermountain West. There is currently no international legal agreement on ozone or its precursors that would effectively deal with long-range transport, despite the recommendations by the National Academy of Sciences (2009) and the Task Force on Hemispheric Transport of Air Pollution (2010) that such an agreement be sought."*

Despite CASAC's and other comments, EPA has conducted limited research and made little progress in addressing the issue of background ozone concentrations in the intermountain west. The WRAP's *West-wide Jumpstart Air Quality Modeling Study (WestJumpAQMS)* from September 2013 (Attachment 2), has analyzed background levels throughout the west. As part of the *WestJumpAQMS*, spatial maps were developed using the contributions of anthropogenic emissions of ozone for the highest (1st max) and fourth highest (4th max) days when the total ozone is greater than or equal to the following five thresholds: 76, 70, 65, 60, and 0 ppb. The 4th max ozone maps correspond to the form of the NAAQS (three year average of the 4th max ozone) and 76 ppb corresponds to the current NAAQS, whereas 70, 65 and 60 ppb represent possible future NAAQS levels and the 0 ppb threshold gives the contributions from throughout the domain. The spatial map developed for the daily maximum of greater than or equal to the 0 ppb threshold for New Mexico shows that anthropogenic sources of ozone within much of New Mexico only contributed 5-10 ppb (Figure 1).

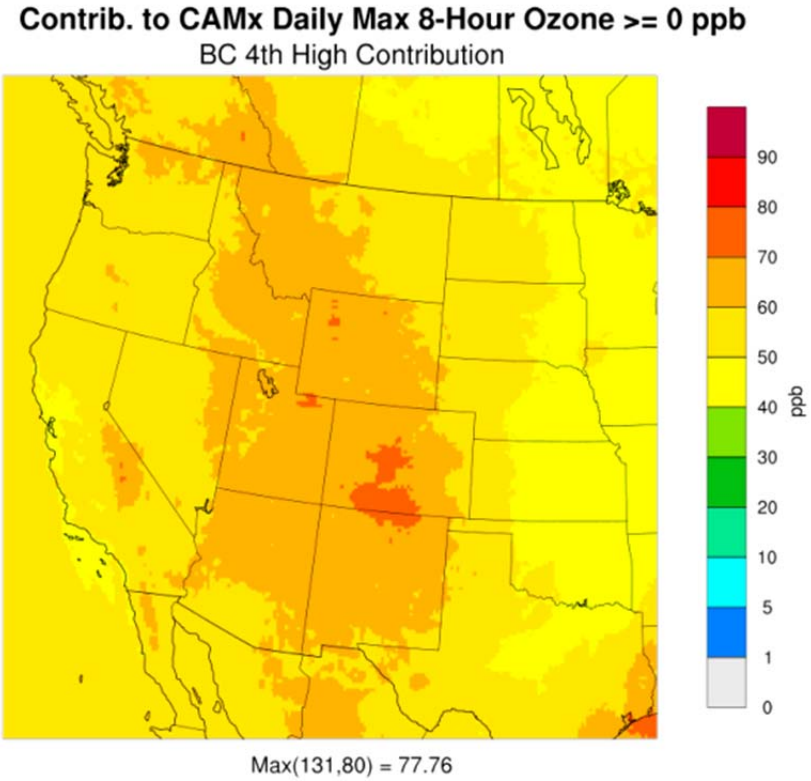
The study also shows that background ozone in New Mexico contributes 50-70 ppb for the daily maximum of greater than or equal to 0 ppb threshold (Figure 2). Based on this study, New Mexico, as well as other areas in the intermountain west, is at a huge disadvantage compared to the rest of the nation. New Mexico requests that EPA take this into consideration in setting the ozone standard at any level. This issue was apparently not anticipated in the development of the Clean Air Act, and requires a novel approach to ensure that areas within New Mexico and the intermountain west are not burdened with the impossible requirements of controlling anthropogenic sources of volatile organic compounds (VOCs) and nitrogen oxides (NOx) that do not exist within the state.

Figure 1: New Mexico - Ozone Contributions from Anthropogenic Sources



Source: West-wide Jump-Start Air Quality Modeling Study (WestJumpAQMS) – Final Report (**PDF**), September 30, 2013.

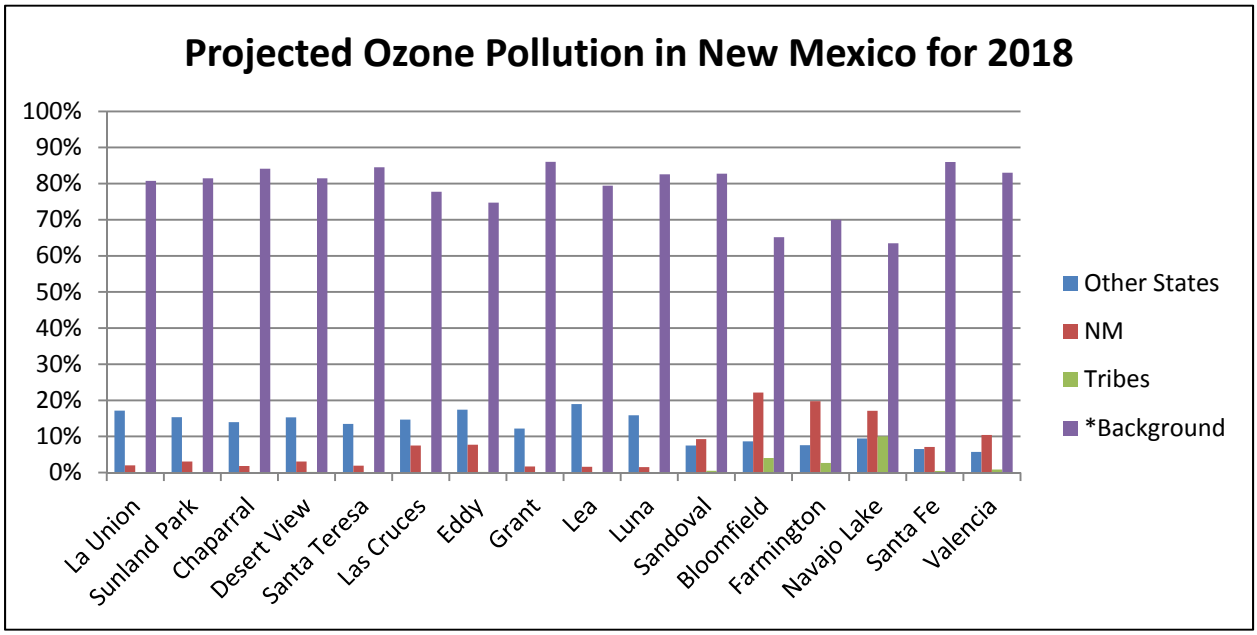
Figure 2: New Mexico - Ozone Contributions from Background



Source: West-e Jump-Start Air Quality Modeling Study (WestJumpAQMS) – Final Report (**PDF**), September 30, 2013.

Recent modeling studies conducted by EPA for the 2008 ozone NAAQS further show that the ozone levels in New Mexico along with the rest of the intermountain west are impacted significantly by background concentrations. In the preliminary modeling developed by EPA for the *Air Quality Modeling Technical Support Document for the 2008 Ozone NAAQS Transport Assessment* (TSD) released in January 2015, the majority of the ozone contribution in New Mexico is from background or what the TSD refers to as boundary conditions. See Appendix C of the TSD, Contributions to 2018 8-Hour Ozone Design Values. The modeling conducted by EPA shows that for all monitoring sites in New Mexico, 63-86 percent of ozone impacts are from high background concentrations (Figure 3).

Figure 3: Predicted 2018 Ozone Contributions for New Mexico's Monitoring Network



*Background includes Boundary Conditions, Biogenics, and Other emissions.

The ozone modeling conducted by EPA also indicates that background concentrations vary regionally, with the highest background concentrations being seen in the border region and areas of higher elevation (Figures 4-7).

Figure 4: Predicted 2018 Ozone Contributions for Northwestern New Mexico

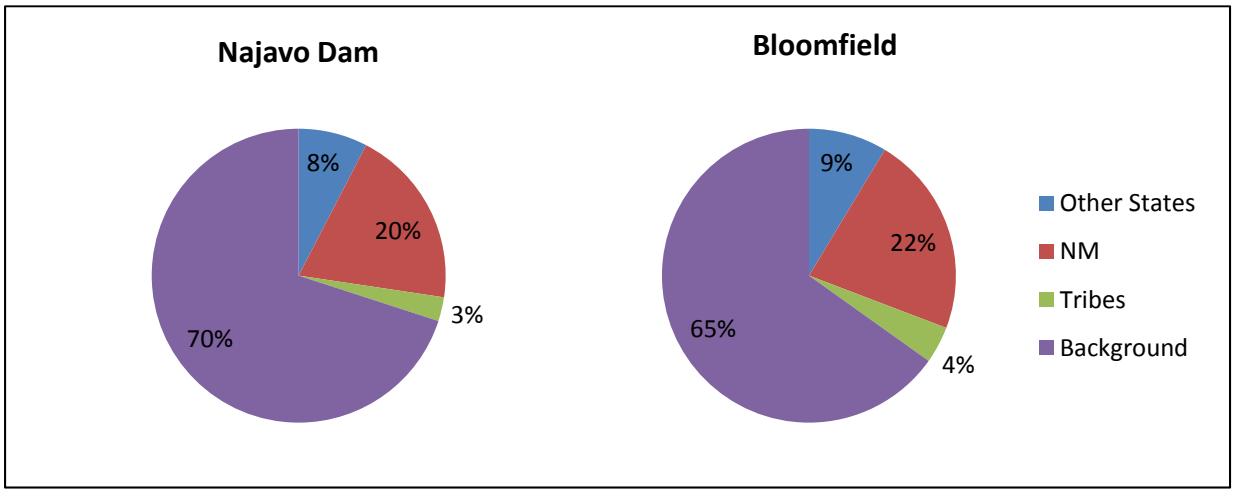


Figure 5: Predicted 2018 Ozone Contributions for Southeastern New Mexico

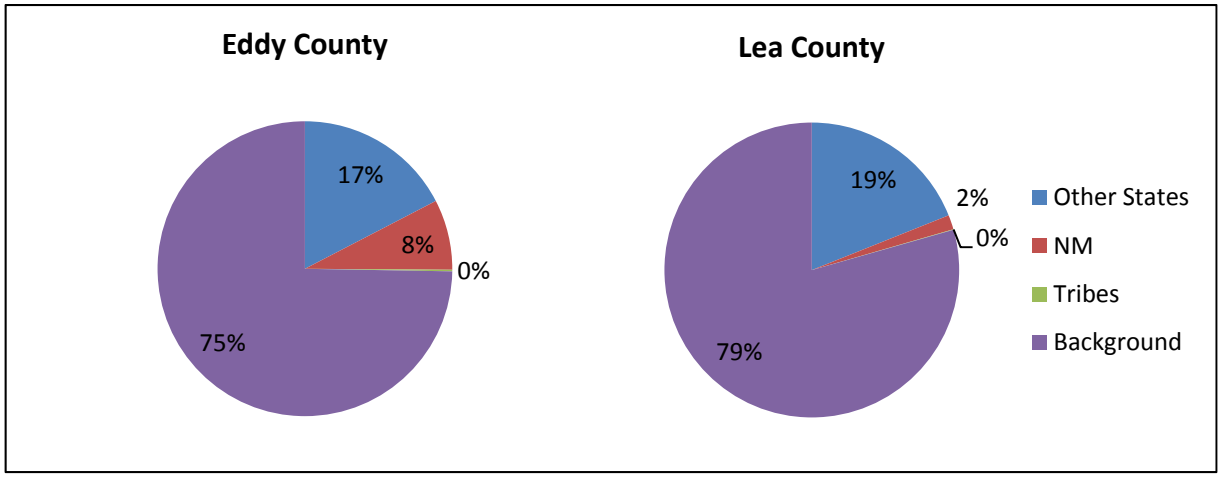


Figure 6: Predicted 2018 Ozone Contributions for the Border Region in New Mexico

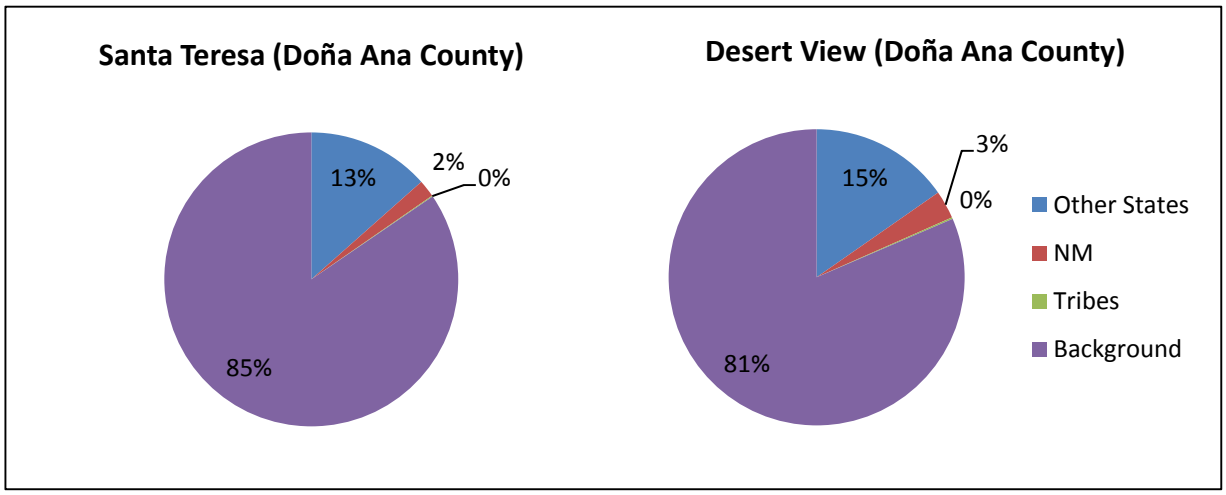
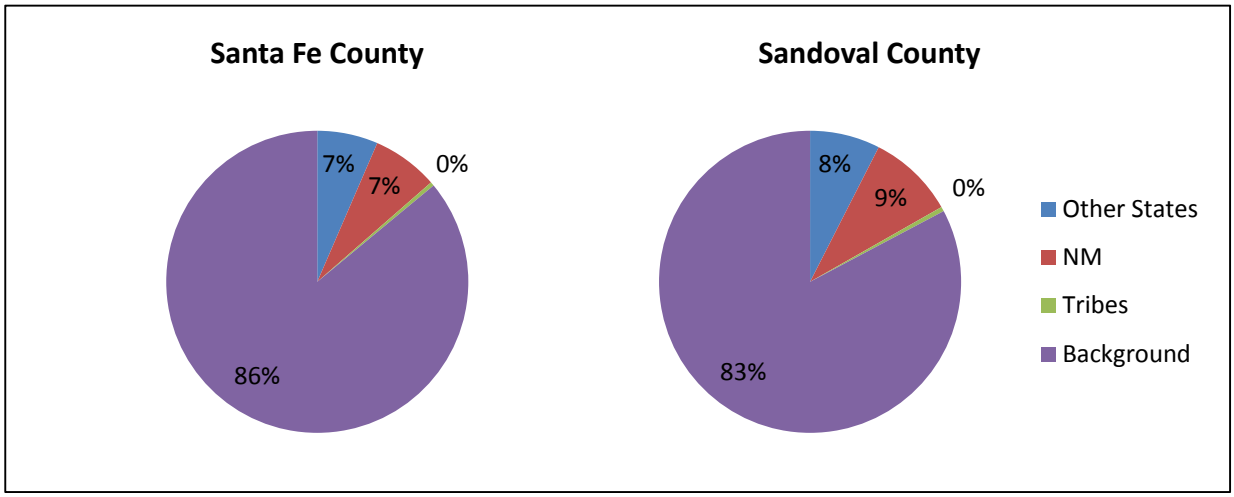


Figure 7: Predicted 2018 Ozone Contributions for High Elevation Areas in New Mexico



New Mexico again requests that EPA work with the states in the intermountain west to logically address the issue of high background ozone concentrations. This issue puts the intermountain west states at a significant disadvantage to comply with an ozone standard that, in many instances, is not threatened by in-state sources. Although New Mexico understands that ground level ozone pollution is unhealthy regardless of where it is generated, we do not feel it is appropriate to designate areas nonattainment for ozone contributions that are outside of the state's control, subjecting these areas to control strategy requirements that do not meaningfully contribute to NAAQS attainment.

Exceptional Events

Under Section 319 of the CAA, the highest priority of implementing the Exceptional Events Rule (EER) is to protect public health. Contrary to this guiding principal, past experience shows that New Mexico's resources have been inordinately consumed by investigating, analyzing and preparing demonstrations for suspected exceptional events. Due to the number of work hours required to prepare these demonstrations, few resources are left to focus on providing public health protections. Furthermore, Congress adopted revisions to Section 319 to avoid nonattainment designations or continued nonattainment where the associated nonattainment requirements are not the appropriate planning processes due to data affected by exceptional events.

EPA states in the Proposed NAAQS Ozone Rule that "as the levels of alternative prospective standards are lowered, background will represent increasingly larger fractions of total O_3 levels, and may subsequently complicate efforts to attain these standards." 79 Fed. Reg. at 75,383. EPA acknowledges this will largely affect rural locations in the west. *Id.* Where background levels are already close to the NAAQS, the need for exceptional event demonstrations to exclude data affected by wildfire and stratospheric ozone intrusion will increase. Although exceptional event demonstrations are appropriate and necessary under the Act, the time and expense required to develop such a demonstration rivals that of developing a nonattainment SIP. Modeling of exceptional events will likely play a large role in meeting the rule's technical requirement for showing "there would have been no exceedance or violation but for the event."

New Mexico does not have the staff with the expertise to run ozone models for exceptional events, nor do we have the staffing levels required to maintain an updated emissions inventory for modeling. New Mexico would likely need to hire additional staff or contract the work out, both difficult in a time of constrained budgets, tight deadlines and increased workloads. In order for states to utilize the provisions of the EER in a practical fashion, EPA must streamline the onerous process, provide the tools and guidance required to prepare demonstrations and respond to demonstrations in a timely fashion.

As evidence of using the EER as a regulatory relief mechanism, EPA provides two examples of recently approved demonstrations (one for stratospheric ozone intrusion and one for wildfire impacts). This limited number of examples provides states little confidence that their efforts to prepare a demonstration will result in concurrence by EPA. New Mexico's previous experience with exceptional event demonstrations has shown that EPA regional office reviews are not consistent with one another, nor is the same regional office consistent in their reviews from year to year. EPA is also suffering from constrained resources and in New Mexico's experience, has

not acted timely upon exceptional event submissions. Timely action is critical because it affects our area designations and planning process. Therefore, it is imperative that EPA issue a revised EER that streamlines the demonstration process with clearly defined requirements and timelines to provide certainty to the planning process. In addition, concurrent guidance should be issued on preparing exceptional events demonstrations for exceedances caused by wildfires and stratospheric ozone intrusion.

In New Mexico, most ozone exceedances occur during the summer months during the wildfire season, while stratospheric ozone intrusions typically occur in the late winter and spring. With drought conditions, wildfires in the west can also occur during non-summer months, leading to an influence on ozone levels. As a result, and as EPA has noted, the timeline for developing demonstrations for exceptional events for area designations is extremely tight. In order to exclude data for area designations, New Mexico would have to review three years of data (i.e., 2013-2015), flag candidate data and provide initial descriptions of the event by July 1, 2016. In order to meet the October 1, 2016 deadline to submit demonstrations and area designations, New Mexico would only have two months to finalize a demonstration for three years of data, given that a thirty day comment period is required. If EPA intends to use 2016 data in final designations, as expected, the timeframe to investigate exceptional events, flag data and submit demonstrations could be as short as two to five months. This extremely shortened timeframe for exceptional events demonstrations may prove to be unattainable and result in nonattainment designations due to data influenced by exceptional events.

Implementation of the proposed ozone NAAQS and associated use of the EER will require more resources than New Mexico currently has. EPA must insure adequate federal funding to provide the staffing, financial and technical resources to enable us to abide by our regulatory obligations and fulfill our mission to protect public health.

Clean Air Act Section 179B

One of the mechanisms that EPA references to address high background levels of ozone in the intermountain west is CAA Section 179B. Section 179B applies to international transport of air pollution, which may contribute to high background levels for certain international border regions. Section 179B allows EPA to approve a SIP that does not demonstrate attainment or maintenance of the NAAQS as long as all required measures have been implemented if the state demonstrates that the plan would have met the standard “but for” the impact of international emissions. Section 179B provides some regulatory relief by preventing automatic bump-ups to higher nonattainment classifications and sanctions for not attaining the standard. However, Section 179B still leaves communities with significant burdens to implement regulatory requirements that may have little air quality benefit.

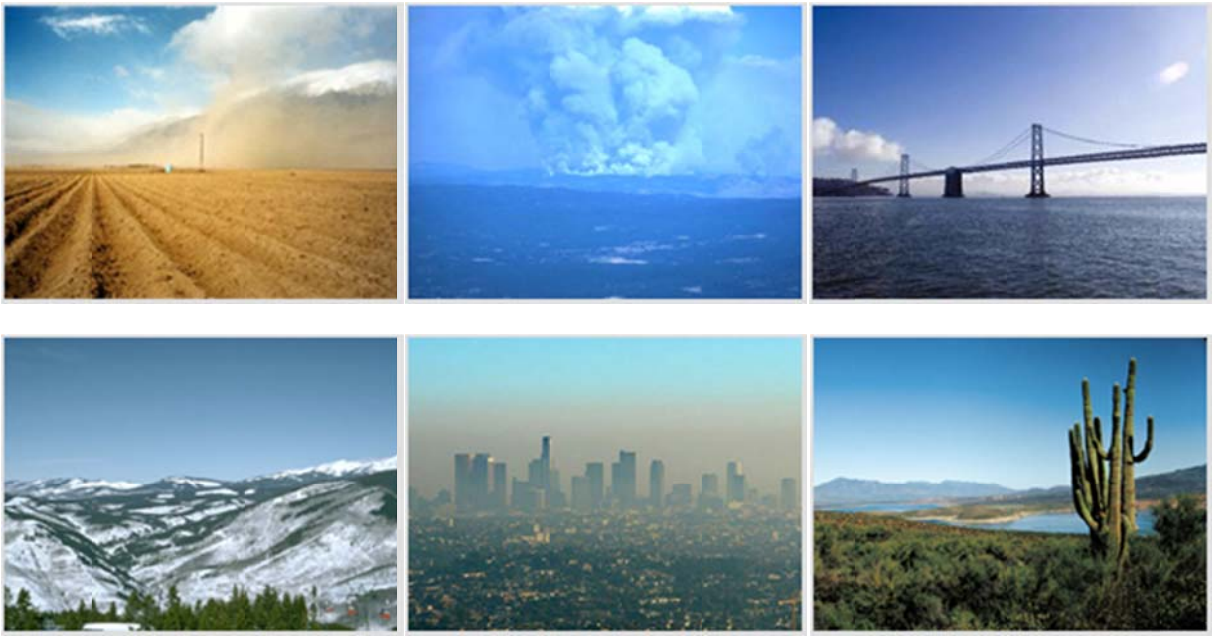
New Mexico has past experience with international transport and the limitations of Section 179B. An example of this was the 1-hour ozone nonattainment area in Sunland Park, New Mexico. Sunland Park is located in the Paso del Norte air shed, which also includes El Paso, Texas, and Ciudad Juarez, Mexico. Sunland Park is a small community with a population of 13,000, and contributes only about three percent of the total ozone precursor emissions within the Paso del Norte air shed. It therefore had almost no control over the emissions that caused the area to be designated nonattainment, but was still required to abide by the nonattainment

requirements under the CAA including general conformity, nonattainment NSR, and transportation conformity, even though these requirements provided limited, if any, benefit in reducing ozone levels within the Paso del Norte air shed.

There is also a question as to how this provision would relate to international transport from countries that do not border the U.S., such as China. As research has shown, the U.S., particularly the western region, is impacted by transported ozone pollution from Asia. Even more concerning, that impact is increasing by approximately 0.63 ppb per year. (Cooper et al., 2010 Nature)

EPA states in its supporting materials for the proposed ozone rule that most areas will be attaining a standard of 70 ppb or 65 ppb for ozone by 2025 through existing and proposed federal rules for VOCs and NOx emissions. This statement is questionable with respect to areas where international transport from Asia is a significant contributor to ozone levels. EPA has not explained how this issue would be addressed under the CAA or how a state would qualify under 179B for emissions from another country that does not border that state. Quantifying the impact of emissions due to global transport will be challenging for states and may require technical expertise and global analyses that states do not have the resources to fund. EPA should develop 179B guidance that specifically addresses global transport from Asia and provide global modeling and technical assistance to states. Otherwise, a 179B demonstration may not be possible for qualifying states to complete.

Attachment 2



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

Final Report

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1.0 INTRODUCTION

ENVIRON International Corporation (ENVIRON), Alpine Geophysics, LLC (Alpine) and the University of North Carolina (UNC) at Chapel Hill Institute for Environment conducted the West-wide Jump-start Air Quality Modeling Study (WestJumpAQMS) 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, BP, and the Western Regional Air Partnership (WRAP) to begin the next round of regional modeling to support western U.S. air quality planning.
- Continue work conducted at the WRAP Regional Modeling Center (RMC[1]) from 2001-2009 to provide regionally complete and consistent emissions and air quality modeling for the western U.S.
    - The RMC modeling products became the basis for many state and federal land manager air analyses in the West, including numerous National Environmental Policy Act (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}, including both primary and secondary PM), 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 NEPA);
3. Perform a comprehensive source apportionment analysis to evaluate local, regional, international, and natural source impacts on ozone and fine particulate matter ($PM_{2.5}$) concentrations 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

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

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 was designed to be a regional photochemical modeling study whose databases will be available to all. WRAP has been working with its partners and has developed a plan for 2011-2013 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 an 8-hour ozone National Ambient Air Quality Standard (NAAQS) with a threshold of 0.08 ppm (84 ppb). On March 12, 2008, EPA promulgated a more stringent 0.075 ppm (75 ppb) 8-hour ozone NAAQS. In January 2010, EPA announced that they were considering lowering the 8-hour ozone NAAQS to within a range of 0.060 ppm to 0.070 ppm. In August 2011, EPA announced that the 8-hour ozone NAAQS would remain at the March 2008 0.075 ppm level. An initial implementation Memorandum was released by EPA on September 22, 2011 (McCarthy, 2011[2]) identified 52 potential areas that would be violating the 0.075 ppm 8-hour ozone NAAQS based on 2008-2010 observations, including many in the western U.S. EPA finalized the designations of ozone nonattainment areas on March 30, 2012[3]. EPA has also initiated the next round of Ozone NAAQS review with the new Ozone NAAQS currently scheduled to be proposed in 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 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 and there are large areas in the western U.S. with no Federal Reference Method (FRM) ozone monitoring data. 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; since 2009 there is a general trend toward increased ozone concentrations in the west.

On December 14, 2012, EPA revised the $PM_{2.5}$ primary NAAQS by lowering the annual $PM_{2.5}$ NAAQS threshold from 15.0 µg/m^3 to 12.0 µg/m^3[4]. EPA retained the 24-hour $PM_{2.5}$ primary NAAQS at 35 µg/m^3. EPA is setting the secondary $PM_{2.5}$ NAAQS at 15 µg/m^3 annual and 35 µg/m^3 24-hour. The 24-hour coarse PM NAAQS (PM_{10}) is also retained at 150 µg/m^3. EPA considered the adoption of a secondary $PM_{2.5}$ NAAQS to protect against visibility impairment in urban areas with a proposed threshold in the 28 to 30 deciview range and an averaging time in the range of 4 to 24 hours. However, EPA determined that the 35 µg/m^3 24-hour $PM_{2.5}$ secondary NAAQS provides visibility protection equal or better than a 30 deciview (dv) standard. Figure 1-2 displays counties that are violating the old 15.0 µg/m^3 annual $PM_{2.5}$ NAAQS and the additional counties that would violate the new 12.0 µg/m^3 annual $PM_{2.5}$ NAAQS (as well as a 13 µg/m^3 threshold that EPA was considering) based on 2008-2010 measurements. Based on 2008-2010 there would be no new $PM_{2.5}$ nonattainment counties in the western U.S. under the new annual $PM_{2.5}$ NAAQS 12 µg/m^3 level.

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

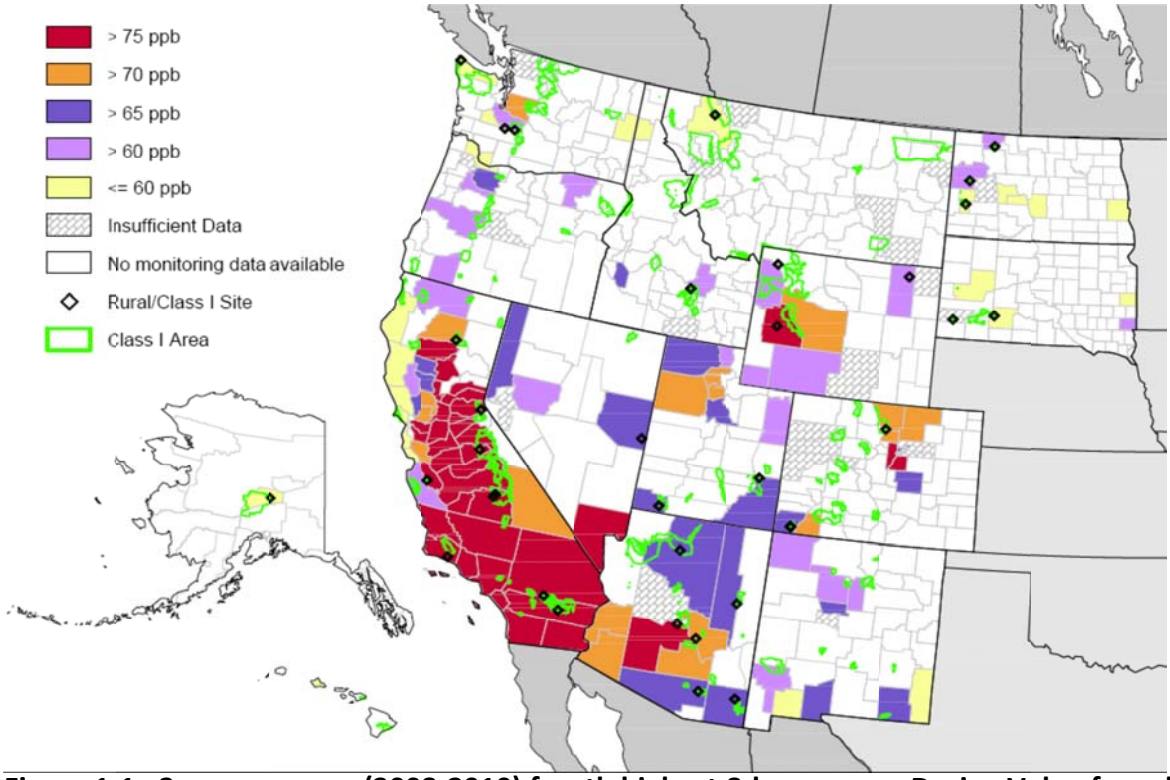


Figure 1-1. 3-year average (2008-2010) fourth highest 8-hour ozone Design Value for selected counties with color scheme indicating whether the Design Value exceeds (red) or is below the March 2008 ozone NAAQS (EPA AQS Federal Reference Method [FRM] data from the monitoring site with the highest ozone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

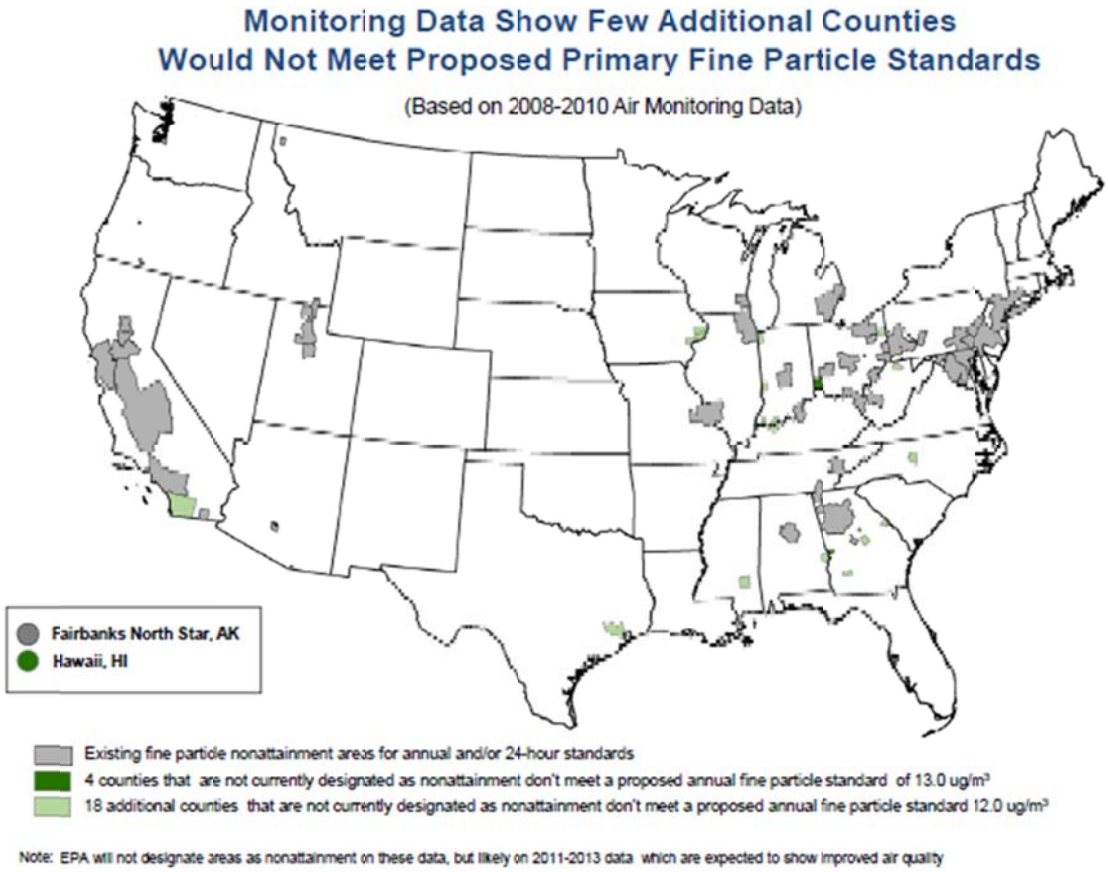


Figure 1-2. Counties that are violating the old 15.0 µg/m^3 $PM_{2.5}$ NAAQS and additional counties that would violate the new 12.0 µg/m^3 $PM_{2.5}$ NAAQS as well as a 13.0 µg/m^3 threshold EPA was considering (dark green) based on 2008-2010 observations (source: http://www.epa.gov/pm/actions.html#jun12).

1.2 OVERVIEW OF APPROACH

The procedures for conducting the WestJumpAQMS were outlined in a draft Modeling Protocol near the beginning of the project (ENVIRON, Alpine and UNC, 2012[5]). Comments were received on the WestJumpAQMS draft Modeling Protocol from Federal, State and local agencies and other stakeholders and a Response-to-Comments document was prepared (WRAP, 2013[6]). The WestJumpAQMS Modeling Protocol was then finalized reflecting the comments received from the stakeholder review (ENVIROM, Alpine and UNC, 2013[7]). Below we summarize the procedures used in the WestJumpAQMS; details are provided in the final Modeling Protocol.

1.2.1 Episode Selection

The 2008 calendar year was selected for the WestJumpAQMS photochemical grid modeling (PGM) because it satisfied the most criteria in EPA's PGM episode selection recommendations (EPA, 2007) at the time the

5 http://www.wrapair2.org/pdf/WestJumpAQMS_Modeling_Protocol_and_SourceApportionment_Design_Draft_Final.pdf
6 http://www.wrapair2.org/pdf/Response-to-Comments_WestJump_Draft_Modeling_Protocol_May1_2013.pdf
7 http://www.wrapair2.org/pdf/WestJumpAQMS_Modeling_Protocol_and_Source%20Apportionment_Design_FinalMay.pdf

project was initiated. These include meteorological conditions conducive to photochemical pollutant formation, availability of the 2008 National Emissions Inventory (NEI) and fairly typical emission conditions (e.g., not greatly affected by the recession). Ten spin-up days at the end of 2007 are used to initial the PGM for the 2008 modeling period.

1.2.2 Model Selection

The WestJumpAQMS model selection methodology followed EPA's guidance for regulatory modeling in support of ozone and $PM_{2.5}$ attainment demonstration modeling and showing reasonable progress with visibility goals (EPA, 2007) that recommends models be selected based on:

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

The WestJumpAQMS modeling used three general types of models for simulating ozone and other gaseous pollutants, particulate matter, visibility and deposition:

- 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.

Table 1-1 summarizes the main models selected for the WestJumpAQMS modeling with details on the justification for their selection provided in the final Modeling Protocol (ENVIRON, Alpine and UNC, 2013). The WRF meteorological and SMOKE emissions models were selected for developing the Photochemical Grid Model (PGM) inputs for the 2008 modeling period. Additional emissions models were used for on-road mobile sources (MOVES) and biogenic emissions (MEGAN). Two PGMs were applied in the WestJumpAQMS: the CAMx PGM was selected as the primary PGM due to the availability of ozone and PM source apportionment capabilities. The CMAQ PGM was also applied and the model performance will be compared with CAMx and reported at a later date on the Three-State Data Warehouse (3SDW) website.

Table 1-1. Summary of models selected for the WestJumpAQMS.

Model Type	Selected Model
Meteorological Model	Weather Research Forecasting (WRF[8])
Emissions Model	Sparse Matrix Operator Kernel Emissions (SMOKE[9])
Emissions Model – On Road Sources	MOtor Vehicle Emissions Simulator (MOVES[10])
Emissions Model – Biogenic Sources	Model for Emissions of Gases and Aerosols in Nature (MEGAN[11])
Photochemical Grid Models	Comprehensive Air-quality Model with extensions (CAMx[12]) Community Multiscale Air Quality (CMAQ[13])

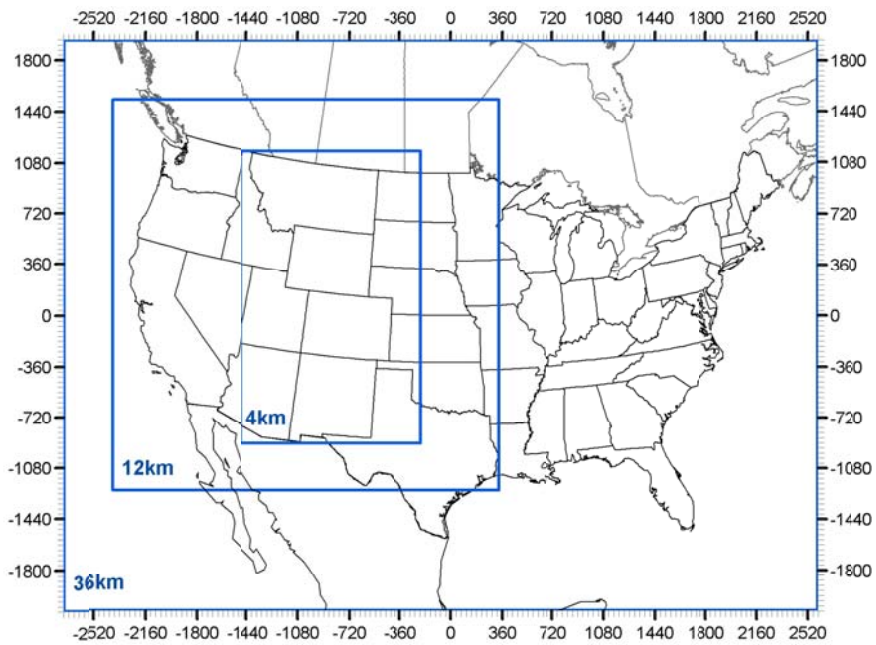
1.2.3 Modeling Domain Selection

The WestJumpAQMS modeling domains were selected as a trade-off between the need to have high resolution modeling for sources in the Inter-Mountain West versus ability to perform regional ozone and particulate matter source apportionment modeling of all the western states with reasonable computation times. Accordingly, a 36/12/4 km nested grid structure was selected for the WestJumpAQMS meteorological, emissions and air quality modeling. The WRF meteorological model requires use of an odd nesting ratio so the 36/12/4 km domains are using a 3:1 grid-nesting ratio. A Lambert Conformal Projection (LCP) was used for the WestJumpAQMS 36/12/4 km horizontal modeling domains using the parameters in Table 1-2. Figure 1-3 defines the 36/12/4 km modeling domains for which PGM (i.e., CAMx and CMAQ) model inputs were prepared. The WRF meteorological model 36/12/4 km domains were defined slightly larger than the PGM modeling domains in order to eliminate any artifacts introduced along the boundaries of the meteorological model domains that may occur as the boundary conditions come into dynamic balance with the WRF numerical algorithms. The following types of 36/12/4 km domains were used in the WestJumpAQMS:

- A 36 km continental U.S. (CONUS) domain (Figure 1-3) 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 (Figure 1-3) that is larger than used in WRAP and contains all of the WRAP and adjacent states as well as extending into portions of Canada and Mexico.
- There were several types of 4 km modeling domains used in the WestJumpAQMS:
    - A large 4 km Inter-Mountain West Domain (IMWD) processing domain (Figure 1-3) that covers all of the areas of primary interest for which PGM meteorological and emissions inputs were prepared.
    - A 4 km Detailed Source Apportionment Domain (DSAD; Figure 1-4) that is 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 throughout the 36/12/4 km CONUS region into the 4 km DSAD, as well as downwind transport of emissions from the DSAD and other regions on downwind ozone and PM concentrations. The 4 km DSAD covers key oil and gas development areas and receptor regions (e.g., Class I areas) in Colorado, Utah, Wyoming and northern New Mexico (see Figure 1-4b).

8 http://www.wrf-model.org/index.php
9 http://www.smoke-model.org/index.cfm
10 http://www.epa.gov/otaq/models/moves/index.htm
11 http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm
12 http://www.camx.com/
13 http://www.cmaq-model.org/

- An Impact Assessment Domain (IAD) that is a larger 4 km domain designed for conducting stand-alone 4 km photochemical grid modeling using boundary conditions (BCs) from the 36/12 km CONUS/WESTUS modeling. The IAD is defined for performing air impact assessments of sources within the IAD 4 km domain on receptors within the IAD 4 km domain. Although initially several IADs were defined, in the end only one large IAD photochemical grid modeling database (Figure 1-5) was developed. The stand-alone 4 km IAD CAMx modeling database was developed to address impacts of BLM emission sources in Colorado and northwestern New Mexico as part of the BLM Colorado Air Resource Management Modeling Study (CARMMS) being conducted for the BLM Colorado State Office (COSO).



Modeling Domain

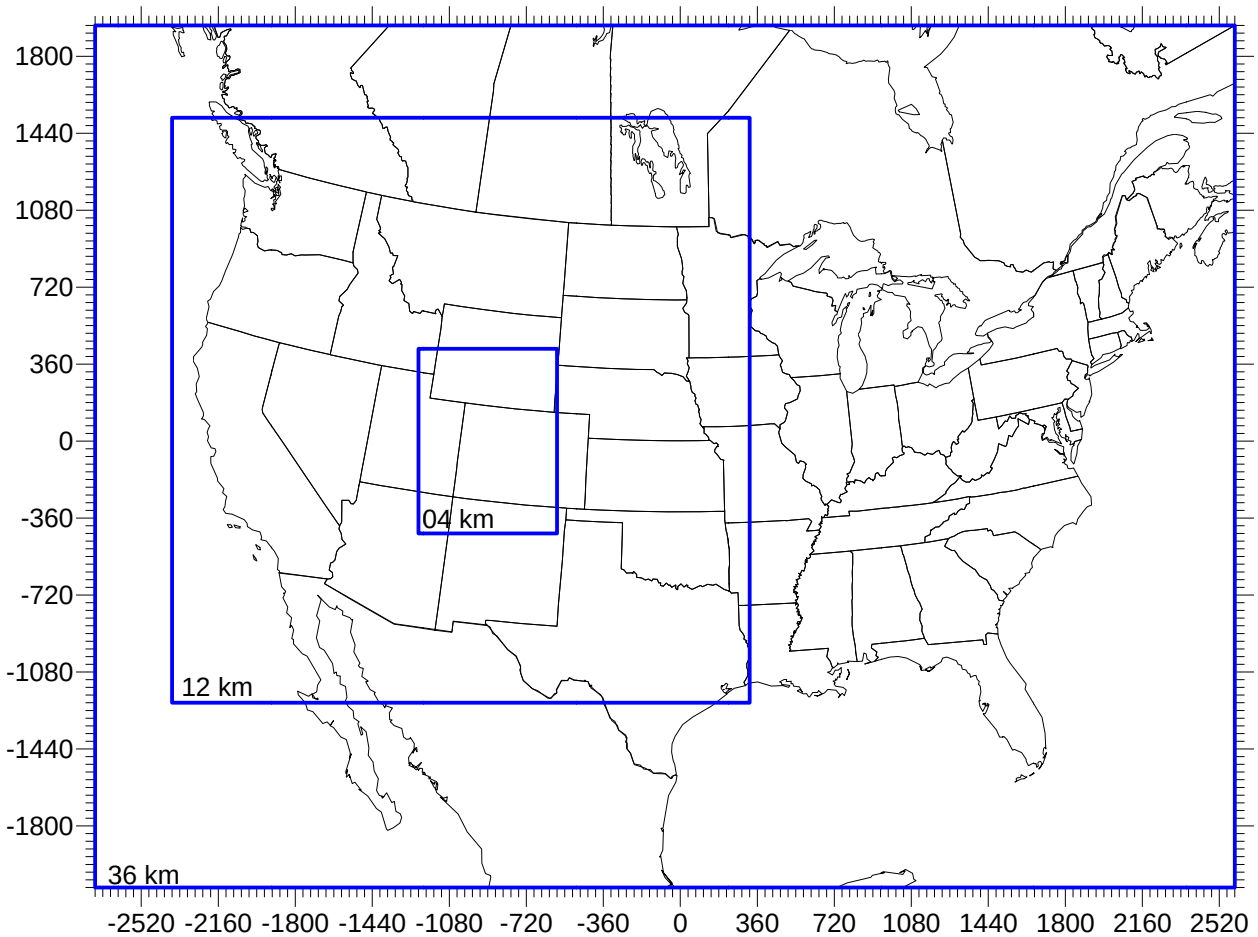
36km: 148 x 112 (-2736, -2088) to (2592, 1944)
12km*: 227 x 230 (-2388, -1236) to (336, 1542)
04km*: 317 x 515 (-1480, -904) to (-212, 1156)

* includes buffer cells

Figure 1-3. 36 km CONUS, 12 km WESTUS and 4 km IMWD processing domains used for developing PGM meteorological and emission inputs.

Table 1-2. Map projection parameters for the WestJumpAQMS 36/12/4 modeling domains.

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



CAMx Modeling Domain

36 km : 148 x 112 (-2736, -2088) to (2592, 1944)
12 km*: 227 x 230 (-2388, -1236) to (336, 1524)
04 km*: 164 x 218 (-1228, -436) to (-572, 436)

* includes buffer cells

Figure 1-4a. Definition of the 4 km Detailed Source Apportionment Domain (DSAD) that is in a two-way grid nest with the 12 km WESTUS and 36 km CONUS domains.

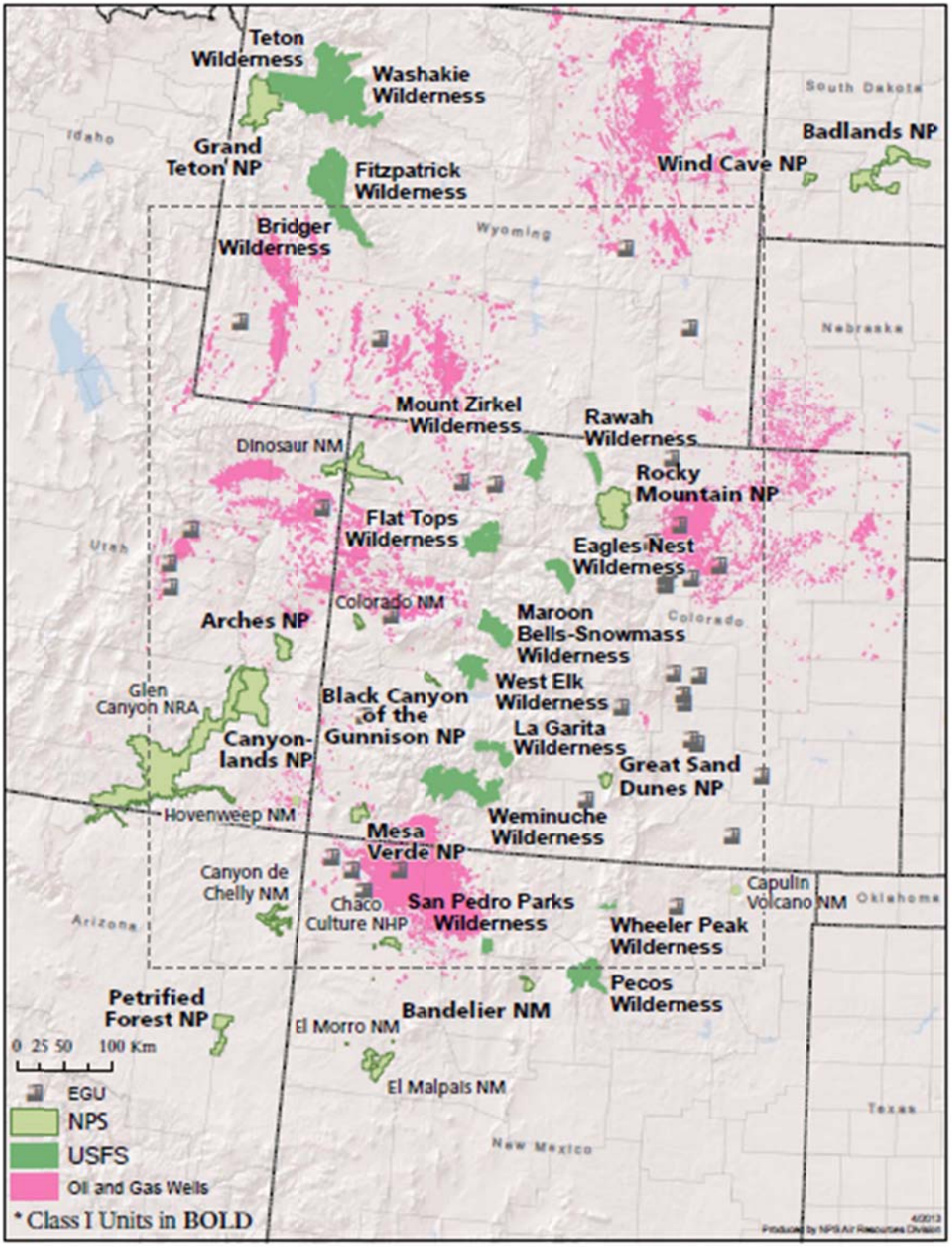
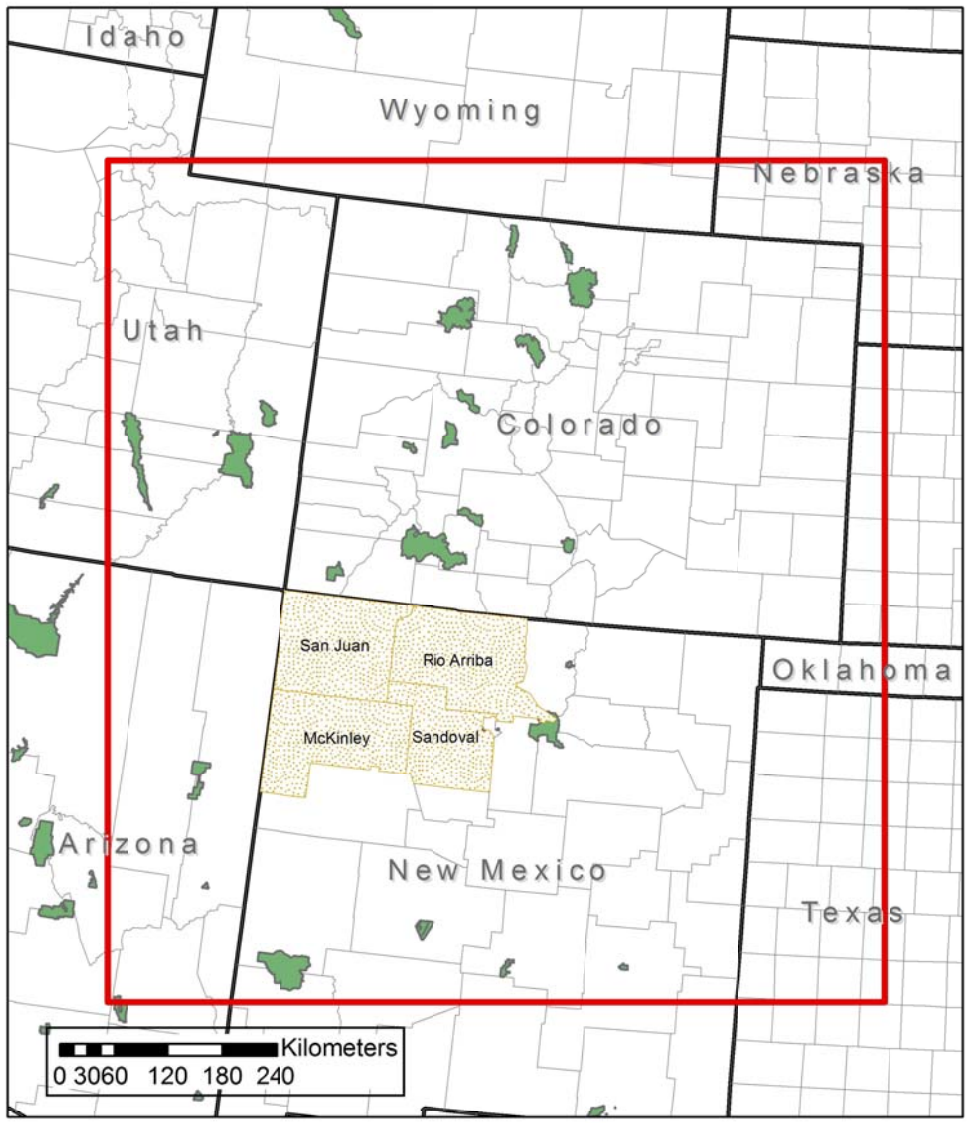


Figure 1-4b. 4 km DSAD Pilot Study domain with locations of oil and gas development (pink), Electrical Generating Units (EGUs) and key Class I (bold) and sensitive Class II receptor areas (green). (Note: Savage Run is another sensitive Class I area in Wyoming note depicted).



Legend

- Proposed 4km Domain
- NM RMP Counties
- Class I Areas

Coordinates of 4km Domain:

SW Corner: (-1260,-720) km
NE Corner: (-396,216) km
(nx,ny) = (216,234)

Projection = Lambert Conformal
parameters:(-97, 40, 33, 45)

Figure 1-5. 4 km Impact Assessment Domain (IAD) for the BLM Colorado Air Resource Management Modeling Study (CARMMS).

The CAMx vertical domain structure depends 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 a pressure level of 50 millibars (mb; ~19-km AGL) (ENVIRON and Alpine, 2012[14]). A layer averaging scheme is adopted for the CAMx simulations whereby multiple WRF layers are combined into one CAMx layer to reduce the air quality model computational time. Table 1-3 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 1-3 is collapsing two WRF layers into one CAMx/CMAQ 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 resulting in overstated surface concentrations. For example, NO_X emissions are caused by combustion, so are buoyant and have plume rise that in reality could take them out of the first layer if it is defined too shallow. However, there is concern that layer collapsing of the lowest WRF layers may introduce uncertainties or errors in the modeling.

The Denver ozone SIP planning modeling of the May-August 2008 period used the same vertical layer structure as being used in WestJumpAQMS and the same 36 WRF to 25 CAMx layer collapsing strategy. They conducted a no layer collapsing CAMx sensitivity test (36 vertical layers) and found it had essentially no effect on the afternoon and daily maximum 8-hour ozone concentration estimates (Morris et al., 2012a). The 36 layer CAMx sensitivity tests produced lower nighttime ozone at many sites, but it tended to degrade rather than improve ozone model performance. The 36 layer sensitivity tests also took 22% more time to run than the 25 vertical layer base case. The Allegheny County Health Department (ACHD) Liberty-Clairton $PM_{2.5}$ SIP modeling[15] also used the same 36 WRF to 25 CAMx layer collapsing strategy as used in the WestJumpAQMS. ACHD also did a no layer collapsing sensitivity test and found essentially no difference in the CAMx-estimated $PM_{2.5}$ concentrations (Morris, Koo, Jung, Loomis and McNally, 2012). The BLM Continental Divide-Creston (CD-C) oil and gas development Environmental Impact Statement (EIS) study in southwestern Wyoming also performed a layer collapsing sensitivity test. Although CD-C layer collapsing strategy was slightly different than WestJumpAQMS as CD-C was collapsing 34 MM5 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 WestJumpAQMS 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 no 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.

14 http://www.wrapair2.org/pdf/WestJumpAQMS_2008_Annual_WRF_Final_Report_February29_2012.pdf
15 http://www.achd.net/air/index.php

Table 1-3. 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	

1.2.4 Meteorological Modeling

The WRF meteorological model was applied for the 2008 calendar year, with 10-day spin-up, on a 36/12/4 km modeling domain to develop PGM modeling inputs for the 36/12/4 km domains depicted in Figure 1-3. Chapter 2 of this report summarizes the WRF meteorological model application and model performance evaluation with more details provided in the WestJumpAQMS WRF Application/Evaluation Report (ENVIRON and Alpine, 2012).

1.2.5 Emissions

The SMOKE emissions model was used to generate the hourly gridded speciated emission inputs for the 2008 base case, the CAMx PGM, the 2008 calendar year and the 36/12/4 km modeling domains. The main source of the 2008 emissions was the 2008 NEI[16] that was augmented with other emissions sources such as the WRAP Phase III oil and gas emission inventories. Chapter 3 of this report summarizes the development of the 2008 base case emissions with more details presented in 16 Technical Memorandums[17] prepared as part of the WestJumpAQMS that focus on each major emissions source category.

1.2.6 Boundary Conditions

Boundary Conditions (BCs) for the 36 km CONUS domain were based on the MOZART[18] global chemistry model. Considerations were also given to using BCs based on the GEOS-Chem[19] or AM3[20] global chemistry models. However, at the time of the WestJumpAQMS PGM input development, only 2008 MOZART global chemistry model output was available. Processors were used to interpolate the MOZART concentration output from the MOZART horizontal and vertical coordinate system to the CAMx/CMAQ LCP coordinate system and vertical layer structure and to map the MOZART chemical species to the CB05 chemical mechanisms used by CAMx. During the course of the WestJumpAQMS output from a 2008 GEOS-Chem simulation became available and a GEOS-Chem BC PGM sensitivity test was conducted that is summarized by Morris, Jung and Koo (2013[21]).

1.2.7 Model Performance Evaluation

The CAMx 2008 base case simulations were compared against observed ambient air quality and wet deposition observations as part of a model performance evaluation. The CAMx 2008 base case modeling and model performance evaluation is presented in Section 4 of this report. A comparison of the CAMx and CMAQ model performance is under preparation and will be posted on the WRAP website at a later date.

1.2.8 Source Apportionment Modeling

The CAMx Anthropogenic Precursor Culpability Assessment (APCA) version of the Ozone Source Apportionment Technology (OSAT) and the Particulate Source Apportionment Technology (PSAT) probing tools were applied to estimate the contributions of states and major source categories to ozone and $PM_{2.5}$ concentrations in the western U.S. under 2008 base case emission conditions. Two types of ozone and $PM_{2.5}$ source apportionment modeling were conducted:

- State-Specific ozone and $PM_{2.5}$ source apportionment modeling analysis that was performed in a similar manner as EPA's Cross State Air Pollution Rule (CSAPR) to assess the contributions of upwind state anthropogenic emissions on downwind state elevated ozone and $PM_{2.5}$ concentrations; and

16 http://www.epa.gov/ttnchie1/net/2008inventory.html
17 http://www.wrapair2.org/WestJumpAQMS.aspx
18 http://www.acd.ucar.edu/wrf-chem/mozart.shtml
19 http://acmg.seas.harvard.edu/geos/
20 http://www.gfdl.noaa.gov/atmospheric-model
21 http://www.wrapair2.org/pdf/Morris_MOZART-GEOS_WestJumpAQMS_Jul10_2013_Draft1.pdf

- Source Category-Specific ozone and $PM_{2.5}$ source apportionment modeling that assessed the contributions of the following six major source categories to ozone and $PM_{2.5}$ concentrations in the western states:
    - Natural Emissions (Biogenic, Lightning, Sea Salt and Windblown Dust);
    - Fires (Wild Fires, Prescribed Burns and Agricultural Burning);
    - Upstream Oil and Gas Sources;
    - Mobile Sources (On-Road, Non-Road and Commercial Marine Vessels);
    - Point Sources (Electrical Generating Units [EGUs] and non-EGU point sources, except oil and gas);
    - Remainder Sources (e.g., Area Sources, Ammonia and Fugitive Dust).

The State-Specific ozone and $PM_{2.5}$ source apportionment results are presented in, respectively, Chapters 5 and 6 and the Source Category-Specific ozone and $PM_{2.5}$ source apportionment modeling results are presented in Chapter 7.

1.2.9 Database Archiving and Distribution

The WestJumpAQMS 2008 modeling databases and modeling results will be archived by the Three State Data Warehouse (3SDW) where they will be available to users on request.

1.2.10 Project Participants

The WestJumpAQMS was performed by the contracting team of ENVIRON International Corporation, Alpine Geophysics, LLC and University of North Carolina (UNC) at Chapel Hill Institute for the Environment under the direction of the Western Regional Air Partnership (WRAP). Tom Moore of WRAP was the contract manager and technical coordinator. Ralph Morris of ENVIRON was project manager and ENVIRON served as the prime contractor. Ralph Morris, Dennis McNally and Zac Adelman directed the activities within the, respectively, ENVIRON, Alpine and UNC modeling centers. At ENVIRON, Ralph Morris was assisted by Bonyoung Koo, Jeremiah Johnson, Jaegun Jung, Tanarit Sakulyanontvittaya, Amnon Bar-Ilan, John Grant, Yesica Alvarez, Rajashi Parikh, James King and Justin Zagunis. At Alpine, Dennis McNally was assisted by Cyndi Loomis and James Wilkinson. And at UNC, Zac Adelman was assisted by Mohammed Omary, B. H. Baek, Dongmei Yang and Aijun Xiu.

2.0 METEOROLOGICAL MODELING

2.1 METEOROLOGICAL MODELING APPROACH

The WestJumpAQMS used the WRF meteorological model to generate the CAMx and CMAQ meteorological inputs for the 2008 calendar year and 36/12/4 km modeling domains (Figure 1-3). The WRF computational domains were defined to be slightly larger than the PGM modeling domains to eliminate the occurrence of boundary artifacts in the PGM meteorological inputs.

The WRF model contains many different physics options, and achieving the best model performance for any particular year and region is accomplished by performing model sensitivity tests using different options. As part of the post-2008 Denver ozone SIP modeling, Alpine Geophysics, LLC and ENVIRON conducted numerous WRF meteorological sensitivity simulations to determine the best performing configuration for simulating meteorology in the Inter-Mountain West region (Morris et al., 2011). The final WRF configuration used for the 2008 Denver ozone modeling was also used for the WestJumpAQMS WRF modeling. Below we summarize the WestJumpAQMS WRF application and evaluation, more details are presented in the WestJumpAQMS WRF Application/Evaluation Report (ENVIRON and Alpine, 2012[22]).

2.2 METEOROLOGICAL MODEL METHODOLOGY

Model Selection: The most recent publicly available version of WRF (Version 3.3.1) at the time of the WestJumpAQMS WRF modeling was used (note that a more recent version is 3.4.1 was released August 16, 2012 during the study). The WRF Processing System (WPS) preprocessor programs including GEOGRID, UNGRIB, and METGRID will be used to develop model inputs.

Horizontal Domain Definition: The computational domain on which WRF was applied for WestJumpAQMS included a 36 km CONUS, 12 km WESTUS and 4 km Inter-Mountain West Domain (IMWD). The grid projection is Lambert Conformal with a pole of projection of 40 degrees North, -97 degrees East and standard parallels of 33 and 45 degrees, the so-called RPO projection (Table 1-2). The datum (size and shape of earth) is a perfect sphere with radius 6370.0 km.

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 1-3.

Topographic Inputs: Topographic information for WRF were developed using the standard WRF terrain databases. The 36 km domain is based on the 10 minute (18 km) global data. The 12 km domain is based on the 2 minute (~4 km) data. The 4 km domain will be based on 30 second (~900 m) data

Vegetation Type and Land Use Inputs: Vegetation type and land use information were developed using the most recently released WRF databases provided with the WRF distribution. Standard WRF surface characteristics corresponding to each land use category were employed.

Atmospheric Data Inputs: The first guess fields were taken from the 12 km North American Model (NAM) database.

Diffusion Options: Horizontal Smagorinsky first-order closure (km_opt = 4) with sixth-order numerical diffusion and suppressed up-gradient diffusion (diff_6th_opt = 2) were used.

Lateral Boundary Conditions: Lateral boundary conditions were specified from the initialization dataset (12 km NAM) on the 36 km domain with continuous updates nested from the 36 km domain to the 12 km

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

domain and continuous updates nested from the 12 km domain to the 4 km domain, using one-way nesting (feedback = 0).

Top and Bottom Boundary Conditions: The top boundary conditions were selected as an implicit Rayleigh dampening for the vertical velocity. Consistent with the model application for non-idealized cases, the bottom boundary condition were selected as physical, not free-slip.

Water Temperature Inputs: The water temperature data were taken from the National Centers for Environmental Prediction (NCEP) Real Time Global (RTG) global one-twelfth degree analysis[23].

FDDA Data Assimilation: The WRF model was run with a combination of analysis and observation nudging (i.e., Four Dimensional Data assimilation [FDDA]). Analysis nudging was used on the 36 km and 12 km domain using the 12 km NAM dataset. For winds and temperature, analysis nudging coefficients of $5x10^{-4}$ and $3.0x10^{-4}$ were used on the 36 km and 12 km domains, respectively. For mixing ratio, an analysis nudging coefficient of $1.0x10^{-5}$ was used for both the 36 km and 12 km domains. The nudging uses both surface and aloft nudging with nudging for temperature and mixing ratio not performed in the lower atmosphere (i.e., within the boundary layer and at the surface). Observation nudging was performed on the 4 km grid domain using the Meteorological Assimilation Data Ingest System (MADIS)[24] observation archive. The MADIS archive includes the National Climatic Data Center (NCDC)[25] observations and the National Data Buoy Center (NDBC) Coastal-Marine Automated Network C-MAN[26] 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.

Physics Options: The WRF model contains many different physics options. The physics options chosen for the WestJumpAQMS application are presented in Table 2-1.

Application Methodology: The WRF model was executed in 5½ day blocks initialized at 12Z every 5 days. Model results were output every 60 minutes. The first twelve (12) hours of each 5 ½ day block is used for model spin-up and not used in the PGM model inputs or in the WRF model performance evaluation. WRF was configured to run in distributed memory parallel mode.

23 Real-time, global, sea surface temperature (RTG-SST) analysis. http://polar.ncep.noaa.gov/sst/oper/Welcome.html
24 Meteorological Assimilation Data Ingest System. http://madis.noaa.gov/
25 National Climatic Data Center. http://lwf.ncdc.noaa.gov/oa/ncdc.html
26 National Data Buoy Center. http://www.ndbc.noaa.gov/cman.php

Table 2-1. Physics options used in the WestJumpAQMS 2008 WRF simulation modeling.

WRF Treatment	Option Selected	Notes
Microphysics	Thompson scheme	New with WRF 3.1.
Longwave Radiation	RRTMG	Rapid Radiative Transfer Model for GCMs includes random cloud overlap and improved efficiency over RRTM.
Shortwave Radiation	RRTMG	Same as above, but for shortwave radiation.
Land Surface Model (LSM)	NOAH	Two-layer scheme with vegetation and sub-grid tiling.
Planetary Boundary Layer (PBL) scheme	YSU	Yonsie University (Korea) Asymmetric Convective Model with non-local upward mixing and local downward mixing.
Cumulus parameterization	Kain-Fritsch in the 36 km and 12 km domains. None in the 4 km domain.	4 km can explicitly simulate cumulus convection so parameterization not needed.
Analysis nudging	Nudging applied to winds, temperature and moisture in the 36 km and 12 km domains	Temperature and moisture nudged above PBL only.
Observation Nudging	Nudging applied to surface wind only in the 4 km domain	Surface temperature and moisture observation nudging can introduce instabilities.
Initialization Dataset	12 km North American Model (NAM)	Also used in analysis nudging

2.3 METEOROLOGICAL MODEL PERFORMANCE EVALUATION

The WestJumpAQMS WRF model performance evaluation is documented in a "WRF Application/Evaluation" report (ENVIRON and Alpine, 2012[27]). The WestJumpAQMS 2008 WRF model performance evaluation 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 fields using graphical outputs. The quantitative approach was to examine tabulations and graphical displays of the average 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. The statistics were calculated using the publicly available METSTAT evaluation tool, which calculates the statistical performance metrics and can produce time series of predicted and observed meteorological variable and performance statistics. The observed database for winds, temperature, and water mixing ratio that were used in this analysis is from the National Oceanic and Atmospheric Administration (NOAA), Earth System Research Laboratory (ESRL) Meteorological Assimilation Data Ingest System (MADIS). The locations of the MADIS monitoring sites within the 36 and 12 km WRF modeling domains are shown in Figures 2-1 and 2-2. The rain observations were taken from the NOAA CPC[28] retrospective rainfall archives.

The WestJumpAQMS 2008 WRF Application/Evaluation report evaluated the WRF surface meteorological parameters using METSTAT across the 36 km CONUS, 12 km WESTUS and 4 km IMWD modeling domains and compared them against meteorological model performance benchmarks. Provided with the WestJumpAQMS WRF Application/Evaluation report was the evaluation of the WRF model performance at each individual surface monitoring site in the inter-mountains western states[29].

27 http://www.wrapair2.org/pdf/WestJumpAQMS_2008_Annual_WRF_Final_Report_February29_2012.pdf
28 http://www.cpc.ncep.noaa.gov/products/precip/realtime/retro.shtml
29 http://www.wrapair2.org/WestJumpAQMS.aspx

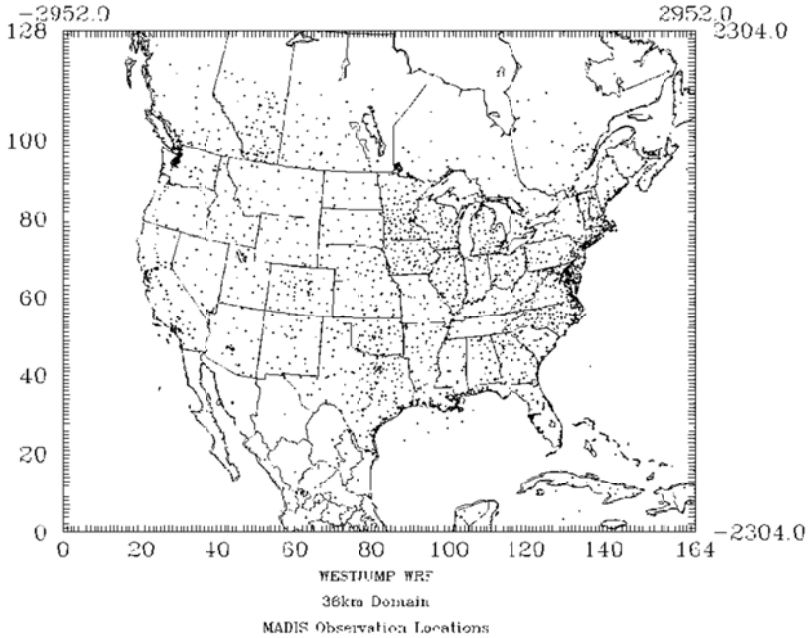


Figure 2-1. Locations of MADIS surface meteorological modeling sites within the WestJumpAQMS WRF 36 km CONUS modeling domain.

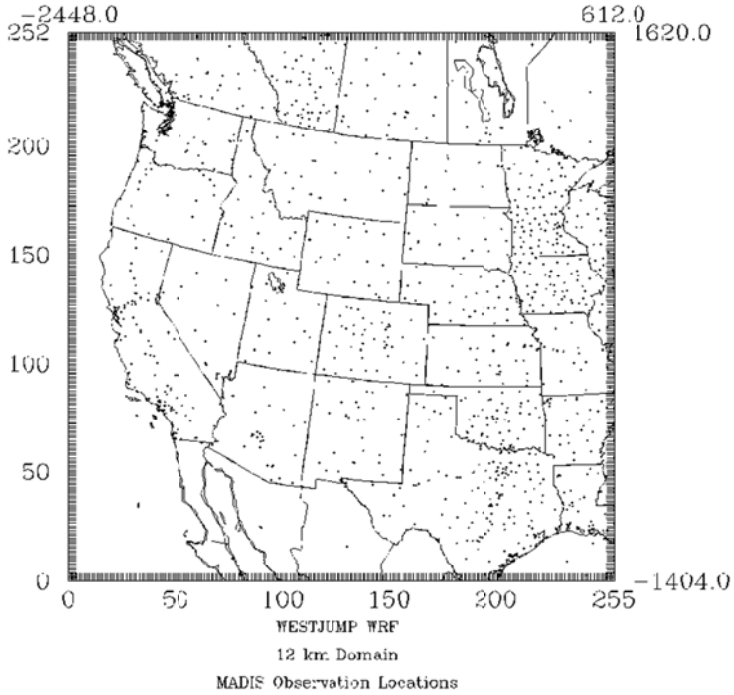


Figure 2-2. Locations of MADIS surface meteorological modeling sites within the WestJumpAQMS WRF 12 km WESTUS modeling domain.

2.4 METEOROLOGICAL MODEL PERFORMANCE BENCHMARKS

Meteorological model performance evaluation benchmarks have been developed after examining the model performance of ~30 meteorological model simulations that produced "good" air quality model performance, primarily to support ozone SIPs (Emery et al., 2001). The key to the benchmarks is to understand how good or poor the results are relative to other model applications run for the U.S. These meteorological model performance benchmarks include measures of bias and error in surface temperature, wind speed and direction and water vapor mixing ratio. Because the benchmarks were developed primarily for meteorological model simulations to support urban ozone planning, they represent model performance under fairly "simple" conditions. That is, usually fairly flat terrain (although sometimes with coastal locations) with simple meteorological conditions (e.g., stationary high pressure). Meteorological model performance within the complex terrain of the Inter-Mountain West would not be expected to be as good as in these simple conditions. Thus, for some of the meteorological model performance metrics (i.e., temperature) more "complex" performance benchmarks have been developed (Kemball-Cook et al., 2005; McNally, 2009).

The equations for bias, error and Root Mean Squared Error (RMSE) are given below. Table 2-2 list the simple and complex meteorological model performance benchmarks that the WRF 2008 simulation model performance was compared against. It is important to emphasize that the benchmarks are not passing/failing grades; rather they are metrics that allow the intercomparison of meteorological model performance.

$$\text{Bias} = \frac{1}{N}\sum_{i=1}^{N}\left(P_i - O_i\right)$$

$$\text{Error} = \frac{1}{N}\sum_{i=1}^{N}\left|P_i - O_i\right|$$

$$\text{RMSE} = \left[\frac{1}{N}\sum_{i=1}^{N}\left(P_i - O_i\right)^2\right]^{1/2}$$

Table 2-2. Simple and complex meteorological model performance benchmarks for surface meteorological model performance evaluation.

Meteorological Benchmark			
Variable	**Simple (Emery et al., 2001)**	**Complex (McNally, 2009)**	**Complex (Kemball-Cook et al., 2005)**
Temperature Bias	≤±0.5°K	≤±1.0 K	≤±2.0 K
Temperature Error	≤2.0°K	≤3.0 K	≤3.5 K
Mixing Ratio Bias	≤±1.0 g/kg	--	NA
Mixing Ratio Error	≤2.0 g/kg	--	NA
Wind Speed Bias	≤±0.5 m/s	--	≤±1.5 m/s
Wind Speed RMSE	≤2.0 m/s	--	≤2.5 m/s
Wind Direction Bias	≤±10 degrees	--	NA
Wind Direction Error	≤30 degrees	--	≤±55 degrees

2.4 SUMMARY OF WRF 2008 MODEL PERFORMANCE EVALUATION

The WestJumpAQMS WRF Application/Evaluation report evaluated WRF across the 36 km CONUS, 12 km WESTUS and 4 km IMWD modeling domains as well as several preliminary Impact Assessment Domains focused on the Inter-Mountain West. WRF was even evaluated down to the individual meteorological monitoring site in the 4 km IMWD on a monthly basis with results available on the WRAP/WestJumpAQMS website. Below we summarize the 2008 WRF monthly model performance for the 36 km CONUS, 12 km WESTUS and 4 km IMWD domains using soccer plots. Soccer plots plot two model performance statistical measures against each other (e.g., temperature bias versus error) along with the model performance benchmarks. When the model performance measures achieve the benchmarks they fall within the box (i.e., score a goal). More detailed WRF 2008 model performance is contained within the WRF Application/Evaluation Report (ENVIRON and Alpine, 2012).

2.4.1 Surface Meteorological Model Performance

Figure 2-3 display soccer plots of monthly humidity (mixing ratio) and temperature model performance within the 36, 12 and 4 km modeling domains. The WRF 36, 12 and 4 km monthly humidity model performance achieves the Simple Performance Benchmark within all three modeling domains (Figure 2-3, left). The WRF monthly humidity performance is exhibiting near zero bias and very low error that achieves the Performance Benchmarks, albeit with a slight dry bias for the warmer and wet bias for the cooler months.

The WRF 36 km temperature performance has a bias that achieves the ≤±1.0 K McNally and ≤±2.0 K Kemball-Cook Complex Benchmarks (Figure 2-3, right). However, the WRF 12 and 4 km simulation temperature exhibits a positive bias ranging from 0.0 to 1.3 K so that some months fall outside of the McNally but are within the Kemball-Cook Complex Benchmarks. The last four months of the year have a positive bias that is greater than 1.0 K. The WRF 12 and 4 km simulation temperature error falls between the Simple (2.0 K) and Complex 3.0/3.5 K) Benchmarks.

The WRF wind speed bias and error falls between the Simple and Complex benchmarks (Figure 2-4, left). WRF exhibits a low wind speed bias across the 4 km domain with the negative bias greater for the warmer than the cooler months. The WRF 12 and 4 km wind direction has a near zero bias that is always within ±5 degrees and achieves the Simple Benchmark (≤±10 degrees). However, the wind direction error falls between the Simple (≤30 degrees) and Complex (≤55 degree) benchmarks (Figure 2-4, right).

Figures 2-3 and 2-4 suggest that there is a degradation in WRF performance going from coarser (36/12 km) to finer (4 km) grid resolution. However, such seemingly degradation is due to the focus of the 4 km domain on the Rocky Mountains where obtaining good WRF meteorological model performance is a greater challenge than the simpler terrain conditions within the 36 and 12 km domains.

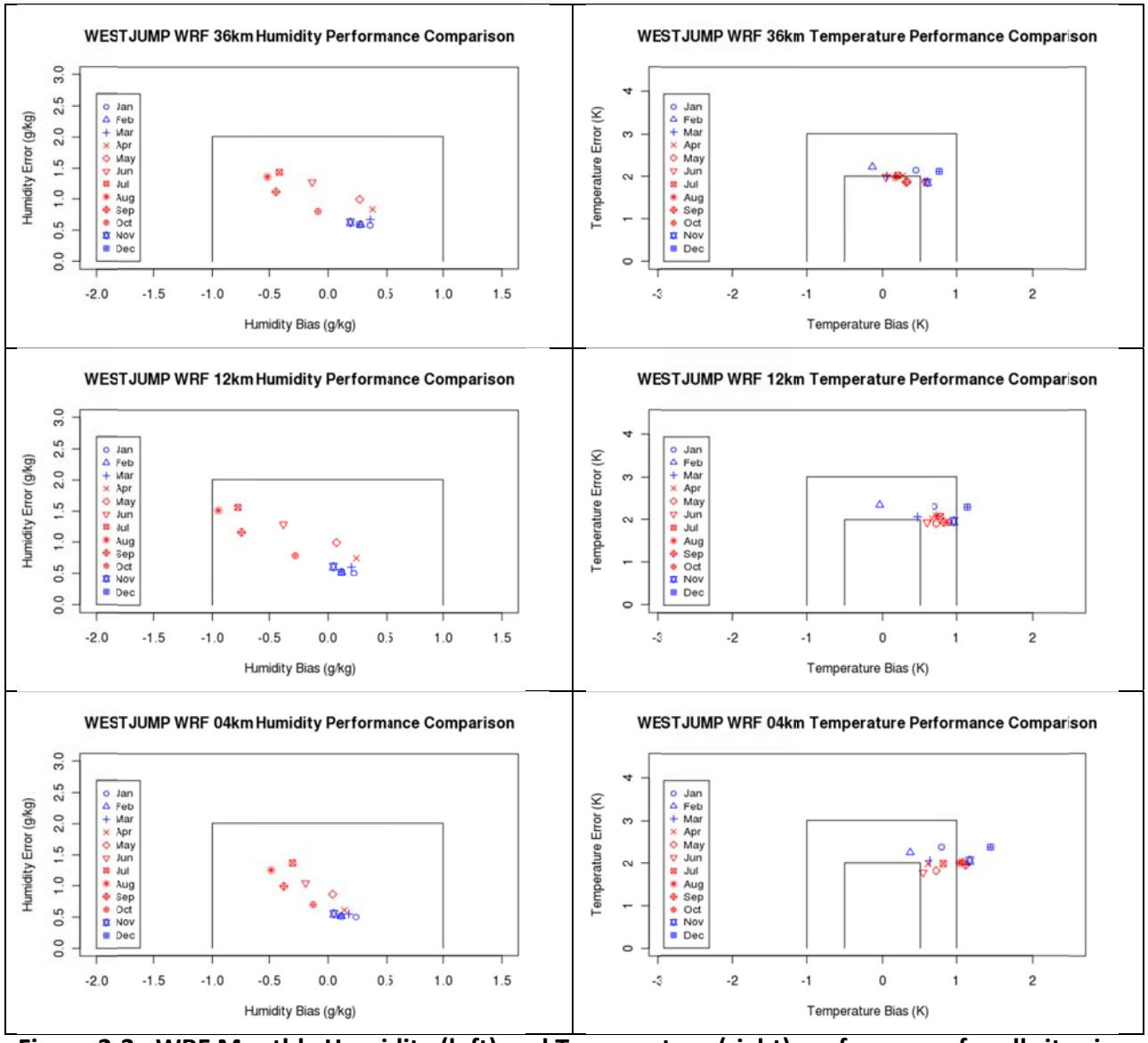


Figure 2-3. WRF Monthly Humidity (left) and Temperature (right) performance for all sites in the 36 km CONUS (top), 12 km WESTUS (middle) and 4 km IMWD (bottom) modeling domains.

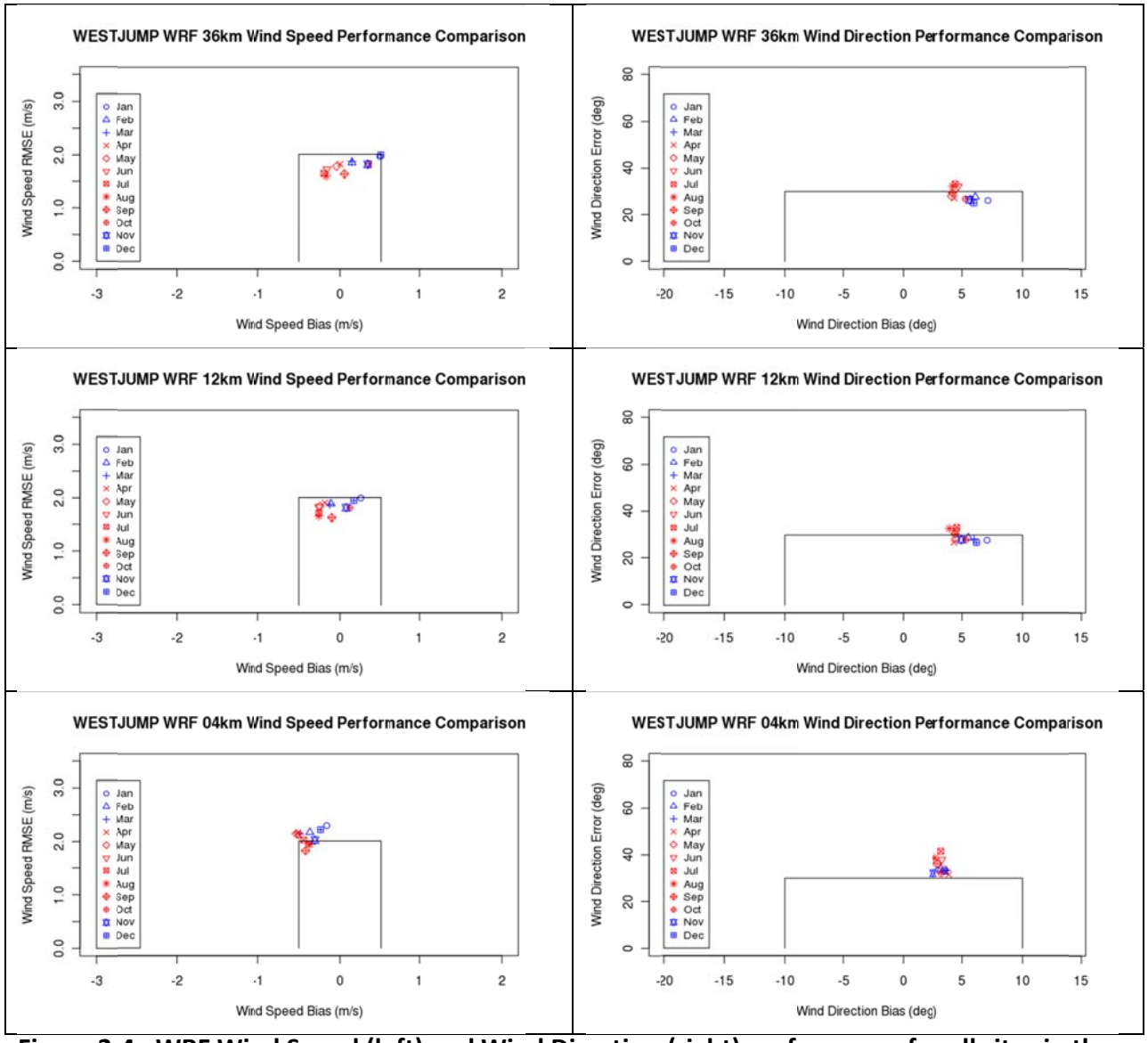


Figure 2-4. WRF Wind Speed (left) and Wind Direction (right) performance for all sites in the 36 km CONUS (top), 12 km WESTUS (middle) and 4 km IMWD (bottom) modeling domains.

2.4.2 Precipitation Evaluation

Figure 2-5 compares monthly total precipitation across the 4 km IMWD for the CPC analysis fields based on observations, the WRF 4 km estimates and the four months of January, April, July and October (see WestJumpAQMS WRF report for remainder of months, ENVIRON and Alpine, 2012). The much higher resolution in the WRF 4 km precipitation fields is readily apparent compared to the coarser CPC fields and must be accounted for in the interpretation of precipitation model performance. In January 2008, the spatial distribution of the CPC and WRF monthly precipitation fields are very similar with most of it occurring in the western half of the 4 km IMWD and much dryer conditions east of the Front Range. The CPC and WRF estimate similar areas of higher precipitation intensity, although the WRF has smaller areas of higher intensity than the CPC analysis fields due to the higher resolution (Figure 2-5a, top).

In April 2008, both the CPC analysis and WRF monthly precipitation exhibit a diagonal northwest to southeast orientation in the precipitation pattern within the IMWD with areas of higher intensity occurring over the Bitterroot Range on the ID-MT border, stretching down along the continental divide and in NB, KS and OK (Figure 2-5a, bottom).

In July 2008, the desert southwest summer monsoon is clearly evident in the CPC and WRF precipitation fields with the highest intensity occurring in Arizona and New Mexico (Figure 2-5b, top). Higher precipitation amounts are also seen in the high plains in the eastern part of the 4 km IMWD, with the Rocky Mountains in the western part of the 4 km IMWD being much dryer.

In October 2008, both the CPC and WRF have very similar spatial patterns of monthly precipitation with the highest intensity precipitation occurring in Kansas stretching down to OK and TX, with WRF estimating higher intensity in OK/TX than seen in the CPC fields (Figure 2-5b, bottom).

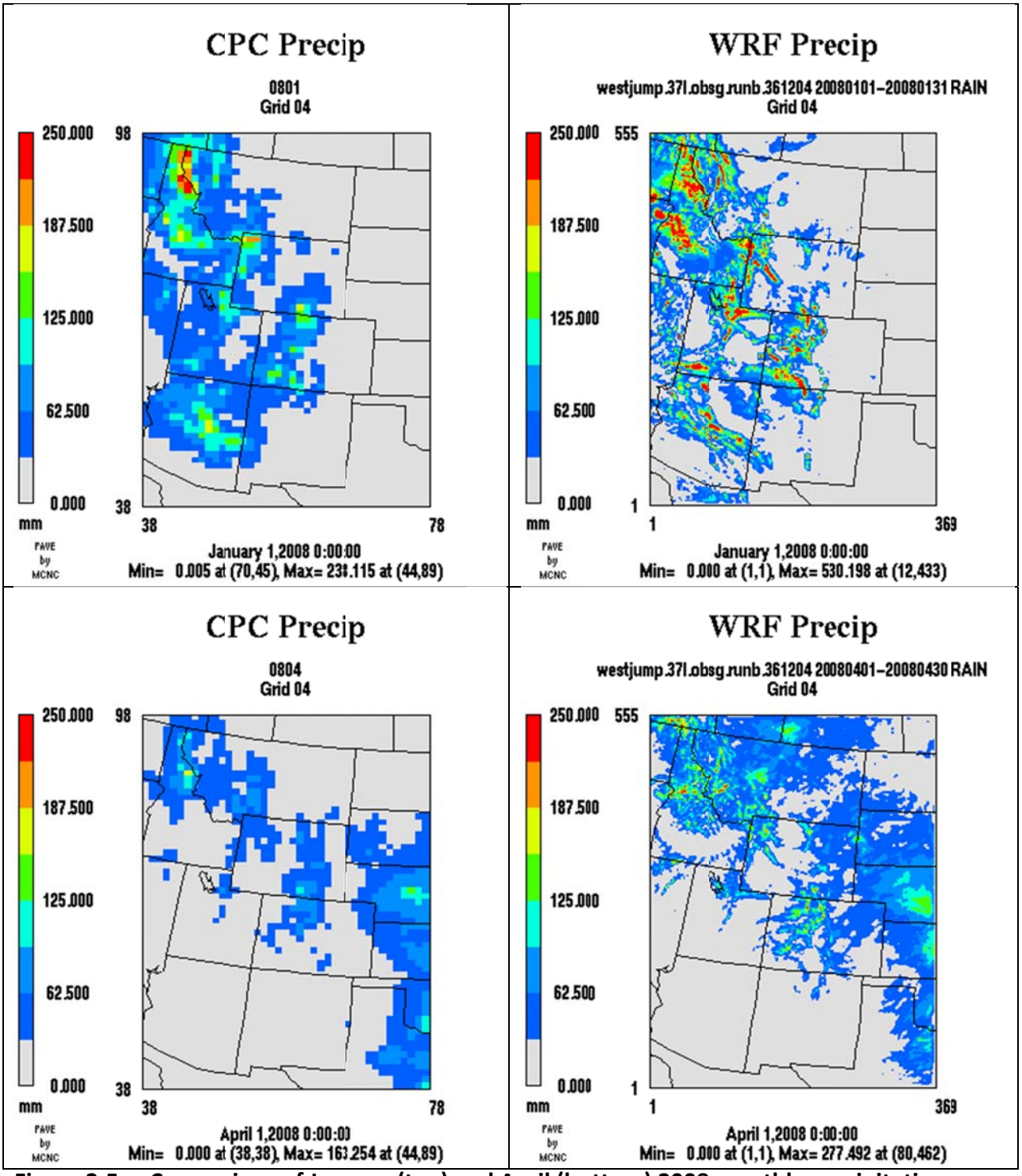


Figure 2-5a. Comparison of January (top) and April (bottom) 2008 monthly precipitation amounts (mm) over the 4 km Inter-Mountain West Domain (IMWD) from the CPC analysis of observations (left) and estimated by the WestJumpAQMS 4 km WRF simulation.

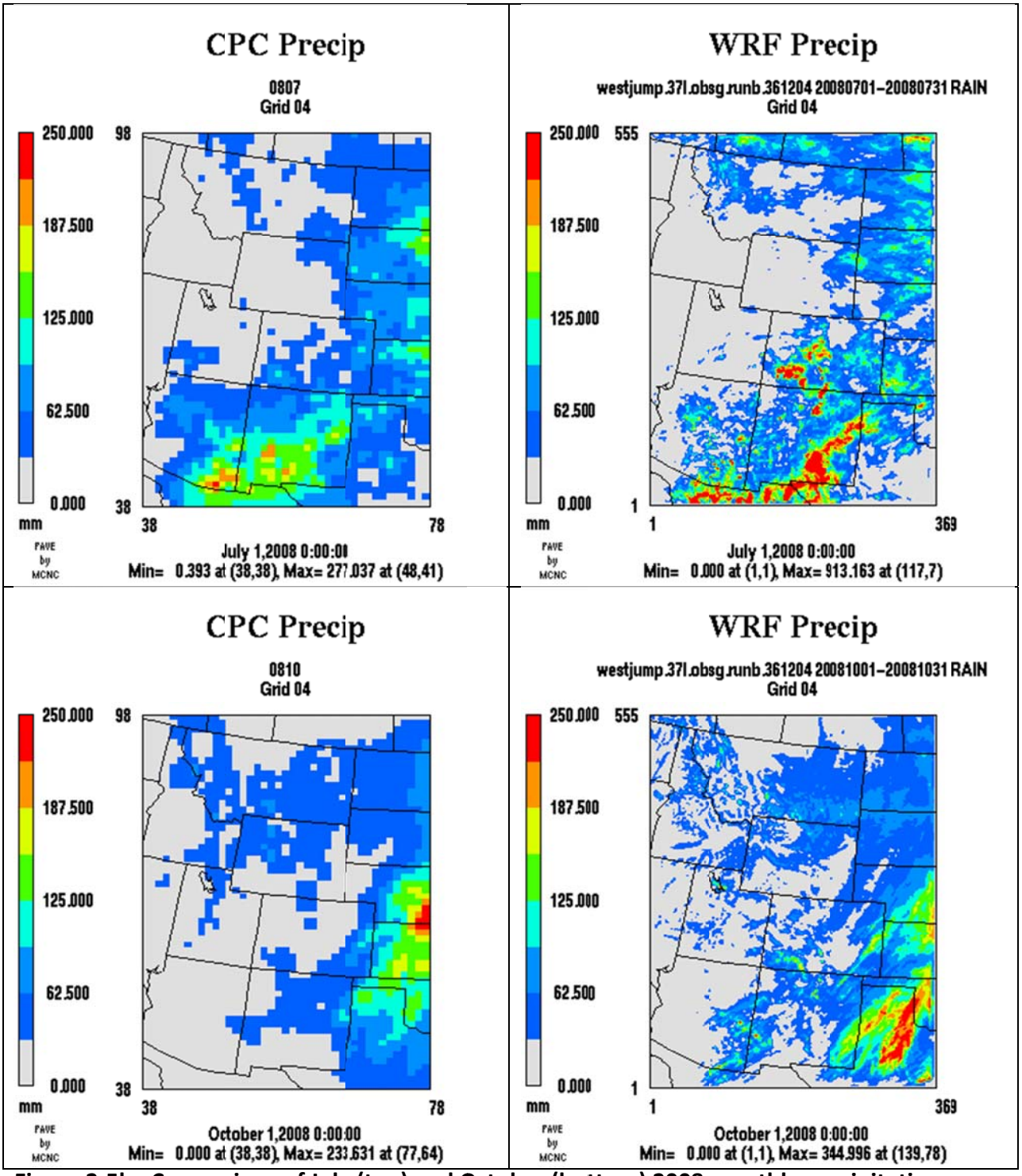


Figure 2-5b. Comparison of July (top) and October (bottom) 2008 monthly precipitation amounts (mm) over the 4 km Inter-Mountain West Domain (IMWD) from the CPC analysis of observations (left) and estimated by the WestJumpAQMS 4 km WRF simulation.

3.0 2008 BASE CASE EMISSIONS

The development of the WestJumpAQMS 2008 base case emissions is summarized below. The primary source for the 2008 base case emissions was Version 2.0 of the National Emissions Inventory (NEIv2.0[30]). For most source categories, the SMOKE emissions modeling system is used to process the emissions into the hourly gridded speciated emissions needed as input for the CAMx and CMAQ PGMs.

3.1 SOURCE OF 2008 BASE CASE EMISSIONS

Table 3-1 summarizes the emission models and sources of 2008 base case emissions that are based primarily on the 2008 NEIv2.0 with the following enhancements:

- Major (≥25 MWe) Electrical Generating Units (EGUs) point source SO_2 and NO_X emissions used Continuous Emissions Monitor (CEM) measurement data that are available online from the EPA Clean Air Markets Division (CAMD[31]). These data are hour-specific for SO_2, NO_x and heat input. The temporal variability of other pollutant emissions besides SO_2 and NO_X (e.g., PM) for the CEM sources were estimated using the hourly CEM heat input data to allocate the annual emissions from the NEIv2.0 to each hour of the year. Emissions, locations and stack parameters for point sources without CEM devices were based on the 2008 NEIv2.0.
- The WRAP-IPAMS Phase III 2006 oil and gas emission inventories were projected to 2008 for all Phase III basins that were available at the time of the WestJumpAQMS 2008 emissions development. In addition, under WestJumpAQMS a new 2008 oil and gas emissions inventory was developed for the Permian Basin in southeastern New Mexico/northwestern Texas.
- Except for California, on-road mobile source emissions were based on the MOVES2010a[32] model with county-specific weekday and weekend day VMT and monthly meteorology for the 2008 base case modeling year. EMFAC2011 2008 on-road mobile source emissions were used for California.
- The WRAP windblown dust (WBD) model[33] was used to generate WBD emissions using day-specific hourly meteorology from the 2008 WRF simulation.
- Sea salt and lightning emissions were generated using the 2008 WRF model hourly gridded output.
- Emissions from fires (wildfires, prescribed burns and agricultural burning) are based on the 2008 fire emissions inventory developed in the Joint Fire Sciences Program (JFSP) Deterministic and Empirical Assessment of Smoke's Contribution to Ozone (DEASCO3[34]) study.
- Biogenic emissions were generated using an enhanced version of the Model of Emissions of Gases and Aerosols in Nature (MEGAN[35]) that was updated by WRAP to better represent biogenic emissions for the western states (Sakulyanontvittaya, Yarwood and Guenther, 2012[36]).
- Mexico emissions were based on the 2008 projections from the 1999 Mexico national emissions inventory.

30 http://www.epa.gov/ttnchie1/net/2008inventory.html
31 http://www.epa.gov/airmarkets/
32 http://www.epa.gov/otaq/models/moves/index.htm
33 http://www.wrapair.org/forums/dejf/fderosion.html
34 https://www.firescience.gov/projects/11-1-6-6/proposal/11-1-6-6_11-1-6_attachment_1_primary.pdf
35 http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm
36 http://www.wrapair2.org/pdf/WGA_BiogEmisInv_FinalReport_March20_2012.pdf

- The Environment Canada 2006 emissions inventory based on the National Pollutant Release Inventory (NPRI) was used for Canada.
- New spatial surrogates for the emissions were developed using the latest 2010 Census and other data that are now available and included population and housing statistics for 2010 and interpolations for the years between 2000 and 2010.

Table 3-1. Summary of sources of emissions and emission models used to generate 2008 base case emissions for the WestJumpAQMS.

Emissions Component	Configuration	Details
Model Code	SMOKE Version 3.1	http://www.smoke-model.org/index.cfm
Oil and Gas Emissions	Update WRAP Phase III 2006 to 2008	Seven WRAP Phase III Basins in CO, NM, UT and WY plus add 2008 Permian Basin O&G Emissions
Area Source Emissions	2008 NEI Version 2.0	Western state updates, then SMOKE processing of http://www.epa.gov/ttn/chief/net/2008inventory.html
On-Road Mobile Sources	MOVES2010a	County specific emissions run for monthly weekday and weekend days. California based on EMFAC2011.
Point Sources	2008 CEM and Non-CEM Sources	Use 2008 day-specific hourly measured CEM for SO_2 and NO_X emissions for CEM sources, 2008 NEIv2.0 for other pollutants and non-CEM sources
Off-Road Mobile Sources	2008 NEIv2.0	Based on EPA NONROAD model http://www.epa.gov/oms/nonrdmdl.htm
Wind Blown Dust Emissions	WRAP Wind Blown Dust (WBD)	WRAP WBD Model with 2008 WRF meteorology adjusted to be consistent with 2002 WBD modeling
Ammonia Emissions	NEIv2.0	Based on CMU Ammonia Model. Updated CAFO location spatial date for Colorado.
Biogenic Sources	MEGAN	Enhanced version of MEGAN Version 2.1 from WRAP Biogenics study http://www.wrapair2.org/pdf/WGA_BiogEmisInv_FinalReport_March20_2012.pdf
Fires	2008 DEASCO3	2008 DEASCO3 fire inventory used. http://www.wrapair2.org/pdf/JSFP_DEASCO3_TechnicalProposal_November19_2010.pdf
Temporal Adjustments	Seasonal, day, hour	Based on latest collected information
Chemical Speciation	CB05 Chemical Speciation	CB6 considered but sensitivity modeling indicated an ozone overestimation issue in the EUSA. (note that CB6 is undergoing revisions).
Gridding	Spatial Surrogates based on landuse	Develop new spatial surrogates using 2010 census data and other data
Quality Assurance	SMOKE QA Tools; PAVE, VERDI plots; Summary reports	Follow WRAP emissions QA/QC plan.

3.2 ON-ROAD MOBILE SOURCES

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

On-road mobile sources include light-duty vehicles, light-duty trucks, heavy-duty vehicles, buses and motorcycles used for transportation of goods and passengers on established roadways. On-road vehicles may be fueled with gasoline, diesel fuel, or alternative fuels such as alcohol blends or natural gas. Below we summarized the development of the on-road mobile source emissions for the WestJumpAQMS 2008 base case modeling. More details can be found in the WestJumpAQMS Technical Memorandum No. 3 (Wilkinson, Loomis and Morris, 2012[37]).

3.2.1 MOVES

The MOtor Vehicle Emissions Simulator (MOVES[38]) is EPA's current tool to construct on-road mobile source emissions estimates for national, state, and county level inventories of criteria air pollutants, greenhouse gas emissions, and some mobile source air toxics from highway vehicles (EPA, 2012a). In addition, MOVES can make projections for energy consumption (total, petroleum-based, and fossil-based). EPA requires that all new regulatory modeling studies use the MOVES model for mobile source emissions and MOVES is also recommended for NEPA studies (EPA, 2012c).

The WestJumpAQMS 2008 on-road mobile source emission modeling was conducted using MOVES2010a. In April 2012, EPA released MOVES2010b after WestJumpAQMS completed its MOVES modeling. According to EPA's documentation, the primary difference between MOVES2010b and MOVES2010a is related to performance issues (e.g., computing run time) and EPA reports that the emission estimates produced by the two versions of MOVES are nearly identical[39]. EPA's technical guidance for State Implementation Plans (SIPs) and transportation conformity notes that studies that started with MOVES2010a do not have to switch to the new MOVES2010b (EPA, 2012b[40]). Given the near identical emissions, EPA's MOVES modeling guidance and the significant effort WestJumpAQMS has invested in its MOVES modeling to date, rerunning with MOVES2010b was not deemed necessary.

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

- Run MOVES in emissions inventory mode using county-specific representative hourly temperature, vehicle miles traveled (VMT) and other inputs (e.g., fleet mix and fuel type) to generate hourly county-level on-road mobile source emissions. The Sparse Matrix Operator Kernel Emissions (SMOKE) emissions modeling system is then used to grid and speciate the hourly county-level MOVES emissions.

37 http://www.wrapair2.org/pdf/Memo_3_MOVES_On-Road_June25_2012_final.pdf
38 http://www.epa.gov/otaq/models/moves/index.htm
39 http://www.epa.gov/otaq/models/moves/documents/420f12014.pdf
40 http://www.epa.gov/otaq/models/moves/documents/420b12028.pdf

- Use the SMOKE-MOVES tool that accesses a MOVES emission factor lookup table using gridded hourly meteorological data and representative VMT, fleet mix, fuel type, etc. for the grid cell to generate gridded hourly on-road emission estimates that are then speciated into the appropriate chemical species. The MOVES lookup table is generated by running MOVES multiple times in emissions factor mode for different temperatures, fuel types, etc.
- Use CONCEPT-MOVES that combine link-based VMT data from a Transportation Demand Model (TDM) with hourly meteorological data and a MOVES emissions factor lookup table to generate hourly gridded speciated on-road mobile source emissions.

For the WestJumpAQMS, MOVES2010a was run in the emissions inventory mode to estimate hourly emissions at the county level for a representative weekend day and weekday for each month of 2008. CONCEPT-MOVES requires link-based TDM data that tends to be limited to urban areas. At the time of the WestJumpAQMS on-road mobile source emissions modeling, SMOKE-MOVES was not fully operational. A modified version of MET4MOVES was run to prepare representative average meteorology for 2008 by month, hour, and county that is suitable for use by MOVES2010a. These new hourly estimates of temperature and relative humidity, based on the WestJumpAQMS 2008 WRF run (ENVIRON and Alpine, 2012), replacing the current default meteorology that exists in the MOVES2010a (movesdb20100830.zonemonthhour database). MOVES2010a was run using the existing MOVES2010a default data sets, with the replacement meteorology, to estimate emissions (tons per hour) for all PM and OZONE pollutants by county/month/weekend day-weekday/hour by appropriate SCC and MOVES2010a process (e.g., extended idle, running exhaust, etc.). The resulting emissions estimates were converted to SMOKE-ready area source, hourly data sets suitable for processing by SMOKE/SMKINVEN. A modified version of SMKINVEN is used to process the hour-specific emissions estimates. For California on-road mobile source emissions, 2008 county-level emissions were based on the EMFAC2011 model that was downloaded from the EMFAC website[41].

3.2.2 SMOKE Modeling of MOVES Estimates

The MOVES/EMFAC estimated county-level on-road mobile source emissions estimates were spatially allocated to the 36/12/4 km modeling domains using the SMOKE emissions model and recent mobile source spatial surrogates developed using the 2010 census and other data. This includes new spatial surrogates specific to new source categories in MOVES (e.g., heavy duty truck idling at rest stops). As MOVES2010a estimates hourly on-road mobile source emissions estimates by county by month for a representative weekend day and weekday, there is no need to temporally allocate the emissions using SMOKE. However, in order for SMOKE to properly utilize the hourly emissions estimates from MOVES, a modified version of SMOKE is required. The MOVES hourly gridded mobile source emissions were chemically speciated to the CB05 chemical mechanism using CB05 chemical speciation profiles based on the SPECIATE4.3 database.

3.3 AREA AND NON-ROAD MOBILE SOURCES

The 2008 NEIv2.0 area and non-road emissions were processed using the SMOKE emissions model with new 2010 census spatial surrogates and default temporal and CB05 speciation adjustments. Several source categories within the area and non-road category were removed from the NEIv2.0 so that they could be replaced or updated and separately processed, which allows a more thorough QA/QC analysis. The source categories that were extracted from the NEIv2.0 area and non-road sources for separate treatment or replacement were as follows:

41 http://www.arb.ca.gov/jpub/webapp//EMFAC2011WebApp/emsSelectionPage_1.jsp

- Oil and gas (O&G) exploration and production sources for locations covered by most of the WRAP Phase III O&G Basins and the Permian Basin were removed from the 2008 NEIv2. They were replaced by the WRAP Phase III 2006 emissions projected to 2008 (see Section 3.4). New 2008 O&G emissions were developed for the Permian Basin in southeastern New Mexico/northwestern Texas. The 2008 NEIv2.0 O&G emissions will be used for the remainder of the U.S. locations, which includes the Williston and Great Plains Basins (North Dakota and Montana) whose WRAP Phase III emissions were not available at the time of the WestJumpAQMS 2008 emissions inventory development.
- Ammonia emissions due to livestock and fertilizer sources were removed from the NEIv2.0 and processed separately.
- Aircraft, locomotive and marine (alm) sources were processed separately as their own source group in the emissions modeling. The marine sources do not include large ocean going (Class 3) vessels (Commercial Marine Vessels, CMV) that will be processed under the off-shore shipping category.
- Fire emissions were removed from the NEIv2.0 and were replaced by 2008 fire emissions developed as part of the DEASCO3 study.
- Fugitive dust emissions were removed from the NEIv2.0 for separate processing.

Below we summarize the processing area and non-road emissions used from the 2008 NEIv2 in the WestJumpAQMS 2008 base case, more details can be found in WestJumpAQMS Technical Memorandum No.2 Area and Non-Road Emissions (Loomis, Morris and Adelman, 2013[42]).

3.3.1 Area Sources

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

3.3.2 Non-Road Sources

The NEIv2.0 Non-Road data categories contain mobile source emissions estimated using the EPA NONROAD[43] model, run within the National Mobile Inventory Model (NMIM[44]). The non-road emissions have been compiled as both annual total emissions, and average day emissions by month. In order to take the best advantage of the monthly and seasonal variability of the non-road emissions sources, we used the monthly options for SMOKE modeling inputs.

Note that emissions data for aircraft, locomotives, and commercial marine vessels are not included in the NEI non-road data category starting with the 2008 NEI. These three non-road mobile source categories were handled as special cases, with separate input processing streams. Aircraft engine emissions occurring during Landing and Takeoff Operations (LTO) and the Ground Support Equipment (GSE) and Auxiliary Power Units (APU) associated with the aircraft are now included in the point data category at individual airports in the

42 http://www.wrapair2.org/pdf/Memo_2_Area_Jan22_2013%20review%20draft.pdf
43 http://www.epa.gov/otaq/nonrdmdl.htm
44 http://www.epa.gov/otaq/nmim.htm

2008 NEI. Emissions from locomotives that occur at rail yards are also included in the point data category. In-flight aircraft emissions, locomotive emissions outside of the rail yards, and commercial marine vessel emissions (both underway and port emissions) are included in the Non-Point data category.

3.4 2008 OIL AND GAS EMISSIONS

For Basins covered by the WRAP-IPAMS Phase III 2006 oil and gas (O&G) emissions[45] available at the time of the 2008 base case emissions development, the WRAP Phase III O&G 2006 emissions were projected to 2008. WestJumpAQMS also developed new 2008 O&G emissions for the Permian Basin in southeastern New Mexico/northwestern Texas. For all other Basins in the U.S. (including Williston and Great Plains Basins whose WRAP Phase III emissions were not available at the time of the 2008 base case development) the 2008 O&G emissions from the NEIv2.0 were used and processed as area and point sources. Extra care was taken to assure that O&G emissions were not double counted using the Phase III and NEI O&G emissions data.

3.4.1 2008 Phase III O&G Emissions Update

The WRAP Phase III 2006 baseline O&G inventories were projected to 2008 for the following eight WRAP Phase III Basins:

- Denver-Julesburg Basin (CO)
- Piceance Basin (CO)
- Uinta Basin (UT)
- North San Juan Basin (CO)
- South San Juan Basin (NM)
- Wind River Basin (WY)
- Powder River Basin (WY)
- Greater Green River Basin (WY)

The 2008 O&G emission update for the WRAP Phase III and Permian Basins used 2008 O&G production statistics from the Enerdeq database published by IHS Global, also referred to as the "PI Dwight's" database. This database 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 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. No new survey work was conducted for the 2008 O&G emissions update so the analysis did not include any updates of company-specific production statistics as was done in the development of the Phase III 2006 O&G emission inventories. The resulting production statistics data were summarized at the county, tribal and basin levels for all basins including the Permian Basin.

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

The 2008 production statistics from the IHS database were used to project the Phase III baseline 2006 O&G inventories. The projections were 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 were developed at the county and tribal levels for all basins. Scaling factors were then matched to all source categories considered as part of the Phase III inventories, using the same cross-referencing analysis as conducted as part of the midterm (2012) projections in the Phase III study. The 2008 to 2006 scaling factors were used to adjust the activity data for the oil and gas emissions.

When activity 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 the 2006 emissions will be reduced and no emission controls assessment is needed (i.e., when activity is reduced between 2006 and 2008, we are assuming that the same equipment is being used in the field, it is just producing less and has lower emissions). In this case, the 2008 emissions will be developed assuming the direct application of the scaling factor with no additional controls.

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 and that new equipment may have been deployed in the field. A controls 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. The controls analysis only considered 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 factors for the specific source category were assumed.

For Colorado Basins, the permitted O&G 2008 emissions were based on the APEN database[46] rather than projected from the WRAP Phase III 2006 O&G emissions. In addition, the Colorado Department of Health and Environment (CDPHE) has determined that not all condensate flash VOC emissions that were assumed to be controlled 95% by flares make it to the flare and some of them are instead vented to the atmosphere. Thus, CDPHE has introduced the concept of a Capture Efficiency (CE) for condensate flare control that assumes only 75% of the condensate Flash VOC emissions are actually controlled by the flare and the other 25% is released directly to the atmosphere. The CDPHE 75% CE assumption was adopted in the WestJumpAQMS 2008 base case O&G emissions in Colorado. The WRAP Phase III 2006 unpermitted condensate tank O&G emissions are either projected to 2008 (D-J Basin) or the 2008 APEN condensate tank emissions are reduced (Piceance Basin) in order for the total 2008 condensate production in the inventory to match the 2008 IHS database production statistics.

Details on the development of the 2008 O&G emissions for the Colorado Basins, the Uinta and South San Juan Basins and the Wyoming Basins can be found in, respectively, Bar-Ilan and Morris (2012a[47]), Bar-Ilan and Morris (2012b[48]) and Bar-Ilan and Morris (2012c[49]).

3.4.2 2008 Emission Inventory for the Permian Basin

A study prepared by Applied EnviroSolutions, Inc. (AES) on 2007 O&G emissions in the New Mexico portion of the Permian Basin along with 2008 O&G emissions from the Texas Commission on Environmental Quality (TCEQ) was used to develop a comprehensive O&G emissions inventory of the Permian Basin. The AES study was commissioned for the Bureau of Land Management (BLM) Carlsbad Field Office (CFO), and used a

46 http://www.colorado.gov/cs/Satellite/CDPHE-AP/CBON/1251596800194
47 http://www.wrapair2.org/pdf/Memo_4a_OG_Jun06_2012_Final.pdf
48 http://www.wrapair2.org/pdf/Memo_4b_OG_June06_2012_Final.pdf
49 http://www.wrapair2.org/pdf/Memo_4c_OG_Jan23_2013_RevisedFinal.pdf

methodology developed by ENVIRON for the Central Regional Air Planning Association (CENRAP)[50]. The preparation of the 2008 inventory for the Permian Basin expanded on the AES study, including both additional emissions estimates in the Permian Basin. The development of the 2008 O&G emissions in the New Mexico and Texas portions of the Permian Basin are summarized in the following two paragraphs, more details can be found in Bar-Ilan and Morris (2012d[51]).

For the New Mexico portion of the Permian Basin, additional O&G area source categories were added to the inventory that were not included in the AES study. The AES study only examined emissions from wellhead/lateral compression, heaters, and flaring. Given the prevalence of both O&G production in the Permian Basin, additional emissions of ozone precursors (nitrogen oxides and volatile organic compounds) are expected from tanks, fugitive emissions, pneumatic devices, dehydrators, drilling, blowdown and completion venting, well workovers, and other source categories. To estimate emissions from these categories, we relied on previous source category emissions estimates from other Phase III basins, and attempted to gather input data from other basin inventories matched as closely as possible to the production type in the Permian Basin. Where applicable, the nearby inventory for the South San Juan Basin served as the primary reference for these additional O&G area source category emission estimates. For the missing source categories in the Permian Basin, we used 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 data were then 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 also accounted for variations in the volatile fraction of produced gas in the Permian Basin relative to the other Phase III basins. The same scaling was 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 was used rather than rerunning the E&P TANK model as there was insufficient data available to rerun the model. For those area sources for which emissions were estimated by AES, the AES emissions were scaled from 2007 to 2008 using scaling factors developed from the production statistics. No control analysis was applied in 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) were gathered by AES as part of the study and were used directly. The previously estimated area source emissions, the newly estimated area source emissions and the point source emissions were aggregated into a single inventory for the New Mexico portion of the Permian Basin. The inventory was formatted similarly to other Phase III basins.

For the Texas portion of the Permian Basin, we used the area source inventory as described above for the New Mexico portion of the basin along with data from the TCEQ, and expanded this approach 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 were scaled by the appropriate production statistic to generate unit-level emissions factors, and these were applied to the production data for the Texas counties. For the permitted sources in Texas, we obtained a database of permitted oil and gas sources that was compiled by the Texas Commission on Environmental Quality (TCEQ). The permitted sources emission data were aggregated with the area source estimates to generate an inventory of the Permian Basin in Texas. It was similarly formatted in the Phase III format, and combined with the New Mexico portion of the basin for a comprehensive Permian Basin inventory.

50 http://www.cenrap.org/html/presentations.php
51 http://www.wrapair2.org/pdf/Memo_4d_OG_Apr24_2013_Final.pdf

3.4.3 2008 O&G Emissions for the Remainder of the U.S.

The WRAP Phase III Basins and Permian Basin O&G emissions described above covers most of an area including northwestern TX, NM, CO, UT and WY. For areas within these states not covered by the WRAP Phase III and Permian Basins, and O&G emissions outside of this region, the O&G emissions from the 2008 NEIv2.0 were used. The areas in the U.S. where the 2008 NEIv2 was used for O&G emissions includes all states outside of the WRAP Phase III and Permian Basins areas (northeast TX, NM, UT, CO, WY, MT and ND). The 2008 NEIv2.0 O&G emissions were also used for the Williston and Great Plains Basins (MT and ND), whose WRAP Phase III 2006 O&G emissions were not available at the time of the WestJumpAQMS 2008 base case emissions development, and the Paradox (UT-CO) and Raton Basins (CO-NM) and Big Horn (WY) basins. Details on the O&G emissions used in the 2008 base case not covered by the WRAP Phase III Basins can be found in WestJumpAQMS Technical Memorandum No. 4e (Loomis, Adelman, Morris and Bar-Ilan, 2013[52]).

3.5 FIRE EMISSIONS

2008 emissions from wild fires, prescribed burns and agricultural burning were based on the comprehensive 2008 fire emissions inventory developed as part of the DEASCO3[53] project sponsored by the Joint Fire Science Program (JFSP). Preliminary WestJumpAQMS PGM modeling used 2008 fire emissions from the Fire INventory from NCAR (FINN[54]) until the DEASCO3 fire emissions were ready. The WestJumpAQMS emissions Technical Memorandum Number 5 (Morris, Tai, Loomis and Adelman, 2012[55]) compared the 2008 FINN fire emissions and the 2008 BlueSky/SMARTFIRE fire emissions available in the NEIv2.0 and selected the FINN for the interim 2008 fire emissions until the DEASCO3 study emissions are ready because: (1) FINN is more complete spatially (e.g., includes Canada); (2) FINN has more complete species; (3) BlueSky/SMARTFIRE may overstate fire emissions; and (4) FINN fires are better documented. Since then, the more detailed and comprehensive DEASCO3[56] 2008 fire emissions inventory has become available and was used for the final WestJumpAQMS 2008 base case and source apportionment modeling presented in this report.

3.6 AMMONIA EMISSIONS

Ammonia emissions were based on the 2008 NEIv2.0 emissions inventory. A vast majority of the ammonia emissions in the 2008 NEIv2.0 were from livestock and fertilizer application that were based on the CMU ammonia model[57]. Updated spatial surrogates for locations of Concentrated Animal Feeding Operations (CAFOs) in Colorado developed as part of the NPS ROMANS study were used to spatially allocate the NEIv2.0 livestock ammonia emissions in Colorado. Details on the development of the ammonia emissions used in the CARMMS 2008 base case can be found in the WestJumpAQMS Technical Memorandum No. 8 (Loomis, Wilkinson, Adelman and Morris, 2013[58]).

3.7 OCEAN GOING VESSELS

Large ships, such as container ships, tankers, bulk carriers and cruise ships are significant contributors to air pollution in many of our nation's cities, ports and coastal regions. There are two types of diesel engines used on large ships: main propulsion and auxiliary engines. The main propulsion engines on most large ships are

52 http://www.wrapair2.org/pdf/Final_Memo_4e_RemainderOG_Mar6_2013.pdf
53 http://www.wrapair2.org/pdf/JSFP_DEASCO3_TechnicalProposal_November19_2010.pdf
54 http://bai.acd.ucar.edu/Data/fire/
55 http://www.wrapair2.org/pdf/Memo_5_Fires_Apr27_2012_Final.pdf
56 http://wrapfets.org/deasco3.cfm
57 http://www.cmu.edu/ammonia/
58 http://www.wrapair2.org/pdf/Memo8_AmmoniaSources_Feb28_2013review_draft.pdf

"Category 3" marine diesel engines, which can stand over three stories tall and run the length of two school buses. Auxiliary engines on large ships typically range in size from small portable generators to locomotive-size engines.

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

Details on the Off-Shore Shipping emissions are provided in a report "Documentation for the Commercial Marine Vessel Component of the National Emissions Inventory – Methodology" prepared by Eastern Research Group (ERG, 2010[59]) dated March 30, 2010. The WestJumpAQMS emissions Technical Memorandum Number 7 (Loomis, Morris and Adelman, 2012[60]) describes the off-shore shipping emissions and how they were processed for input into the photochemical grid model.

It should be noted that the Off Shore Shipping emissions category discussed in this section includes just the Class 3 Commercial Marine source. Smaller vessels (Class 1 and 2) are included with the Non-Road Mobile Source discussed in Section 3.3.2. The latest 2008 emissions inventory for ocean going vessels used in the WestJumpAQMS are similar to what was used for the Emissions Control Area (ECA) analysis[61].

3.8 BIOGENIC EMISSIONS

WRAP performed a Western Biogenic Emissions Update Study that enhanced the MEGAN biogenic emissions model to better simulate biogenic emissions in the western U.S. The WestJumpAQMS used the new enhanced version of MEGAN along with the 2008 WRF 36/12/4 km data to generate hourly gridded speciated biogenic emission inputs. Details on the WRAP Biogenic Emissions Update Study can be found in the study's final report (Sakulyanontvittaya, Yarwood and Guenther, 2012[62]) with a summary provided in the WestJumpAQMS emissions Technical Memorandum Number 9 on biogenic emissions (Sakulyanontvittaya et al., 2012[63]).

3.9 SPATIAL ALLOCATION

New spatial allocation surrogates were developed at 4 km resolution for the CONUS domain using the latest 2010 CENSUS and other new data. The 4 km surrogate distributions were used directly for disaggregating the county-level emissions to the 4 km grid cells in the WestJumpAQMS modeling domain, as well as collapsed to 36 and 12 km resolution for spatial allocation to the 36 km CONUS and 12 km WESTUS domains used in WestJumpAQMS modeling. Table 3-2 summarizes the spatial surrogates to be used for spatial allocation in the WestJumpAQMS SMOKE emissions modeling. More details are provided in the WestJumpAQMS emissions Technical Memorandum Number 13 on SMOKE modeling parameters (Adelman, Loomis and Morris, 2013[64]).

59 http://www.epa.gov/ttn/chief/net/nei08_alm_popup.html
60 http://www.wrapair2.org/pdf/OffshoreShippingEmissionsMemo_7WestJumpAQMS_Jan23_2012.pdf
61 http://www.epa.gov/otaq/oceanvessels.htm
62 http://www.wrapair2.org/pdf/WGA_BiogEmisInv_FinalReport_March20_2012.pdf
63 http://www.wrapair2.org/pdf/Memo_9_Biogenics_May9_2012_Final.pdf
64http://www.wrapair2.org/pdf/Memo13_Parameters_Sep30_2013_final.pdf

Table 3-2. Spatial surrogate distributions to be used in the SMOKE emissions modeling spatial allocations.

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

3.10 TEMPORAL ALLOCATION

Temporal profiles are available from the U.S. EPA for a wide range of emissions sources. While the majority of the temporal profiles available from the EPA represent nationally averaged emissions sources, state-specific monthly profiles exist for prescribed fires, wildfires, livestock, and some mobile sources. For most sources the emissions modeling temporal allocations were based on the U.S. EPA temporal profiles distributed with the 2008 NEIv2.0[65] (filename: amptpro_2008aa_us_can_revised_06oct2011_v0.txt). Several source categories use episode emissions that already have hourly emissions so will not use the temporal allocation profiles. These emissions categories include: large point sources with measured hourly CEM emissions; on-road mobile sources that use the MOVES monthly weekday/weekend day hourly emissions; biogenic emissions from MEGAN; and fire emissions from DEASCO3. The EPA default cross walk file between SCC codes and temporal allocations is available on the 2008 NEIv2.0 website[66].

3.11 CHEMICAL SPECIATION

The U.S. EPA develops speciation profiles from information stored in the SPECIATE database[67]. The current SPECIATE database (version 4.3) is the official repository of volatile organic compound (VOC) and particulate matter (PM) emissions source profiles for different categories of emissions sources. SPECIATE contains 5,592 profiles of chemical mass fractions from source testing conducted by EPA, state agencies, or published in the literature since the 1970's. Of the current profiles in SPECIATE, 3,570 are for PM sources, 1,775 are for VOC sources, and 247 are for other gases, such as mercury. The most recent update to the SPECIATE database occurred with the release of version 4.3 in September 2011. SPECIATE 4.3 include 405 new profiles obtained from a combination of recommendations for EPA Office of Transportation and Air Quality, EPA and state-sponsored studies of various industrial processes, and literature reviews conducted by the SPECIATE workgroup.

65 http://www.epa.gov/ttnchie1/net/2008inventory.html
66 ftp://ftp.epa.gov/EmisInventory/2008v2/doc/scc_eissector_xwalk_2008neiv2.xlsx
67 http://www.epa.gov/ttnchie1/software/speciate/

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

The WestJumpAQMS CAMx and CMAQ photochemical grid modeling is using the Carbon Bond version 05 (CB05) chemical mechanism (Yarwood et al., 2005[68]). The SMOKE emissions modeling will be performed using CB05 speciation profiles, based on the SPECIATE V4.3 database, and ROG-to-TOG conversion factors. The Speciation Tool is an interface to the SPECIATE database that develops CB05 VOC speciation profiles for use in the SMOKE emissions modeling. The exception to using the SPECIATE V4.3 VOC speciation profiles was for the WRAP Phase III Basins where Basin-specific CB05 VOC speciation profiles were used for O&G VOC emissions. Note that we also used some of the WRAP Phase III VOC speciation profiles for O&G emissions in the Permian Basin as they looked more representative than the default VOC speciation profiles used in the SMOKE emissions modeling system.

3.12 QUALITY ASSURANCE AND QUALITY CONTROL

The emissions modeling quality assurance (QA) and quality control (QC) procedures developed as part of the WRAP Regional Modeling Center (RMC) were used in the WestJumpAQMS emissions modeling (Adelman, 2004). The 2008 base case emissions are processed by major source category in several different "streams" of emissions modeling. This is done in order to assist in the QA/QC of the emissions modeling as it is much easier to identify potential issues in the emissions fields when analyzing single source categories at a time. 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 3-3 lists an example of separate streams of emissions modeling by source category that can be used. Also shown in Table 3-3 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)

68 http://www.camx.com/publ/pdfs/cb05_final_report_120805.aspx

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

No.	Emissions Processing Category (Abbr)	Inventory Source	Temporal	Processing Comments
1	Nonpoint/Area (nonpt)	NEI	mwdss_mon	Remove oil & gas, agricultural NH3, and dust,; includes commercial marine and rail
2	Livestock NH_3 (lv)	NEI	mwdss_mon	Do not apply met-based temporal profiles; separate out for possible sensitivity later
3	Fertilizer NH_3 (ft)	NEI	mwdss_mon	Group with lv as a full agricultural NH3 sector (ag)
4	Fugitive and Road Dust (fd)	NEI	mwdss_mon	Includes paved and unpaved road dust; apply transport factors but not met factors
5	Residential Wood Combustion (rwc)	NEI	mwdss_mon	Do not apply met-based temporal profiles; separate out for possible sensitivity later
6	Area Oil & Gas from P3 (ogp3)	WRAP P3	mwdss_mon	Basin specific speciation profiles and spatial surrogates (includes Permian Basin)
7	Area Oil and Gas from NEI (ognei)	NEI	MWDSS_mon	Use default speciation and allocations
8	Nonroad mobile (nr)	NEI	mwdss_mon	Includes NMIM commercial marine and rail
9	MOVES RPD (rpd)	MOVES	hourly met	
10	CEM Point (ptcem)	NEI08/CAMD	daily	Anomalies removed from 2008 CAMD data
11	Non-CEM Point (ptncem)	NEI08	mwdss_mon	Removed oil & gas sources from NEI and transferred to ptognei sector
12	Point Oil & Gas from P3 (ptogp3)	WRAP P3	mwdss_mon	WRAP Phase III inventory and Permian Basin
13	Point Oil & Gas from NEI (ptognei)	WRAP NEI	mwdss_mon	Remove NEI oil and gas emissions for counties in WRAP P3/Permian Basins
14	Point Fires (ptfire)	FINN and DEASCO3	hourly/daily	FINN used in preliminary and DEASCO3 used in final simulations
15	Commercial Marine (ptseca)	NEI	aveday_mon	Latest version from Emissions Control Area (ECA) rule
16	Lightning NO_X (lnox)		hourly met	Gridded hourly NO emissions tied to WRF convective rainfall (optional)
17	Sea salt (ss)		hourly met	Surf zone and open ocean PM emissions (Optional)
18	Windblown Dust (wbd)	TBD	hourly met	WRAP WBD model
19	MEGAN Biogenic (bg)	MEGAN2.1	hourly met	Use new versions of MEGAN V2.10 updated by WRAP for the western U.S.
20	Mexico Area (mexar)	Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2008
21	Mexico Point (mexpt)	Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2013
22	Mexico Mobile (mexmb)	Mexico NEI	mwdss_mon	Mexico inventory projected from 1999 to 2013
23	Canada Area (canar)	Canada NPRI	mwdss_mon	Latest Environment Canada Inventory
24	Canada Point (canpt)	Canada NPRI	mwdss_mon	Latest Environment Canada Inventory
25	Canada Mobile (canmb)	Canada NPRI	mwdss_mon	Latest Environment Canada Inventory
26+	BLM Planning Areas	BLM	Mwdss_mon	Separate processing of O&G and mining emissions in each BLM Planning Area

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

- Spatial plots of the hourly emissions for each major species (e.g., NO_X, VOC, some speciated VOC, SO_2, NH_3, 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 were written to generate the CAMx-ready two-dimensional day-specific hourly speciated gridded emission inputs. The point source and, as available elevated fire, emissions were processed into the day-specific hourly speciated emissions in the CAMx-ready point source format.

The resultant model-ready emissions were subjected to a final QA using spatial maps, vertical plots and diurnal plots to assure that: (1) the emissions were merged properly; (2) CAMx/CMAQ inputs contain the same total emissions as the base emission inputs to SMOKE; and (3) to provide additional QA/QC information.

4.0 2008 BASE CASE MODELING AND MODEL PERFORMANCE EVALUATION

The WestJumpAQMS project performed photochemical grid modeling (PGM) using both the CAMx and CMAQ photochemical grid models (PGMs). Applying both PGMs will provide insight into the capabilities of photochemical modeling for the western U.S. and what features are important. Because a major objective of the study is to address western U.S. ozone and particulate matter (PM) source-receptor relationships using ozone and PM source apportionment techniques, CAMx was the primary model due to its more advanced ozone and PM source apportionment tools (Arunachalam, 2009) and ability to perform two-way grid nesting. The WestJumpAQMS CMAQ analysis is ongoing and will be reported on at a later date. In this Chapter we present the CAMx 2008 base case modeling and model performance evaluation.

Four general types of PGM model simulations were conducted:

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

The WestJumpAQMS photochemical modeling also developed a framework for future air quality modeling in the western U.S. This potentially includes the development of modeling results that can be used to support future State implementation Plan (SIPs) planning and air quality modeling to support the development of Environmental Impact Statements (EISs) and Resource Management Plans (RMPs) to address requirements of the National Environmental Policy Act (NEPA).

4.1 CAMX AND CMAQ SCIENCE AND INPUT CONFIGURATIONS

Table 4-1 summarizes the CAMx and CMAQ science configurations and options used for the 2008 base case simulations. The latest version of CAMx at the time the WestJumpAQMS modeling was initiated, which is Version 5.41 (released November 2012), was used. CAMx was configured to predict both ozone and PM species. The current version of CMAQ (Version 5.0.1 released in July 2012) was used in the WestJumpAQMS modeling.

Many common parameterizations were selected for CAMx and CMAQ. Both models used the Piecewise Parabolic Method (PPM) advection solver for horizontal transport (Colella and Woodward, 1984) along with the spatially varying (Smagorinsky) horizontal diffusion approach. CAMx used K-theory for vertical diffusion using the CMAQ-like vertical diffusivities from WRFCAMx and CMAQ used the analogous vertical mixing approach. The CB05 gas-phase chemical mechanism was selected for both CAMx and CMAQ. Note that CAMx also includes the more recent CB6 gas-phase chemical mechanism that includes updates to the chemical kinetic rates. However, CAMx sensitivity modeling using CB6 found that it had an ozone overestimation tendency, especially in the eastern U.S., so the CB05 chemical mechanism was used. CMAQ V5.0.1 also does not support CB6 so by using the CB05 chemical mechanism for both models simplifies the

interpretation of the CMAQ and CAMx model performance comparison. Additional CAMx and CMAQ inputs were as follows:

Meteorological Inputs: The WRF-derived meteorological fields (ENVIRON and Alpine, 2012) were processed to generate CAMx and CMAQ meteorological inputs using the, respectively, WRFCAMx and MCIP processors.

Initial/Boundary Conditions: The boundary conditions (BCs) for the 36 km CONUS domain simulation were based on the MOZART[69] global chemistry model. Considerations were also given to generating the 2008 36 km CONUS domain BCs using output from the GEOS-Chem[70] or AM3[71] global chemistry models. However, at the start of the WestJumpAQMS PGM modeling we only have access to the 2008 MOZART global chemistry model output. During the course of WestJumpAQMS a GEOS-Chem BC sensitivity test was conducted and compared against results using the MOZART BCs that is discussed in Morris, Jung and Koo (2013). Existing programs were used to interpolate from the MOZART horizontal and vertical coordinate system to the CAMx/CMAQ LCP coordinate system and vertical layer structure and to map the MOZART chemical species to the CB05 chemical mechanism.

Photolysis Rates: Photolysis rate inputs for CAMx were prepared using the Tropospheric Ultraviolet and Visible (TUV[72]) radiation model. Gridded temporally varying albedo/haze/ozone column inputs were prepared for CAMx. Day-specific ozone column data was based on the Total Ozone Mapping Spectrometer (TOMS) data measured using the satellite-based Ozone Monitoring Instrument (OMI[73]). Albedo was based on land use data. For CAMx there is an ancillary snow cover input that will override the land use based albedo input that is based on the WRF day-specific snow cover output data. Average albedo values for snow cover were used. Note that this is in contrast to the highly reflective fresh white snow albedo values that occur during winter high ozone events in southwest Wyoming and the Uinta Basin in Utah; the WestJumpAQMS CAMx and CMAQ modeling is not configured for simulating the winter elevated ozone cold pooling events that require more refined WRF meteorological modeling, higher grid resolution and enhanced snow cover albedo values than being used in WestJumpAQMS. CAMx modeling was conducted to use the in-line TUV option that adjusts the photolysis rates for the effects of cloud cover and aerosol loadings to account for the reduction in UV radiation. With the introduction of CMAQ Version 5 in January 2012 CMAQ has a new in-line option for calculating in-line photolysis rates that was used in the WestJumpAQMS. The user inputs the opacity and photolysis data (absorption cross sections and quantum yields data) and CMAQ internally calculates the photolysis rates during the simulation.

Landuse: Landuse field inputs were developed based on USGS GIRAS data.

Spin-Up Initialization: Ten days of model spin up (e.g., December 21-31, 2007) was used to initialize the CAMx and CMAQ models on the 36 km CONUS domain before adding the 12 km and, when used, 4 km nested domains for the last two days of 2007 before the start of the 2008 calendar year (January 1, 2008).

For the most part, CMAQ was configured in a similar manner as CAMx. However, since CMAQ does not support two-way grid nesting, it was operated using one-way grid nesting. Many CMAQ inputs (e.g., ICBCs and emissions) were generated using the corresponding CAMx inputs and the CAMx2CMAQ processor.

69 http://www.acd.ucar.edu/wrf-chem/mozart.shtml
70 http://acmg.seas.harvard.edu/geos/
71 http://www.gfdl.noaa.gov/atmospheric-model
72 http://cprm.acd.ucar.edu/Models/TUV/
73 http://ozoneaq.gsfc.nasa.gov/

Table 4-1. CAMx (Version 5.41) and CMAQ (Version 5.0.1) model configurations for WestJumpAQMS.

Science Options	Configuration	Details
Model Codes	CAMx V5.41 – November 2012 Release CMAQ V5.0.1 – July 2012 Release	CAMx V6.00 was released in May 2013 CMAQ V5.0.1 is latest version
Horizontal Grid Mesh	36/12/4 km	Many CAMx runs done using just 36/12 km grids
36 km grid	148 x 112 cells	36 km CONUS domain
12 km grid	239 x 206 cells	12 km WESTUS domain
4 km grid	DSAD 4-km domain	Also set up 4 km IAD as a one-way nest
Vertical Grid Mesh	25 vertical layers, defined by WRF	Layer 1 thickness ~24- m. Model top at ~19-km above MSL
Grid Interaction	36/12/4 km two-way nesting for CAMx	One-way grid nesting for CMAQ
Initial Conditions	10 day spin-up on 36 km grid	Clean initial conditions
Boundary Conditions	36 km from global chemistry model	MOZART GCM used, GEOS-Chem GCM BCs used in sensitivity test.
Emissions		
Baseline Emissions Processing	SMOKE, MOVES and MEGAN	
Sub-grid-scale Plumes	Plume-in-Grid not used, waiting for improvements in CAMx V6.1 PiG	CMAQ has no subgrid-scale Plume-in-Grid module
Chemistry		
Gas Phase Chemistry	CB05	CB6 sensitivity test
Meteorological Processor	WRFCAMx and MCIP 4.1	Compatible with CAMx V5.4 and CMAQ V5.0.1
Horizontal Diffusion	Spatially varying	K-theory with Kh grid size dependence
Vertical Diffusion	CMAQ-like in WRF2CAMx	ACM2 for CMAQ V5.0.1
Diffusivity Lower Limit	Kz_min = 0.1 to 1.0 m^2/s or 2.0 m^2/s	
Deposition Schemes		
Dry Deposition	Zhang dry deposition scheme (CAMx) M3Dry Pleim dry deposition (CMAQ)	Zhang 2003
Wet Deposition	CAMx and CMAQ-specific formulation	rain/snow/graupel/virga
Numerics		
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) -- Fast Solver	EBI implemented in both CAMx and CMAQ
Vertical Advection Scheme	Implicit scheme w/ vertical velocity update (CAMx) New vertical velocity scheme (CMAQ)	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	PPM in both CAMx and CMAQ
Integration Time Step	Wind speed dependent	~0.1-1 min (4 km), 1-5 min (1 -km), 5-15 min (36 km)

4.2 CAMX MODEL PERFORMANCE EVALUATION

Below we present the procedures and results of the CAMx model performance evaluation.

4.2.1 Overview of Model Performance Evaluation Procedures

The 2008 base case simulation ozone, total $PM_{2.5}$ mass and speciated $PM_{2.5}$ concentrations were evaluated against concurrent measured ambient concentrations using graphical displays of model performance and statistical model performance measures that are compared against established model performance goals and criteria. The model performance evaluation follows the procedures recommended in EPA's photochemical modeling guidance documents (e.g., EPA, 1991; 2007). Note that EPA is currently updating their modeling guidance, but the basic features on how to evaluate a photochemical grid model is expected to be similar.

After the initial overview of the model performance evaluation focusing on ozone and $PM_{2.5}$ is performed, a more detailed model performance evaluation was conducted that also includes ozone/$PM_{2.5}$ precursor species (e.g., NO, NO_2, NO_X and SO_2), related species (e.g., HNO_3), visibility and deposition and use of higher (4 km) model resolution. The more detailed evaluation was focused on the 4 km IAD.

4.2.2 Aerometric Data for the Model Evaluation

The following routine air quality measurement data networks operating in in 2008 were used in the WestJumpAQMS model performance evaluation:

> EPA AQS Surface Air Quality Data: Data files containing hourly-averaged concentration measurements at a wide variety of state and EPA monitoring networks are available in the Air Quality System (AQS[74]) 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 were reformatted for use in the model evaluation software tools and used in the evaluation of the modeling system across the western U.S. There are several types of networks within AQS that measure different species. The standard hourly AQS AIRS monitoring stations typically measure hourly ozone, NO_2, NO_X and CO concentration and there are thousands of sites across the U.S. The Federal Reference Method (FRM) network measures 24-hour total $PM_{2.5}$ mass concentrations typically using a 1:3 day sampling frequency, with some sites operating on an everyday frequency. The Chemical Speciation Network (CSN) measures speciated $PM_{2.5}$ concentrations including SO_4, NO_3, NH_4, EC, OC and elements at 24-hour averaging time period using a 1:3 or 1:6 day sampling frequency. Figures 4-1 and 4-2 display 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.

74 http://www.epa.gov/ttn/airs/airsaqs/aqsweb/

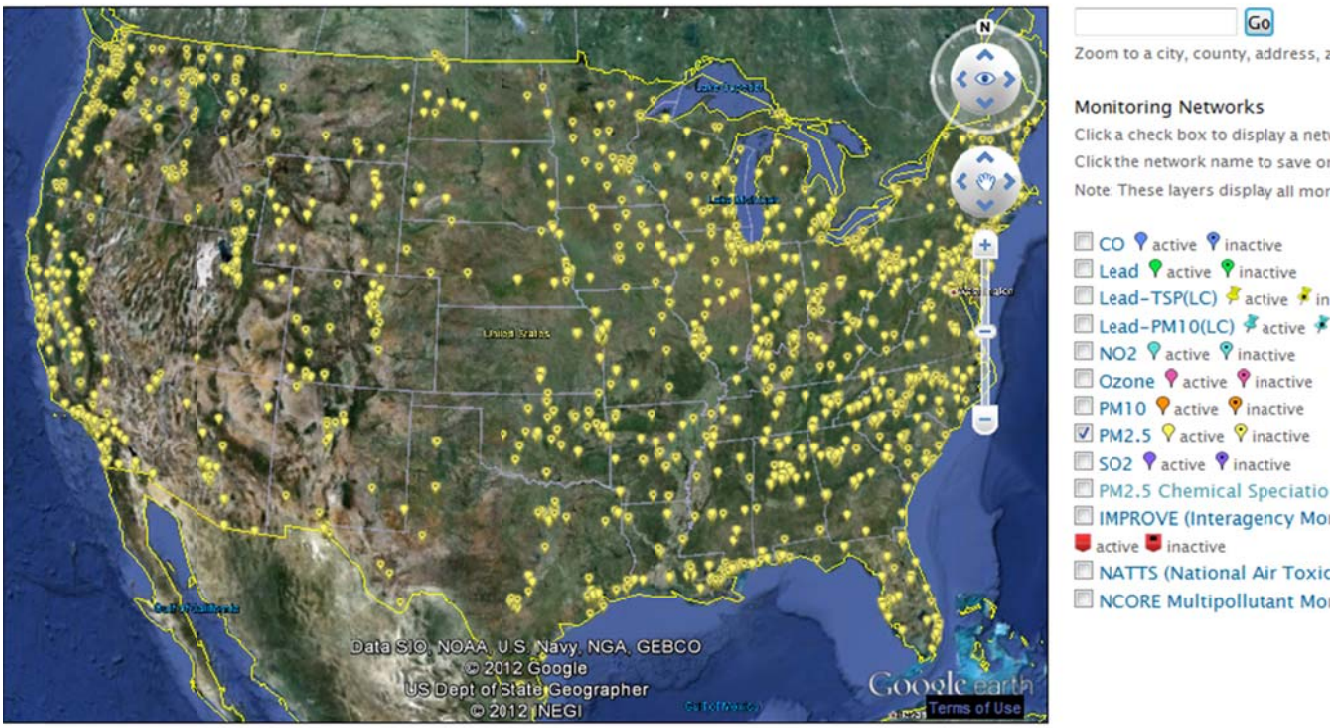


Figure 4-1. Locations of FRM $PM_{2.5}$ mass monitoring sites showing active and inactive (with black dot) sites (source: http://www.epa.gov/airquality/airdata/ad_maps.html).

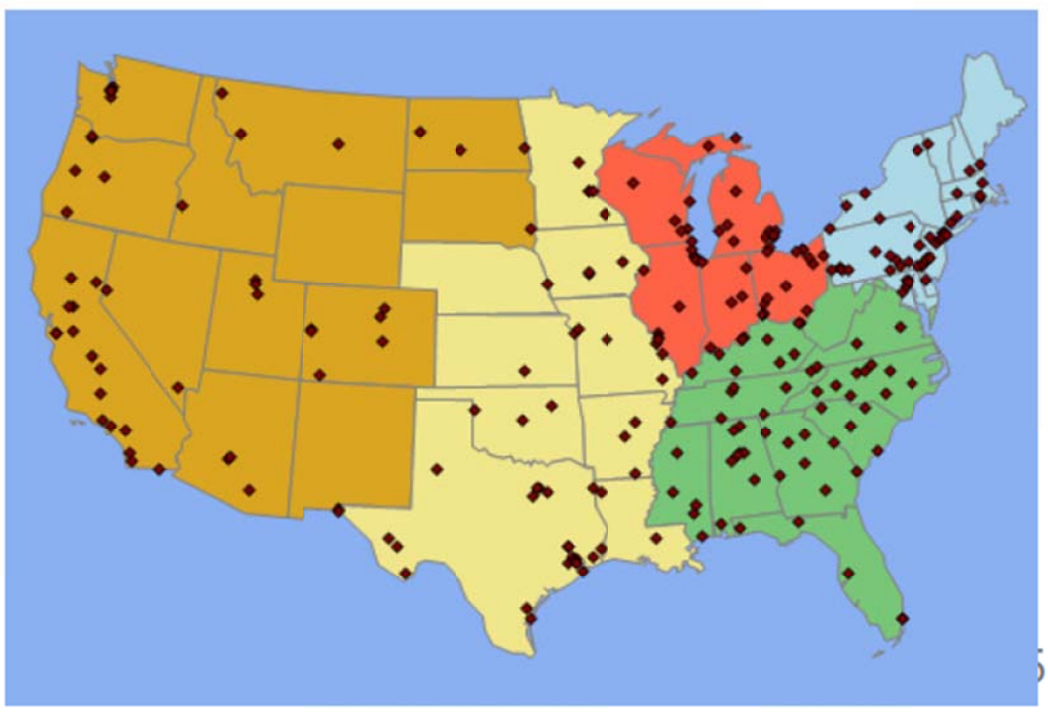


Figure 4-2. Locations of CSN speciated $PM_{2.5}$ monitoring sites (source: http://www.epa.gov/ttn/amtic/speciepg.html).

IMPROVE Monitoring Network: The Interagency Monitoring of Protected Visual Environments (IMPROVE[75]) network collects 24-hour average $PM_{2.5}$ and PM_{10} mass and speciated $PM_{2.5}$ concentrations (with the exception of ammonium) using a 1:3 day sampling frequency. IMPROVE monitoring sites are mainly located at more rural Class I area sites that correspond to specific National Parks and Wilderness Areas 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 4-3 shows the locations of the approximately 150 IMPROVE and IMPROVE protocol sites across the U.S.

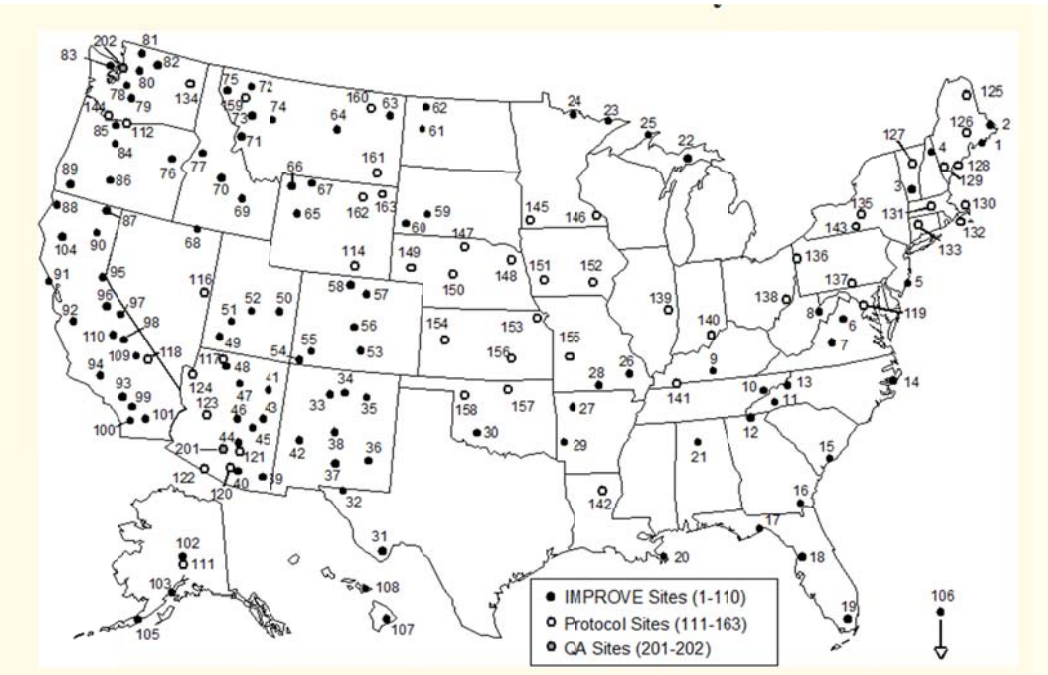


Figure 4-3. Locations of IMPROVE monitoring sites (source: http://vista.cira.colostate.edu/IMPROVE/)

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

CASTNet Monitoring Network: The Clean Air Status and Trends Network (CASTNet[76]) operates approximately 80 monitoring sites in mainly rural areas across the U.S. CASTNet sites typically collected hourly ozone, temperature, wind speed and direction, sigma theta, solar radiation, relative humidity, precipitation and surface wetness. CASTNet also collects weekly (Tuesday to Tuesday) samples of speciated $PM_{2.5}$ sulfate, nitrate, ammonium and other relevant ions and weekly gaseous SO_2 and nitric acid (HNO_3). Figure 4-4 displays the locations of the ~80 CASTNet sites across the U.S.

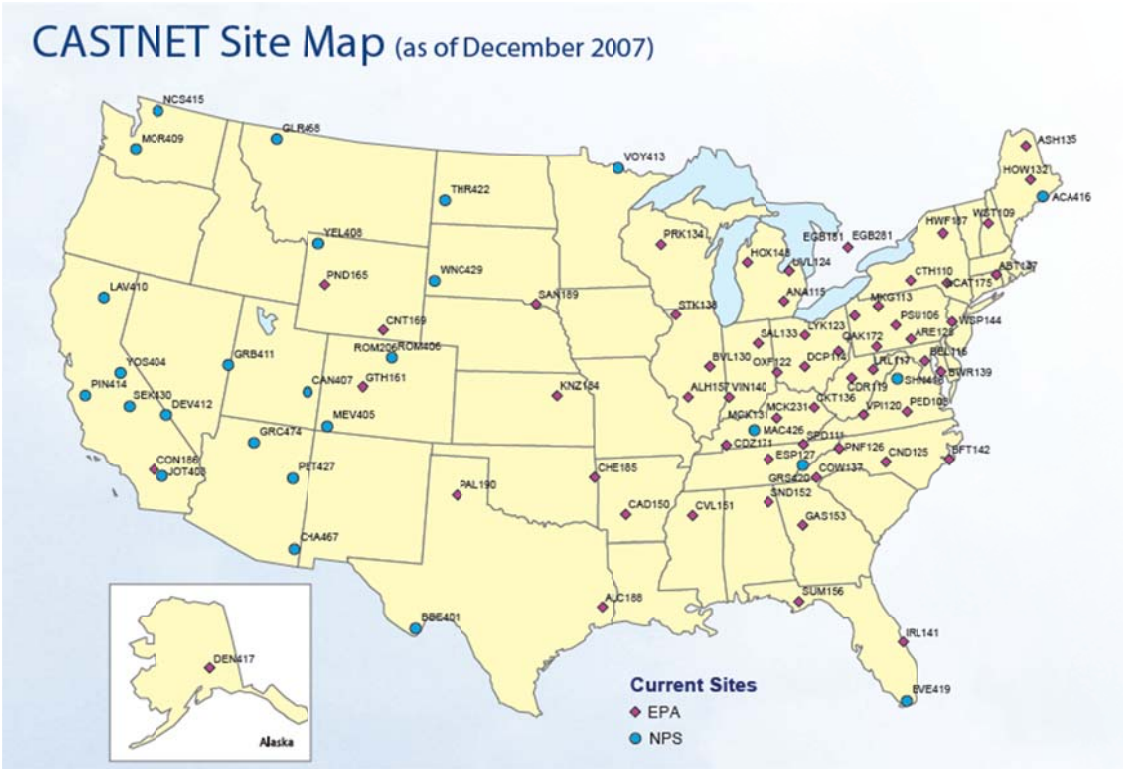


Figure 4-4. Locations of CASTNet monitoring sites (source: http://epa.gov/castnet/javaweb/index.html).

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

NADP Network: The National Acid Deposition Program (NADP[77]) collects weekly samples of SO_4, NO_3 and NH_4 in precipitation (wet deposition) in their National Trends Network (NTN) at over a 100 sites across the U.S. that are mainly located in rural areas away from big cities and major point sources. Seven NADP sites also collect episodic daily wet deposition measurements (AIRMON) when precipitation occurs. Over 20 of the NADP sites also collect weekly mercury (MDN) samples. Figure 4-5 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 dry deposition based on atmospheric observations so were not used in the model performance evaluation.

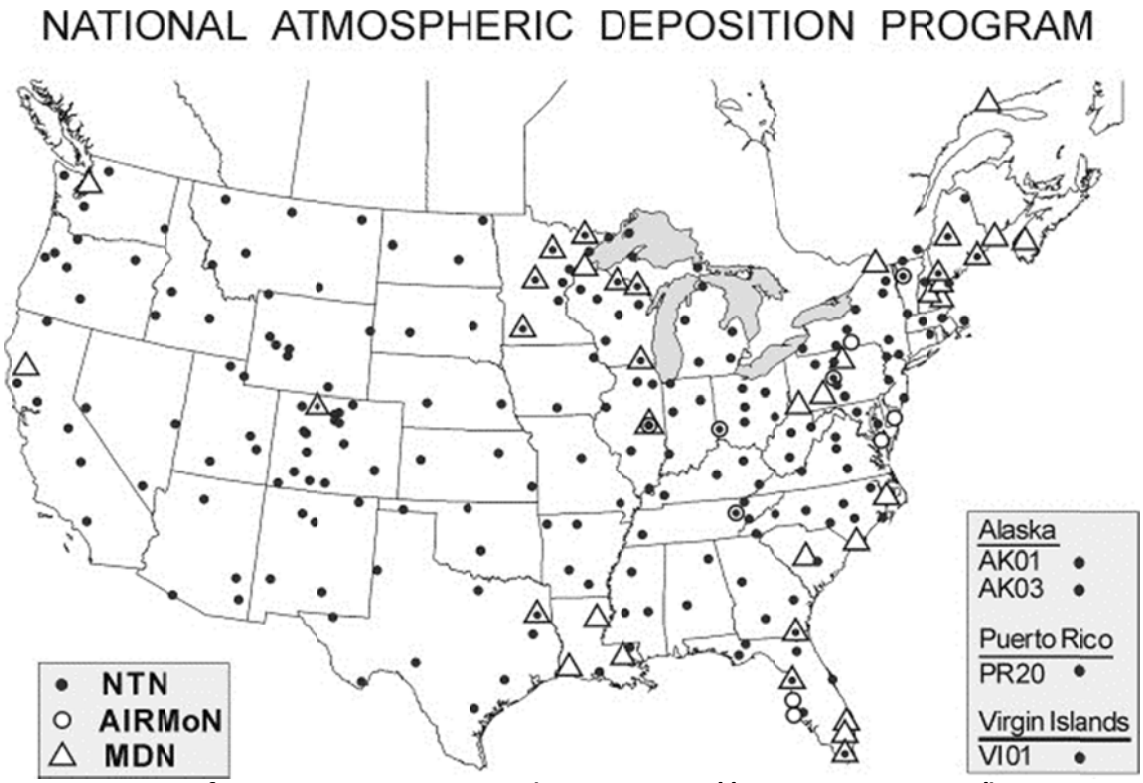


Figure 4-5. Locations of NADP monitoring sites (source: http://nadp.sws.uiuc.edu/).

Ozonesonde Network: The NOAA Earth Systems Research Laboratory (ESRL) operates several ozonesonde sites[78] throughout the world that measure the vertical structure of ozone concentrations throughout the troposphere and into the lower stratosphere. Ozonesonde monitoring sites within the WestJumpAQMS modeling domain include: (1) Trinidad Head on the coast in northern California; (2) Boulder, Colorado; and (3) at the University of Alabama at Huntsville. Due to time and resource constraints, WestJumpAQMS did not perform any evaluation using the ozonesonde data.

77 http://nadp.sws.uiuc.edu/NADP/
78 http://www.esrl.noaa.gov/gmd/ozwv/ozsondes/index.html

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

4.3 MODEL PERFORMANCE STATISTICS, GOALS AND CRITERIA

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

- Unpaired Peak Accuracy (UPA) ≤ ±20%
- Mean Normalized Bias (MNB) ≤ ±15%
- Mean Normalized Gross Error (MNGE) ≤ 35%

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

The MNB/MNGE uses hourly predicted and observed ozone concentrations paired by time and location and is defined as the difference between the predicted and the observed hourly ozone divided by the observed hourly ozone concentrations averaged over all predicted/observed pairs (see Table 4-3) within a given region and for a given time period (e.g., by day, month or modeling period). The MNGE is defined similarly only it uses the absolute value of the difference between the predicted and observed hourly ozone concentrations so is an unsigned metric. As the MNB/MNGE performance metrics divide by the observed hourly ozone concentration, the metric is calculated just using the predicted and observed hourly ozone pairs for which the observed hourly ozone concentration is above a threshold concentration. In the 1991 EPA modeling guidance an observed hourly ozone threshold concentrations of 60 ppb is suggested. Since 1991 these ozone performance goals have been extended to 8-hour ozone concentrations and from urban to more rural areas. Given the large reductions in ozone over the last two decades and the lower ozone concentrations associated with the 8-hour ozone time averaging and rural locations, the observed ozone threshold for 8-hour ozone concentrations has been reduced, with a 40 ppb threshold frequently used.

For PM species, a separate set of model performance statistics and performance goals and criteria have been developed as part of the regional haze modeling performed by several Regional Planning Organizations (RPOs). EPA's modeling guidance notes that PM models might not be able to achieve the same level of model performance as ozone models. Indeed, $PM_{2.5}$ species definitions are defined by the measurement technology used to measure them and different measurement technologies can produce very different $PM_{2.5}$ concentrations. Given this, several researchers have developed PM model performance goals and criteria that are less stringent than the ozone goals that are shown in Table 4-2 (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 4-3.

Table 4-2. PM model performance goals and criteria.

Fractional Bias (FB)	Fractional Error (FE)	Comment
≤±15%	≤35%	Ozone model performance goal that would be considered very good model performance for PM species
≤±30%	≤50%	PM model performance Goal, considered good PM performance
≤±60%	≤75%	PM model performance Criteria, considered average PM performance. Exceeding this level of performance for PM species with significant mass may be cause for concern.

It should be pointed out that these model performance goals and criteria are not used to assign passing or failing grade 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.

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, many were adopted in the WestJumpAQMS 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.

- The model evaluation statistics should be calculated for the highest resolution temporal resolution available and for important regulatory averaging times (e.g., daily maximum 8-hour ozone).

- It is important to report processing steps in the model evaluation and how the predicted and observed data were paired and whether data are spatially/temporally averaged before the statistics are calculated.

- Predicted values should be taken from the grid cell that contains the monitoring site, although bilinear interpolation to the monitoring site point can be used for higher resolution modeling (< 12 km).

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

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

- Evaluation should include more than just ozone and $PM_{2.5}$, such as SO_2, NO_2 and CO.

- Spatial displays should be used in the model evaluation to evaluate model predictions away from the monitoring sites. Time series of predicted and observed concentrations at a monitoring site should also be used.

- It is necessary to understand measurement artifacts in order to make meaningful interpretation of the model performance evaluation.

Table 4-3. Definition of model performance evaluation statistical measures used to evaluate the PGMs.

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

4.4 CAMX OZONE MODEL PERFORMANCE

Figure 4-6 displays the ozone model performance of the CAMx 2008 36/12 km base case simulation for each western state using the AQS and CASTNet monitoring networks. Section 4.5.3 presents CAMx model performance evaluation using 4 km modeling results for the CARMMS domain. Each figure displays scatterplots of predicted and observed daily maximum 8-hour ozone concentrations (DMAX8) matched by location and day for the two monitoring networks along with performance statistics of bias (NMB and FB) and error (NME and FE) calculated using no ozone concentration threshold that are compared against the ≤±15% and ≤35% performance goals, respectively. As recommended by Simon Philips and Baker (2012), we are not using the MNB and MNGE model performance statistics. Below we discuss the CAMx 36 and 12 km ozone model performance for each western state.

Arizona: Figure 4-6a displays the CAMx DMAX8 ozone model performance using 36 and 12 km 2008 base case modeling results in Arizona (AZ). The AZ DMAX8 ozone model performance exhibits low bias (5.8% to 7.3%) and error (13.3% to 14.1%) across the AQS network that achieves the ozone performance goal by a wide margin, albeit with an overestimation tendency. As seen in the AQS scatter plot (Figure 4-6a, left), the overestimation tendency appears to be primarily due to overestimation of the observed low ozone values, which is consistent with not accounting for the full NO titration of ozone due to the coarse grid spacing (36 and 12 km) at the primarily urban based (e.g., Phoenix) AQS monitoring sites. This is supported by the ozone performance at the more rural CASTNet monitors (Figure 4-6a, right) that exhibits even lower bias (1.6% to 2.2%) and error (9.7% to 9.8%) without as large a tendency to overestimate the lower observed DMAX8 ozone concentrations.

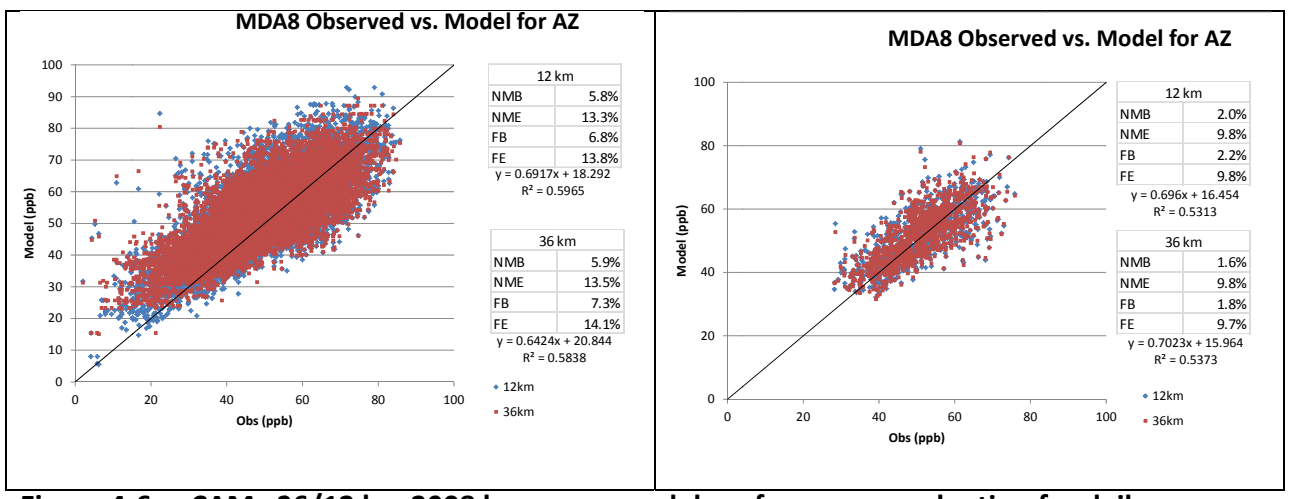


Figure 4-6a. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations in Arizona for the AQS (left) and CASTNet (right) monitoring networks.

California: The ozone performance in California is not as good as seen in AZ. Across the AQS monitors the bias (5.3% to 10.2%) and error (19.6% to 21.5%) are much higher than seen in AZ. Ozone model performance at the CASTNet monitors in CA are characterized by an underestimation bias (-5.1% to -8.5%) especially of the higher observed ozone concentrations. There are more differences in the 12 km (blue) and 36 km (red) ozone model performance in CA than the other states with the 12 km results performing better than the 36 km results. The underestimation of the higher observed DMAX8 ozone concentrations is expected due to the coarse grid resolution used that is unable to simulate the complex ozone formation processes in California (e.g., coastal marine and mountain-valley meteorology).

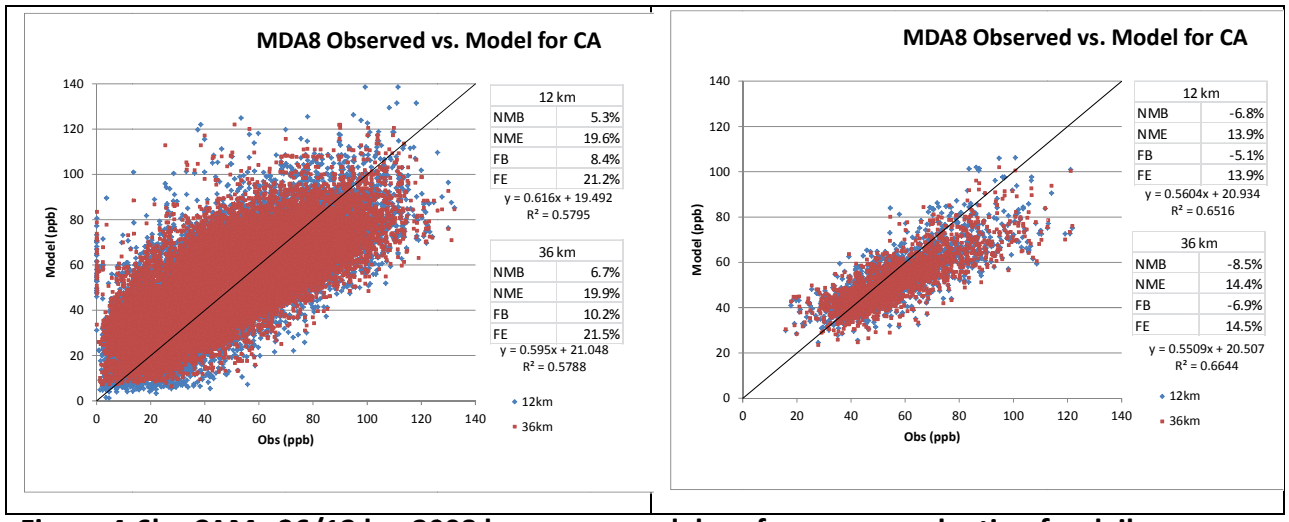


Figure 4-6b. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations in California for the AQS (left) and CASTNet (right) monitoring networks.

Colorado: The Colorado DMAX8 ozone bias across the AQS (8.9% to 12.9%) and CASTNet (8.3% to 8.8%) achieves the ozone performance goal with an overestimations bias. For the AQS network the predicted DMAX8 ozone appears to be 5-10 ppb above the observed values. Better ozone performance is seen across the CO CASTNet monitoring sites, except for occurrences of very low observed DMAX8 ozone (~20-30 ppb) when predicted values are in the 40-80 ppb range. An investigation of the observed ozone for these points revealed that the observed ozone at the Gothic monitoring site was essentially pegged at ~20-30 ppb over many days during the summer of 2008. There were no data quality flags to indicate problems with the ozone measurements during this period, but it should be pointed out that during 2008 the Gothic monitor was not a compliance (SLAMS) monitor so was not subjected to the more rigorous level of quality assurance required for compliance monitors. Thus, in future ozone model performance evaluations (e.g., MOZART versus GEOS-Chem BC sensitivity test comparison presented by Morris, Jung and Koo, 2013) the questionable observed ozone data at Gothic were set to missing.

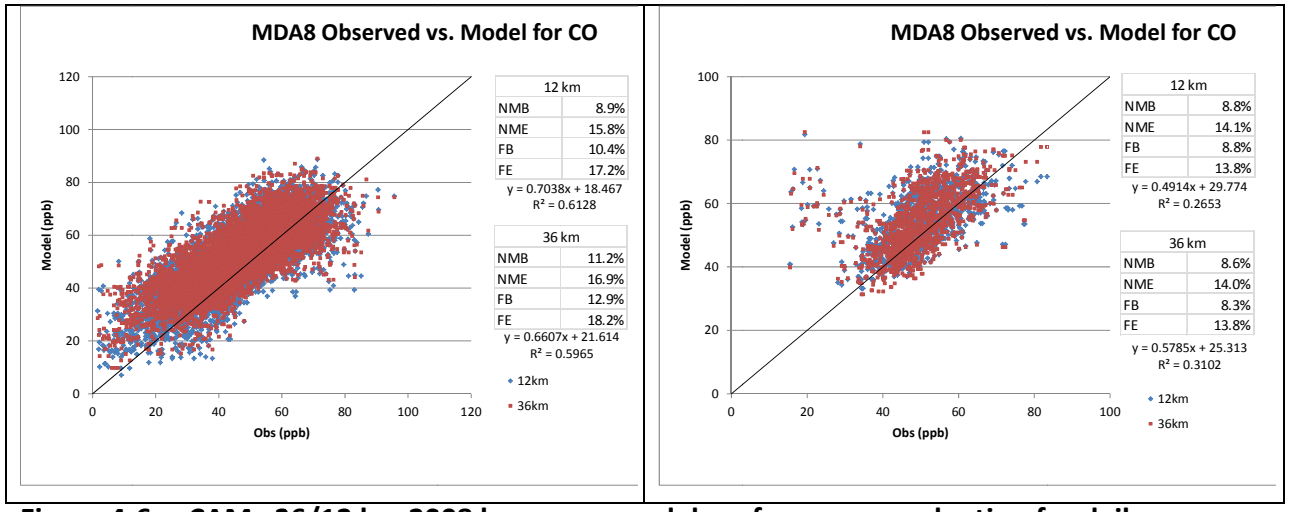


Figure 4-6c. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations in Colorado for the AQS (left) and CASTNet (right) monitoring networks.

Montana: Ozone performance in Montana is characterized by an overestimation bias (22.9% to 29.2%) that exceeds the ozone performance goal across both the AQS and CASTNet networks (Figure 4-6d). Examining the observed ozone data for 2008 in MT reveals that both the AQS and CASTNet networks consist of the same one monitoring site at Glacier National Park. The Glacier CASTNet monitor is operated by the NPS and is part of the compliance network, unlike CASTNet sites operated by EPA in 2008 (although they are now compliance monitors). Although the Glacier ozone monitor is a rural monitor away from any major NO_X sources, the ozone data tends to frequently go down to zero at night that results in lower observed DMAX8 ozone concentrations than predicted. The reasons for this are unclear, but it does explain the seemingly MT ozone model performance overestimation.

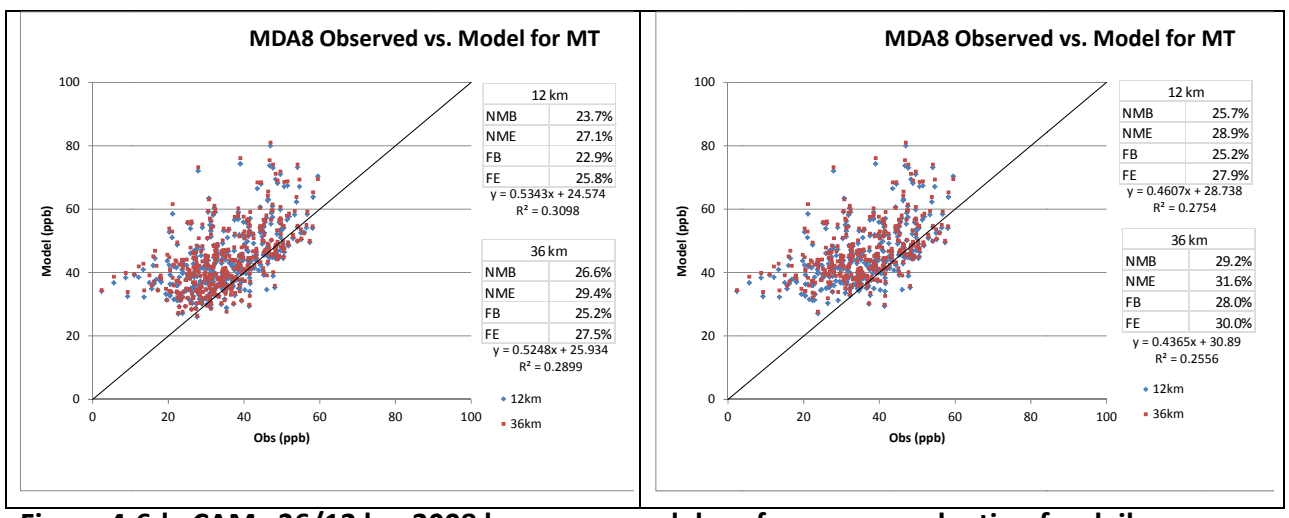


Figure 4-6d. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations in Montana for the AQS (left) and CASTNet (right) monitoring networks.

North Dakota: Ozone performance in North Dakota exhibits an overestimation bias across the AQS (7.0% to 8.3%) and CASTNet (4.3% to 5.6%) monitors that achieves the ozone performance goal (Figure 4-6e). The ND error performance statistics (12.6% to 15.4%) also achieve the performance goal.

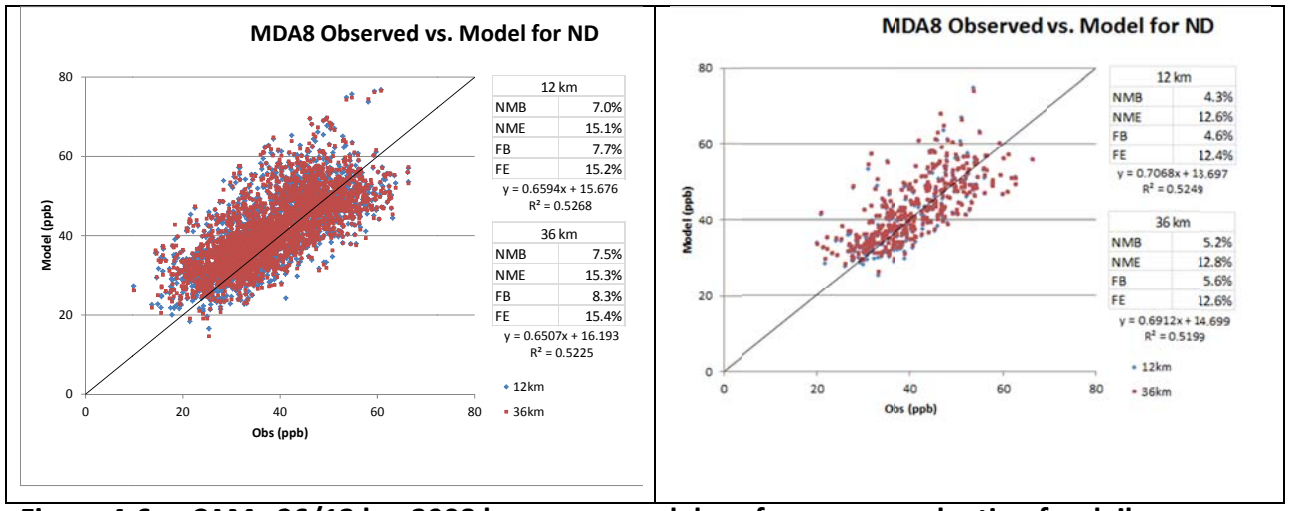


Figure 4-6e. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations in North Dakota for the AQS (left) and CASTNet (right) monitoring networks.

Idaho and New Mexico: The ozone performance across the AQS monitoring sites in Idaho and New Mexico are shown in Figure 4-6f, there are no CASTNet sites in these two states. Ozone performance in Idaho (Figure 4-6f, left) is characterized by very low bias (2.2% to 2.8%) and reasonable error (14.2% to 14.5%) that achieves the ozone performance goals. However, there are some odd predicted and observed ozone pairs including a zero observed DMAX8 ozone value that are highly suspect. New Mexico ozone performance is characterized by an overestimation bias (17.5% to 18.2%) that fails to achieve the ozone performance goal. The predicted DMAX8 ppb ozone appears to be ~10 ppb higher on average than observed. The reasons for the ozone overestimation tendency in New Mexico are not known.

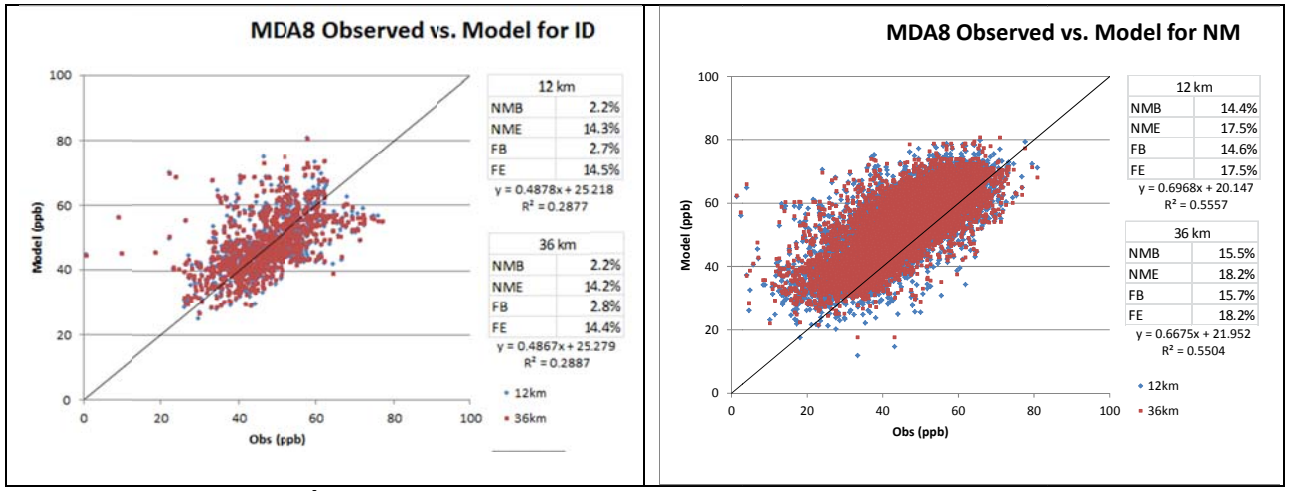


Figure 4-6f. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations at AQS monitors in Idaho (left) and New Mexico (right).

Nevada: Ozone performance across AQS monitors in Nevada is characterized by an overestimation bias (9.7% to 14.6%) that, although fairly high, achieves the ozone performance goal (Figure 4-6g). The overestimation occurs for both low and high observed DMAX8 ozone concentrations, including several points with predicted DMAX8 ozone of ~100 ppb when observed values are in the 60-90 ppb range. Much better ozone model performance is seen for the Nevada CASTNet network (i.e., Big Basin monitoring site) that exhibits extremely low ozone bias (-1.1% to 0.5%) and error (9.1% to 9.4%).

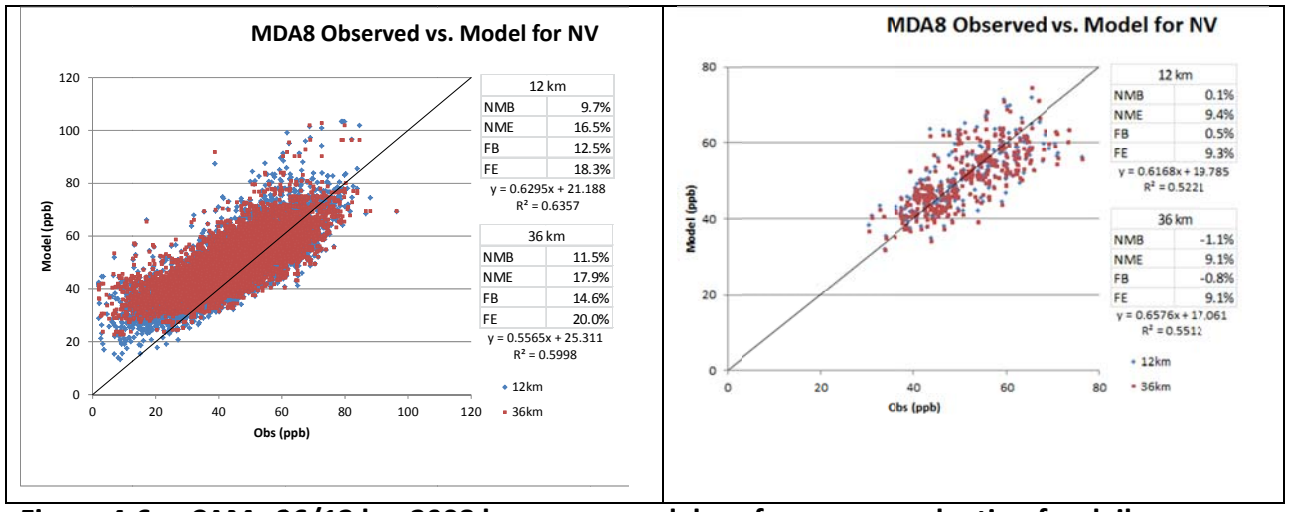


Figure 4-6g. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations in Nevada for the AQS (left) and CASTNet (right) monitoring networks.

South Dakota: Ozone performance across South Dakota has an overestimation bias (8.6% to 14.0%) that barely achieves the ozone performance goal (Figure 4-6h). Ozone performance is better across the CASTNet monitoring sites but still exhibits an overestimation bias.

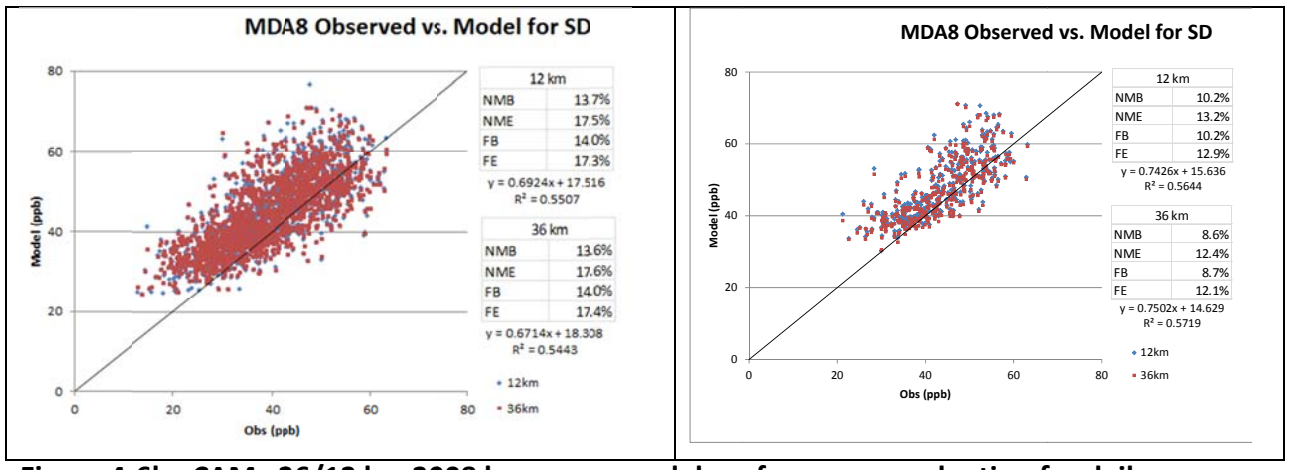


Figure 4-6h. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations in South Dakota for the AQS (left) and CASTNet (right) monitoring networks.

Utah: Across the AQS network in Utah ozone model performance has a overestimation bias (7.2% to 11.1%) that is partly due to an overestimation of the low observed DMAX8 ozone concentrations, which is likely due to ozone titration in Salt Lake City that is not fully captured by the coarse grid spacing used (Figure 4-6i, left). The model fails to capture the highest observed ozone concentrations greater than 80 ppb with modeled values in the 60-80 ppb range. Even with these issues the ozone model performance goals are achieved by a wide margin. Excellent ozone model performance is seen for the Utah CASTNet network (i.e., the Canyonlands monitoring site) with near zero bias (1.0% to 1.4%) and the low error (8.6% to 8.8%).

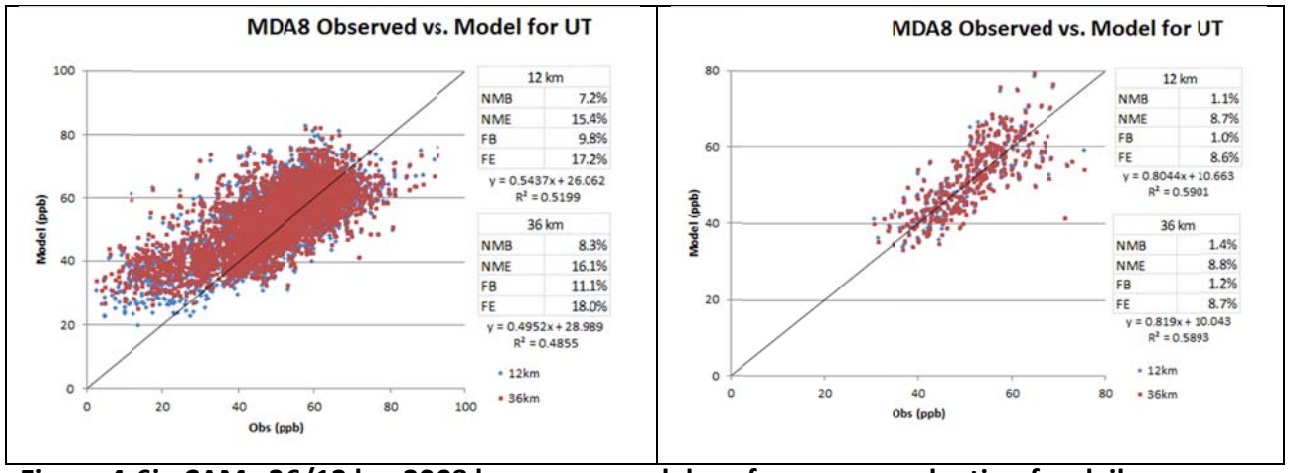


Figure 4-6i. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations in Utah for the AQS (left) and CASTNet (right) monitoring networks.

Oregon and Washington: Ozone performance across the AQS monitors in Oregon and Washington have an overestimation bias that mostly exceeds the performance goal and is greater for the 36 km than 12 km modeling results suggesting that the overestimation bias may be partly due to the coarse grid resolution used (Figure 4-6j). The ozone overestimation bias is so great that, with the exception of Oregon and the 12 km modeling results, the ozone bias performance goals are not achieved. The overestimation bias at the Washington CASTNet monitors (not shown) is even greater (40-50%).

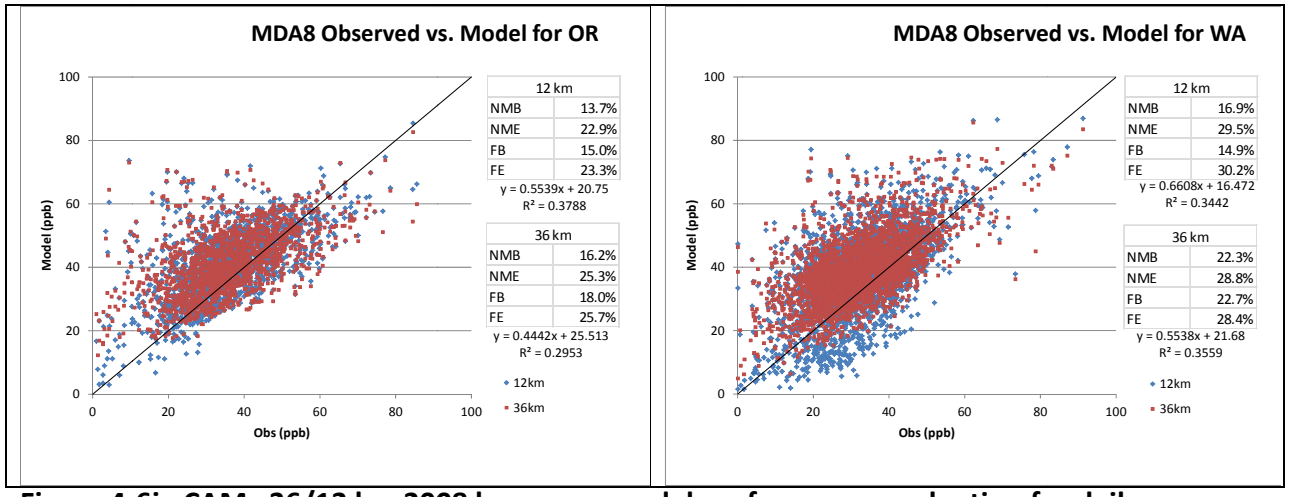


Figure 4-6j. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations in Oregon (left) and Washington (right) for the AQS monitoring network.

Wyoming: Ozone performance at AQS and CASTNet monitors in Wyoming is characterized by low bias (1.3% to 4.8%) and error (10.3% to 13.7%) that achieves the ozone performance goals by a wide margin (Figure 4-6k). In the AQS scatterplot there are occurrences of observed DMAX8 ozone values in the 80-120 ppb range where the modeled values are in the 40-50 ppb range that correspond to winter ozone events in southwestern Wyoming (e.g., Boulder monitoring site) that are not captured by the model. Note that the WestJumpAQMS modeling was not set up to simulate high winter ozone occurrences for which focused higher resolution WRF meteorological modeling would need to be performed to better simulate cold pooling and higher resolution used in CAMx.

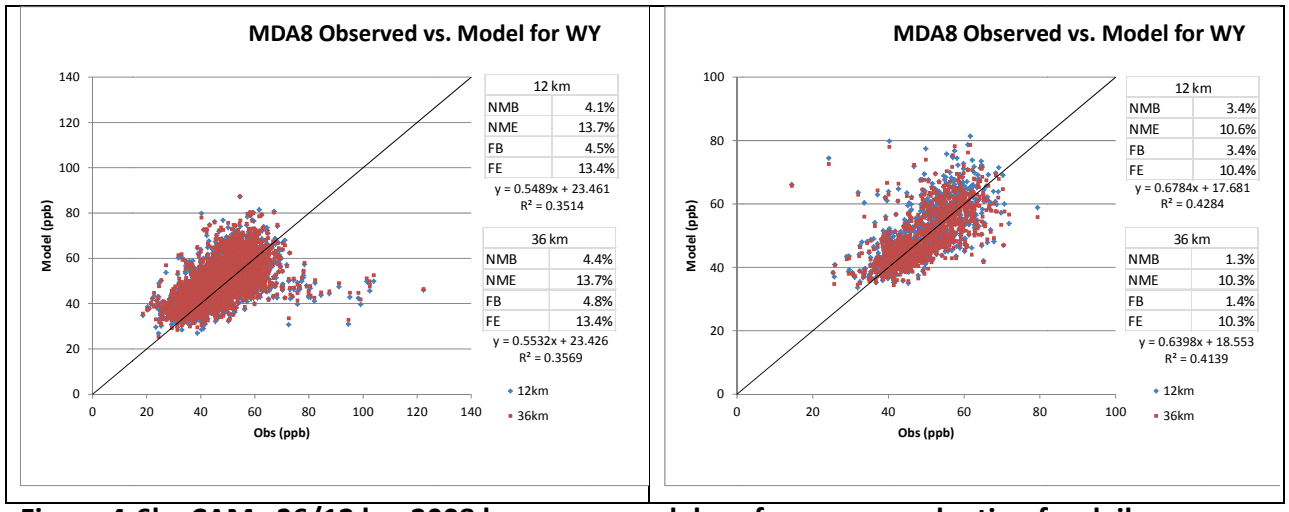


Figure 4-6k. CAMx 36/12 km 2008 base case model performance evaluation for daily maximum 8-hour ozone concentrations in Wyoming for the AQS (left) and CASTNet (right) monitoring networks.

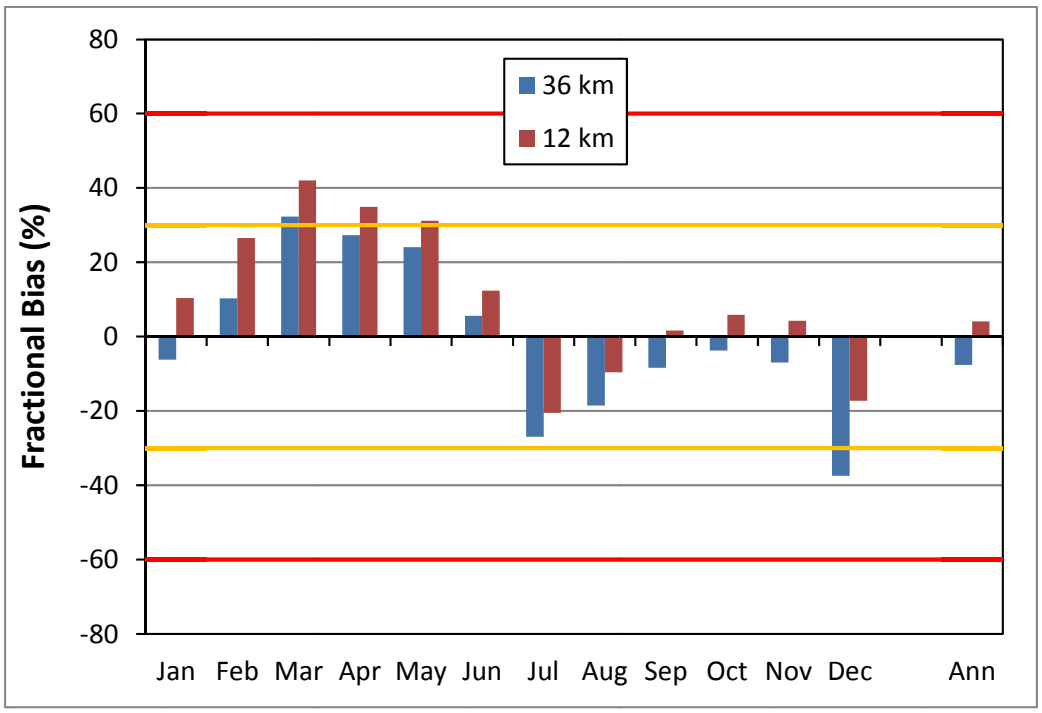
In summary, the CAMx 36/12 km DMAX8 ozone model performance mostly achieves the ozone model performance goals across the western states. With the exception of California, the DMAX8 ozone model performance exhibited an overestimation that in some cases was traced to questionable observations (e.g., Gothic and Glacier CASTNet sites in Colorado and Montana, respectively) and in others occurred across most of the state (e.g., New Mexico, Oregon and Washington). There is some indication that the coarse grid resolution (36/12 km) may be contributing to the overestimation bias in some cases.

4.5 CAMX PM MODEL PERFORMANCE

CAMx 36/12 km PM model evaluation is performed for total $PM_{2.5}$ mass across several networks (e.g., FRM, IMPROVE and CSN) and speciated $PM_{2.5}$ at the IMPROVE and CSN networks. Below we summarize the PM model performance across the WESTUS 12 km domain and then focus on model performance by western U.S. state. The Fractional Bias (FB) and Fractional Error (FE) performance statistics are used and compared with the PM Performance Goals and Criteria presented in Table 4-2. Note that the monthly model performance was calculated down to the individual site in the WESTUS domain as well as by day across all sites in the WESTUS domain. However, these results are too voluminous (~7 Gb and over 300,000 model performance graphics) to present in a report.

4.5.1 PM Performance Across the WESTUS 12 km Domain

Figure 4-7a displays the CAMx 36 km and 12 km model performance for total $PM_{2.5}$ mass across the FRM monitoring network in the WESTUS 12 km domain. Shown are monthly FB and FE model performance statistics that are compared against the PM Model Performance Goals and Criteria. The CAMx 36/12 km monthly FRM $PM_{2.5}$ model performance always achieves the PM Performance Criteria and usually achieves the PM Performance Goals. The model exhibits a $PM_{2.5}$ overestimation bias in the spring and an underestimation bias in the summer and later in the year with the largest underestimation occurring in December 2008. The CAMx 12 km $PM_{2.5}$ modeling results tend to be higher than the 36 km modeling results resulting in degraded model performance when the model overestimates $PM_{2.5}$ and improved model performance when the model underestimates the observed $PM_{2.5}$ concentrations. On an annual basis, CAMx exhibits very low bias with FB values of 4.1% and -7.6% for the 12 km and 36 km modeling results, respectively, and error values of 53-54% that achieves the PM Performance Criterion but just barely falls outside of the PM Performance Goal for bias (≤±50%).



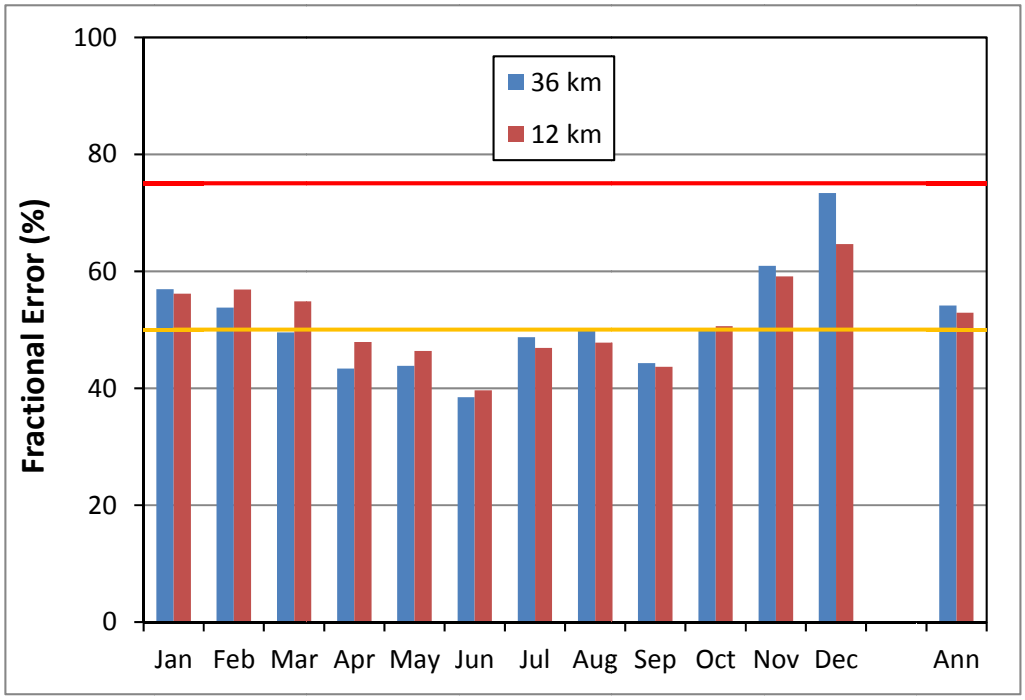


Figure 4-7a. Total $PM_{2.5}$ mass FB (top) and FE (bottom) model performance across the FRM network in the WESTUS domain for the CAMx 36 and 12 km 2008 base case.

Figure 4-7b displays the CAMx 36 km and 12 km total $PM_{2.5}$ mass model performance across the IMPROVE and CSN monitors in the WESTUS domain. With the exception of summer, CAMx exhibits an overestimation bias for $PM_{2.5}$ that is greater at the IMPROVE than CSN monitoring sites. The $PM_{2.5}$ overestimation bias at the IMPROVE sites is large enough that the PM Performance Criteria is not achieved for February and March, although the PM Performance Criteria is achieved for the other 10 months across the IMPROVE and for all months across the CSN network in the western U.S. The CAMx $PM_{2.5}$ model performance achieves the PM Performance Goal for almost all months at the CSN western U.S. monitoring sites but for just the summer months at the IMPROVE monitoring sites.

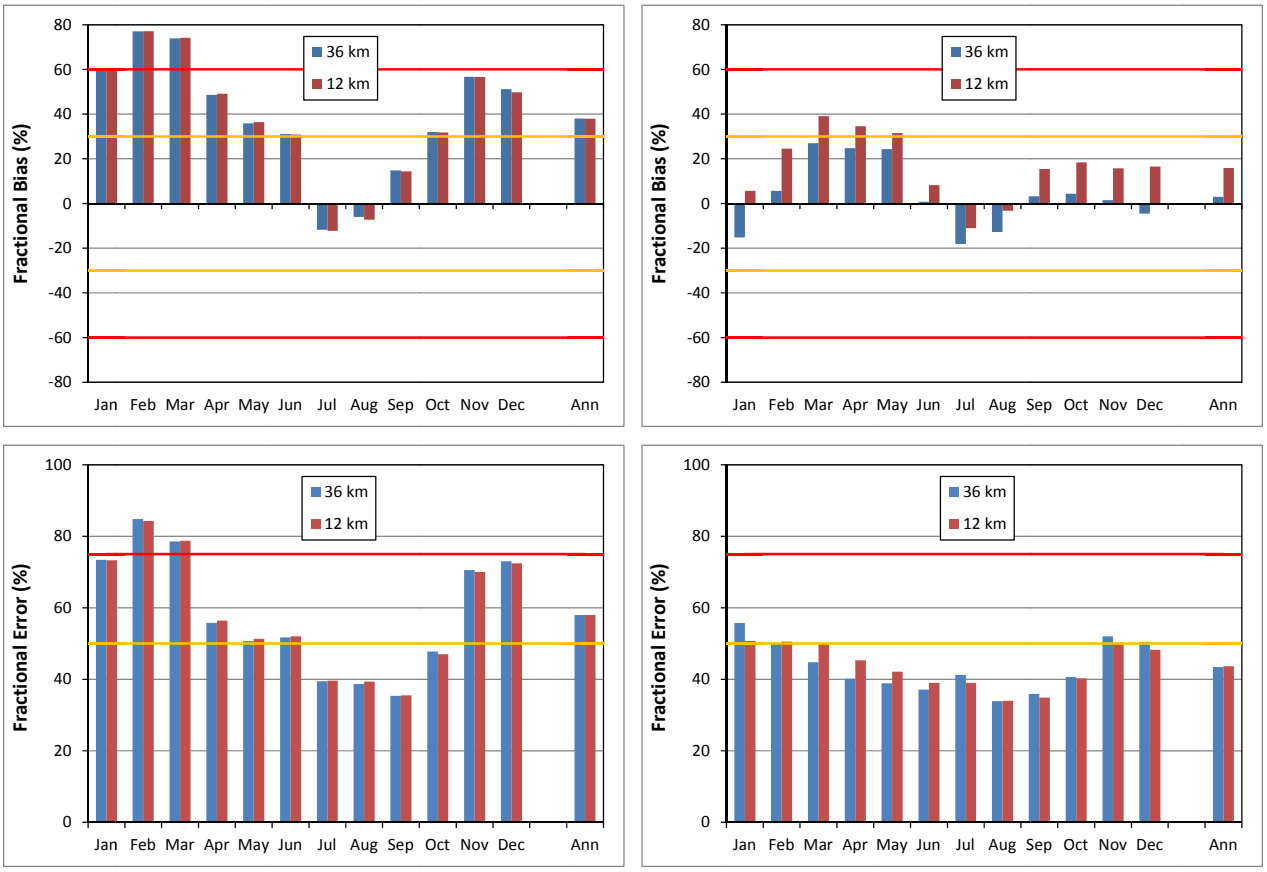


Figure 4-7b. Total $PM_{2.5}$ mass FB (top) and FE (bottom) model performance across the IMPROVE (left) and CSN (right) networks in the WESTUS domain for the CAMx 36 and 12 km 2008 base case.

Figure 4-8a displays the CAMx 36 km and 12 km sulfate (SO4) model performance across the IMPROVE and CSN monitoring sites in the western U.S. CAMx exhibits an SO4 overestimation bias in the winter and an underestimation bias the rest of the year. The CAMx SO4 performance always achieves the PM Performance Criteria across both monitoring networks. The CAMx SO4 model performance achieves the PM Model Performance Goal across the IMPROVE network except for the months of April and May. Whereas across the CSN network the SO4 model performance fails to achieve the PM Performance Goal for the spring and summer months. At the IMPROVE monitors, the CAMx 36 and 12 km results exhibit nearly identical model performance, whereas for the CSN network the CAMx 12 km SO4 model performance is better than the 36 km modeling results.

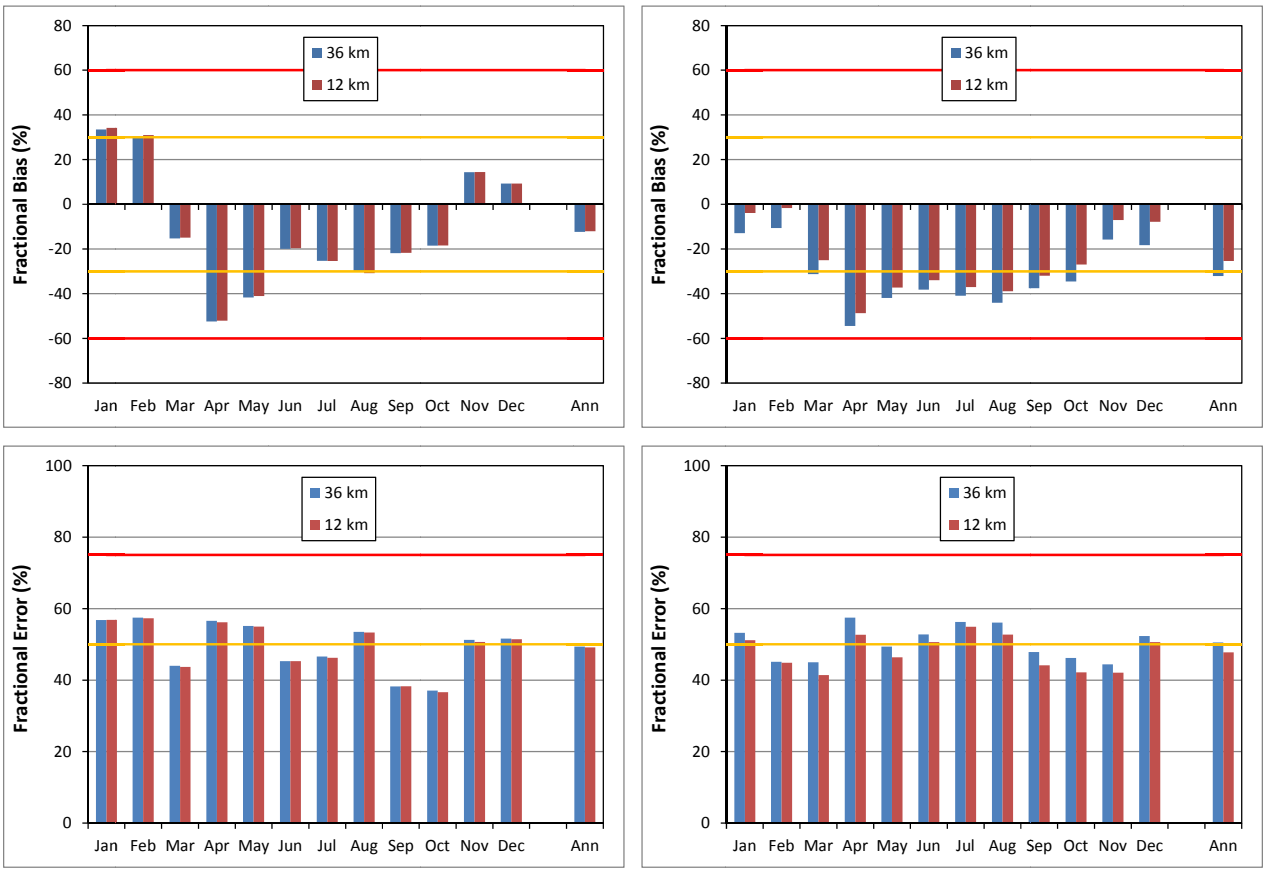


Figure 4-8a. SO_4 FB (top) and FE (bottom) model performance across the IMPROVE (left) and CSN (right) networks in the WESTUS domain for the CAMx 36 and 12 km 2008 base case.

Across the IMPROVE network in the western U.S., the CAMx NO3 model performance exhibits an overestimation bias except for the summer months (Figure 4-8b, left). The NO3 performance always achieves the PM Performance Criteria for FB, although it exceeds the Performance Criteria for FE and most months. The NO3 model performance across the CSN network is characterized by an underestimation bias that is so great in the summer that the PM Performance Criteria is not achieved (Figure 4-8b, right). However, the observed NO3 concentrations are extremely low in the summer and both the observed and modeled NO3 concentrations indicate that it is usually a very small component of $PM_{2.5}$ mass in the summer.

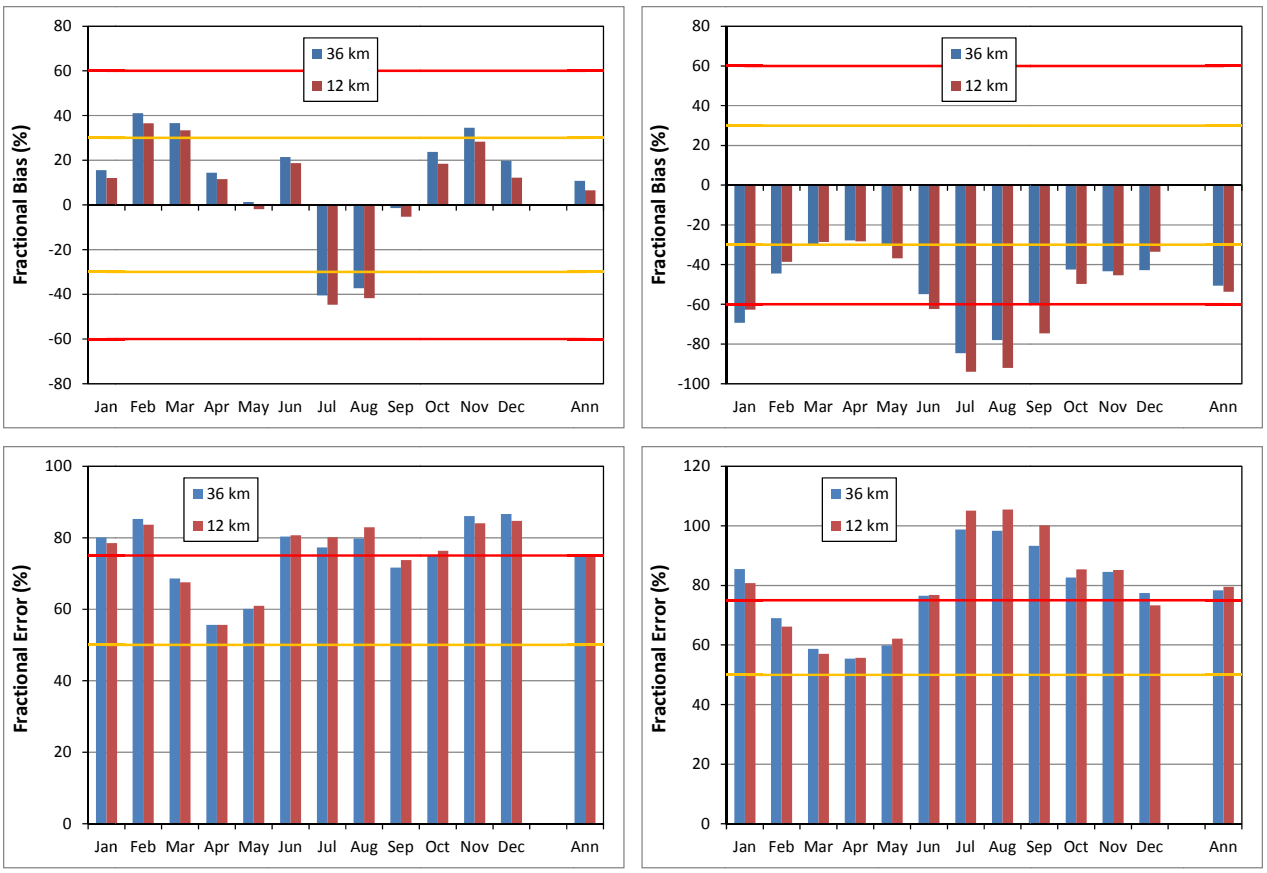


Figure 4-8b. NO_3 FB (top) and FE (bottom) model performance across the IMPROVE (left) and CSN (right) networks in the WESTUS domain for the CAMx 36 and 12 km 2008 base case.

Figure 4-8c displays the western U.S. ammonium (NH4) model performance across the IMPROVE and CSN networks. NH4 is underestimated, which is consistent with the general underestimation of SO4 and NO3. Note that the IMPROVE network does not measure NH4 so the model is evaluated against derived NH4 (NH4d) that is estimated from the SO4 and NO3 measurements assuming they are completely neutralized by NH4. Since SO4 is not always completely neutralized by NH4 and there are other basic compounds that can neutralize SO4 and NO3, then NH4d is an overstatement of actual ambient NH4 concentrations, so the CAMx NH4d underestimation is expected. With the exception of April and May across the IMPROVE network, the CAMx NH4 model performance achieves the PM Performance Goal. The CAMx NH4 performance tends to fall between the PM Performance Goal and Criteria across the IMPROVE network and is right at the PM Performance Goal across the CSN network.

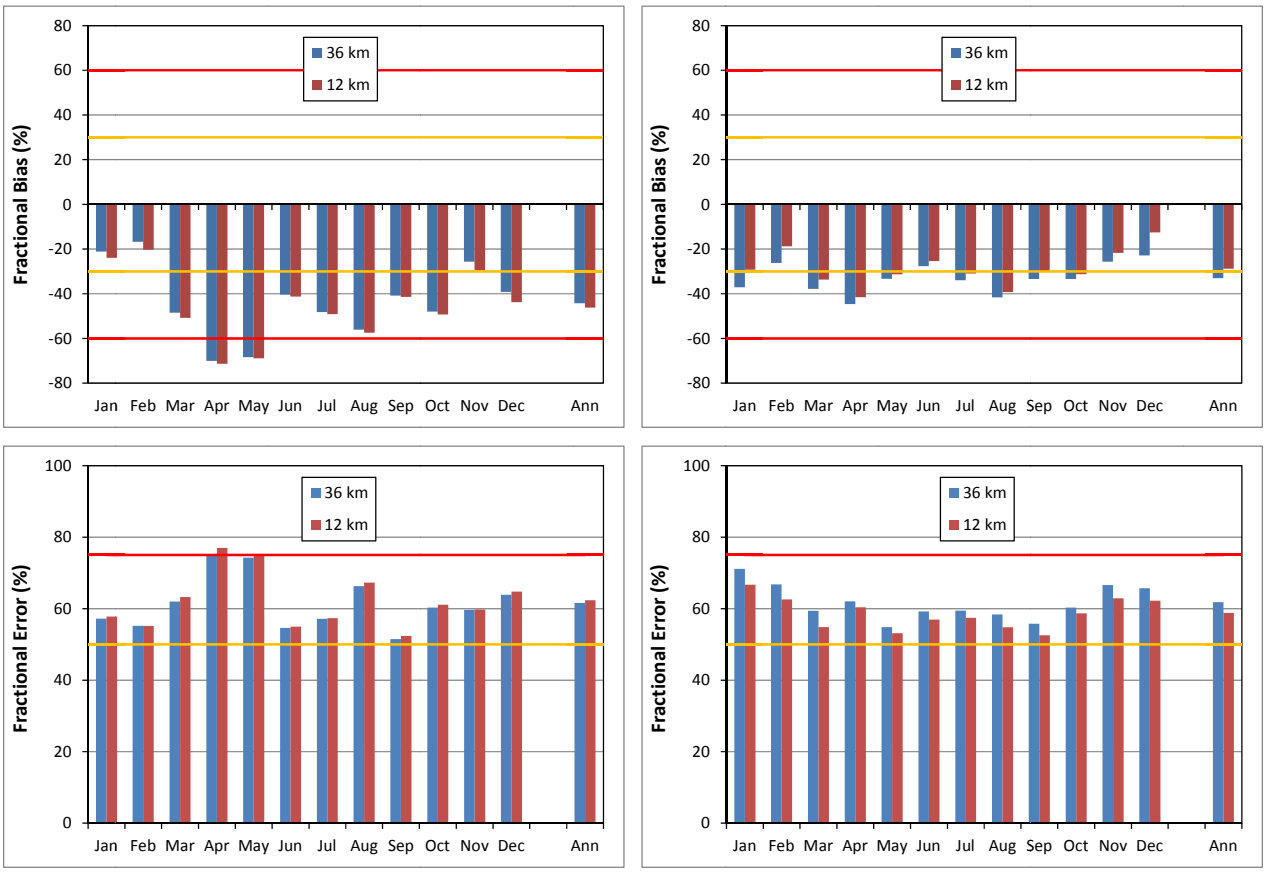


Figure 4-8c. NH_4 FB (top) and FE (bottom) model performance across the IMPROVE (left) and CSN (right) networks in the WESTUS domain for the CAMx 36 and 12 km 2008 base case.

The CAMx elemental carbon (EC) model performance is displayed in Figure 4-8d. The CAMx EC model performance almost always achieves the PM Performance Criteria with the one exception being FE across the IMPROVE network in January. The FE tends to fall between the PM Performance Goal and Criterion whereas the FB achieves the PM Performance Goal for many months at the IMPROVE network. It should be pointed out that in 2008 the CSN used the NIOSH technology to measure EC that has known measurement artifacts. The CSN carbon measurements have now all switched to the TOR technology as used by IMPROVE.

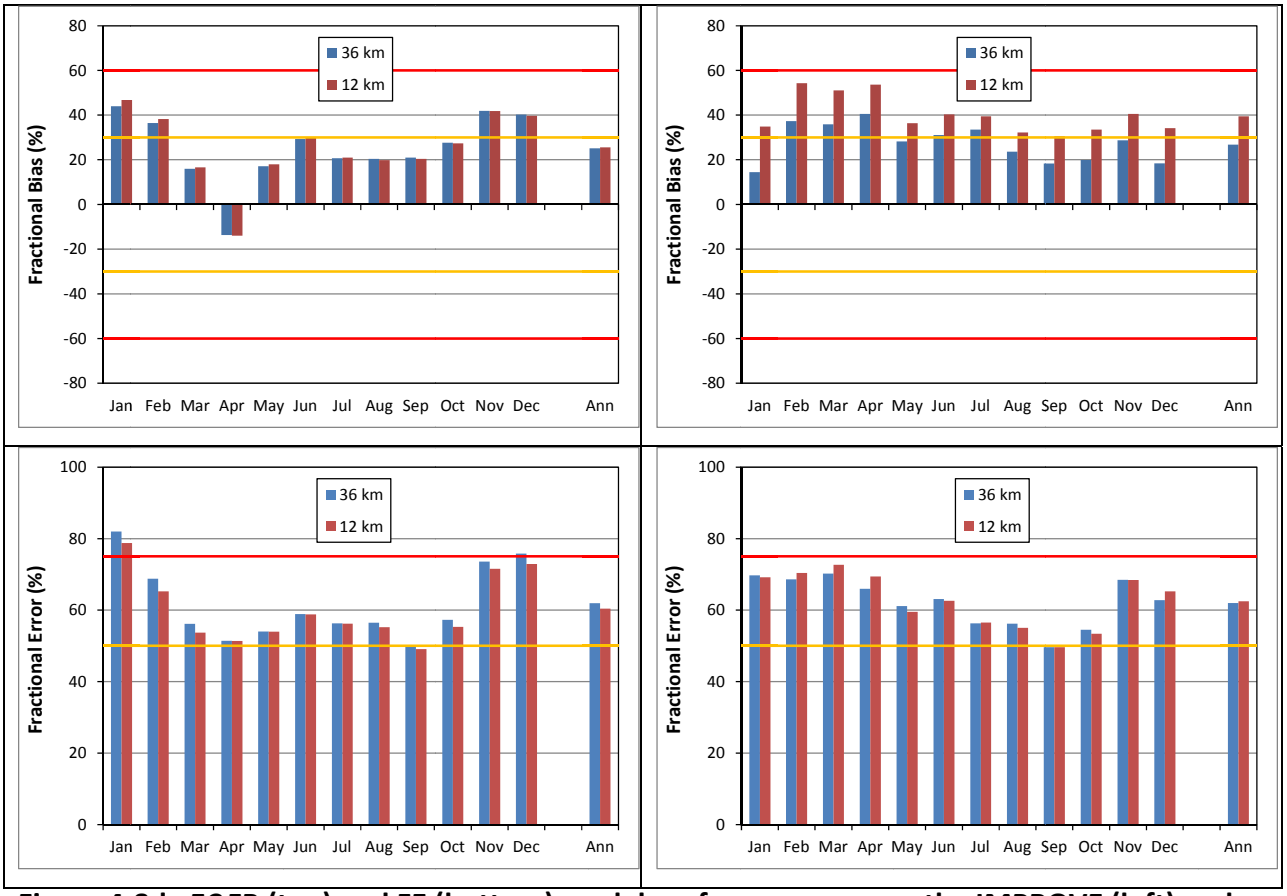


Figure 4-8d. EC FB (top) and FE (bottom) model performance across the IMPROVE (left) and CSN (right) networks in the WESTUS domain for the CAMx 36 and 12 km 2008 base case.

The CAMx Organic Aerosol (OA) model performance exhibits an underestimation bias across both networks that is greatest in the spring and greater for the CSN than IMPROVE network. The OC measurements were converted to OA by increasing them by 40% (OA = 1.4 x OC). In 2008 the CSN measurements using NIOSH have a known positive bias so the higher OA underestimation at CSN compared to IMPROVE is not unexpected. The OA underestimation is likely due to multiple causes:

- Measurement artifacts.
- Missing SVOC emissions and chemical and thermodynamic processes.
- Underestimation of secondary organic aerosol (SOA).
- Lack of blank correction in the measurements.

Note that the EPA SANDWICH methodology to process CSN and IMPROVE speciated $PM_{2.5}$ measurements does not directly use the OC measurements but instead obtains OA using mass balance techniques with the total $PM_{2.5}$ mass and speciated $PM_{2.5}$ measurements.

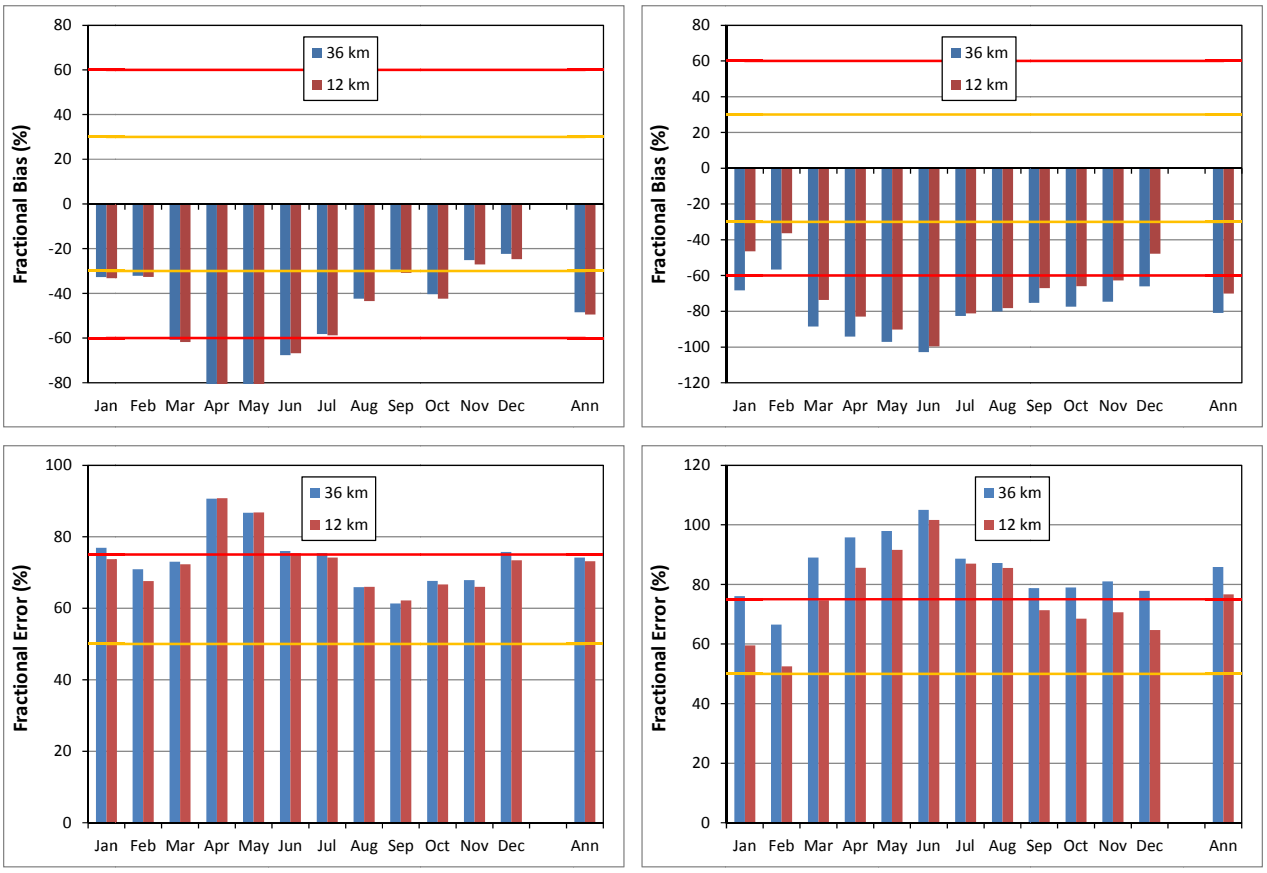


Figure 4-8e. OA FB (top) and FE (bottom) model performance across the IMPROVE (left) and CSN (right) networks in the WESTUS domain for the CAMx 36 and 12 km 2008 base case.

The CAMx model performance for the other $PM_{2.5}$ (OPM2.5) species is shown in Figure 4-8f. The measured OPM2.5 concentrations are defined as the difference between the total $PM_{2.5}$ mass observations minus the speciated $PM_{2.5}$ observations (SO4+NO3+NH4+EC+OA). When a negative OPM2.5 concentration is calculated it is set to zero. In the model the OPM2.5 species is defined from the $PM_{2.5}$ emissions that are not explicitly speciated as SO4, NO3, NH4, EC or OA. Given the two different "observed" and modeled definitions of the OPM2.5 species it is not surprising that the model greatly overestimates OPM2.5. There are likely other PM components in the modeled OPM2.5 species (e.g., OA) that explain these differences. Better understanding of the PM emissions speciation profiles and measurement artifacts are needed to improve the comparisons of the OPM2.5 species.

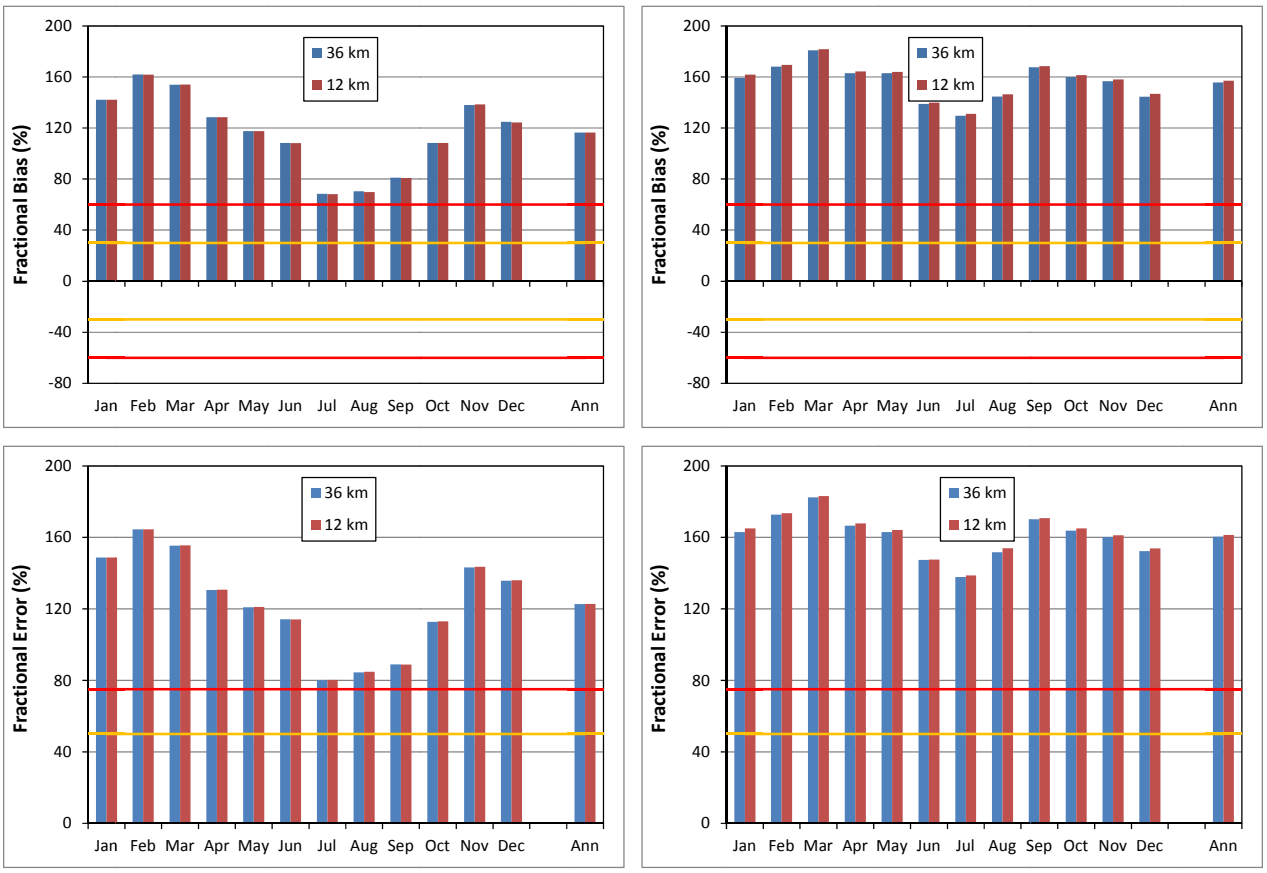


Figure 4-8f. Other $PM_{2.5}$ FB (top) and FE (bottom) model performance across the IMPROVE (left) and CSN (right) networks in the WESTUS domain for the CAMx 36 and 12 km 2008 base case.

4.5.2 CAMx 12 km PM Model Performance by Western U.S. State

Figure 4-9 displays the CAMx 12 km total $PM_{2.5}$ mass model performance across the FRM, CSN and IMPROVE networks for each western U.S. state using soccer plots that plot FB vs. FE and compares them with the PM Model Performance Goals and Criteria. The performance for each $PM_{2.5}$ species across the CSN and IMPROVE networks in the states of Arizona, Colorado, New Mexico and Utah are shown in Figures 4-10 through 4-14. The CAMx state-specific $PM_{2.5}$ performance usually achieves the PM Performance Goals (Figure 4-9). Exceptions to this are overestimation at the IMPROVE network for mainly winter months in AZ, CA, CO, NM, MT, UT and WY. The model frequently also achieves the PM Performance Goals, with ND and SD $PM_{2.5}$ performance being particularly good.

SO4 performance almost always achieves the PM Performance Criteria in AZ, CO, NM and UT with performance in CO and NM usually achieving the PM Performance Goal (Figure 4-10). Both AZ and UT exhibit a SO4 underestimation bias in the summer that sometimes exceeds the PM Performance Criteria in UT.

Very different NO3 performance is seen across the CSN and IMPROVE networks. Across the CSN network NO3 is mostly underestimated, especially during the warmer months (Figure 4-11). However, across the IMPROVE network there is usually low bias, although the summer months are still underestimated and the error is usually at the PM Performance Criterion.

Consistent with the SO4 and NO3 underestimation, NH4 is generally underestimated especially in AZ and UT. As expected, since the IMPROVE uses derived NH4d that will overstate actually observed NH4 concentrations, the model NH4 underestimation bias is greater across the IMPROVE than CSN networks (Figure 4-12).

The TCM (EC+OA) model performance across the IMPROVE network is fairly good with the exception of some underestimation in the spring and summer months in CO and spring in AZ and UT (Figure 4-13). TCM performance across the CSN network exhibits an underestimation bias. The particle carbon measurement technology used by the CSN network in 2008 has known measurement artifacts that likely contributes to the worse model performance using the CSN than IMPROVE carbon measurements.

Finally, the OPM2.5 performance is characterized by an overestimation bias that is greater for CSN than for IMPROVE. This is due in part to the setting of negative calculated "observed" OPM2.5 concentrations to zero using the CSN network that indicates more differences in the measurement artifacts of the CSN total $PM_{2.5}$ mass and speciated $PM_{2.5}$ whose differences are used to define OPM2.5.

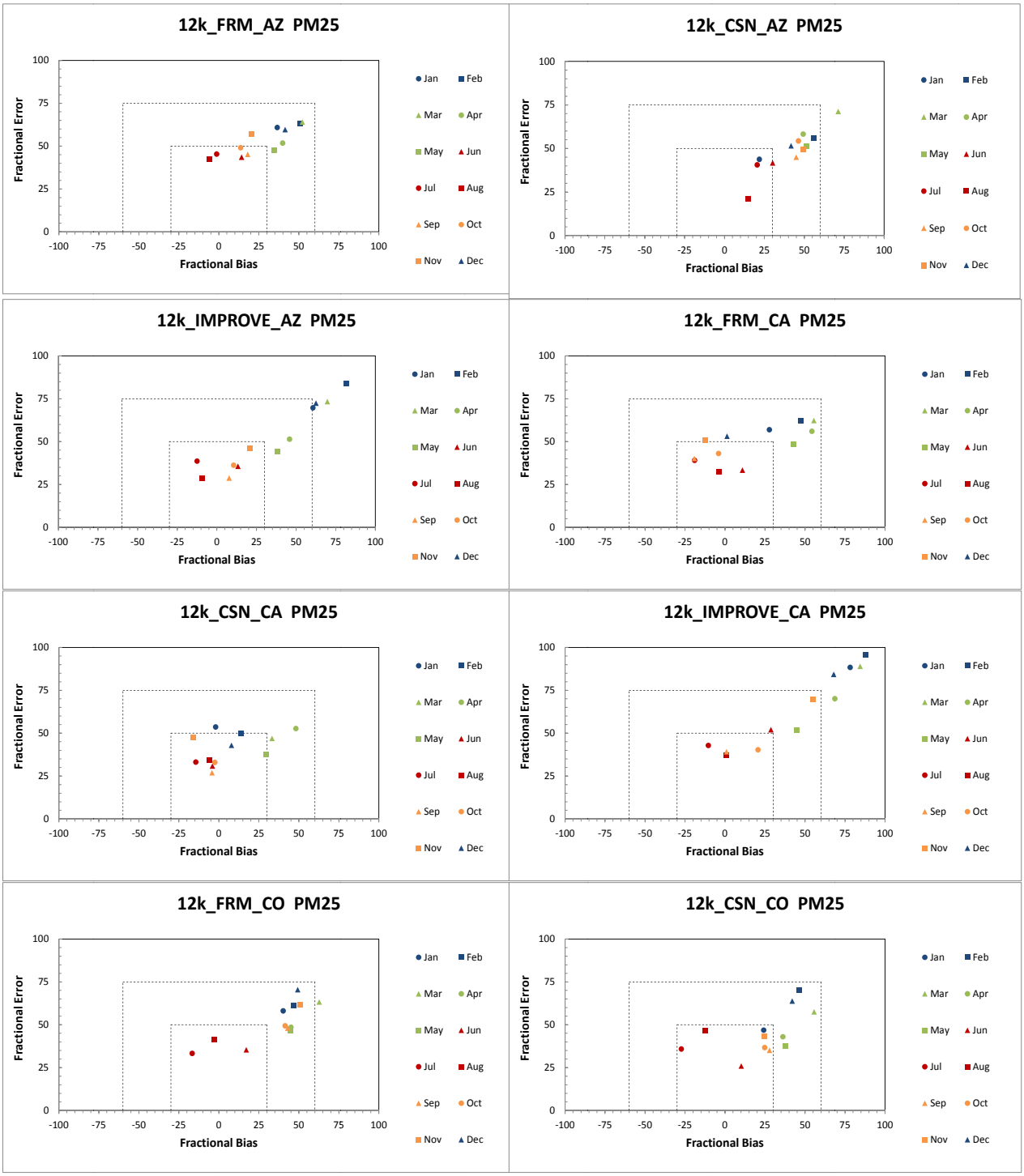


Figure 4-9a. Total $PM_{2.5}$ mass model performance by state for the CAMx 2008 12 km base case simulation and FRM, CSN and IMPROVE networks.

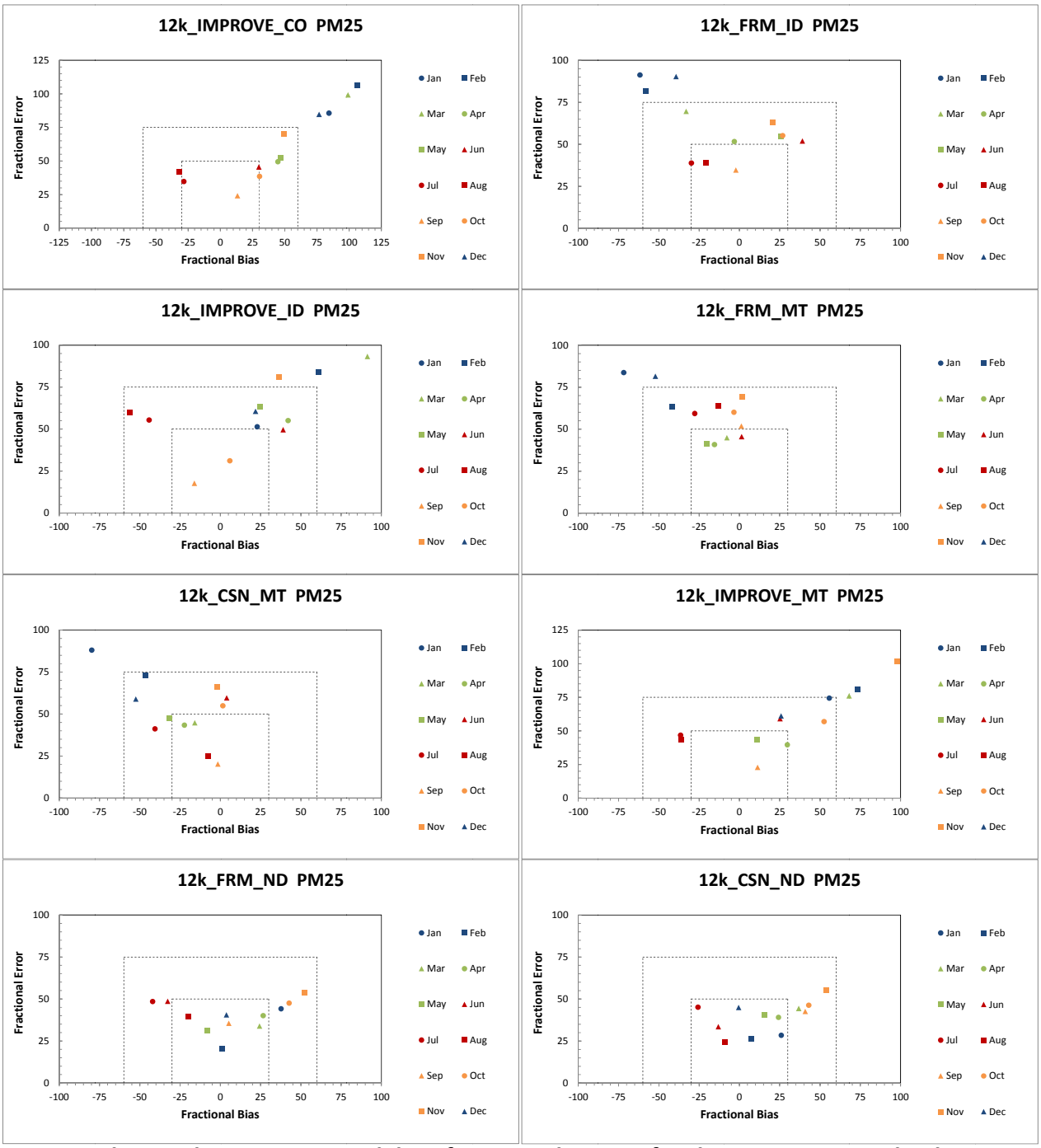


Figure 4-9b. Total $PM_{2.5}$ mass model performance by state for the CAMx 2008 12 km base case simulation and FRM, CSN and IMPROVE networks.

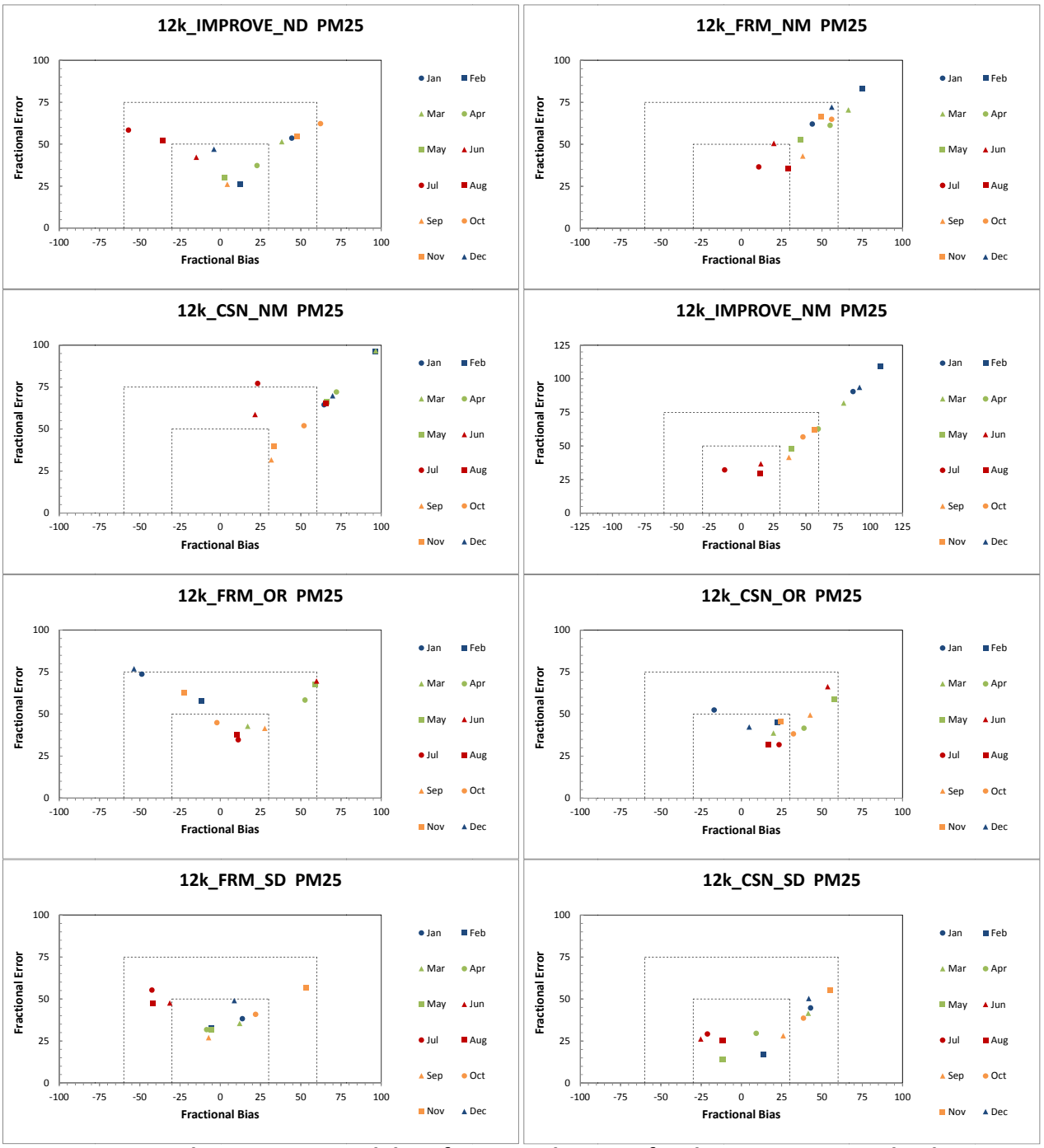


Figure 4-9c. Total $PM_{2.5}$ mass model performance by state for the CAMx 2008 12 km base case simulation and FRM, CSN and IMPROVE networks.

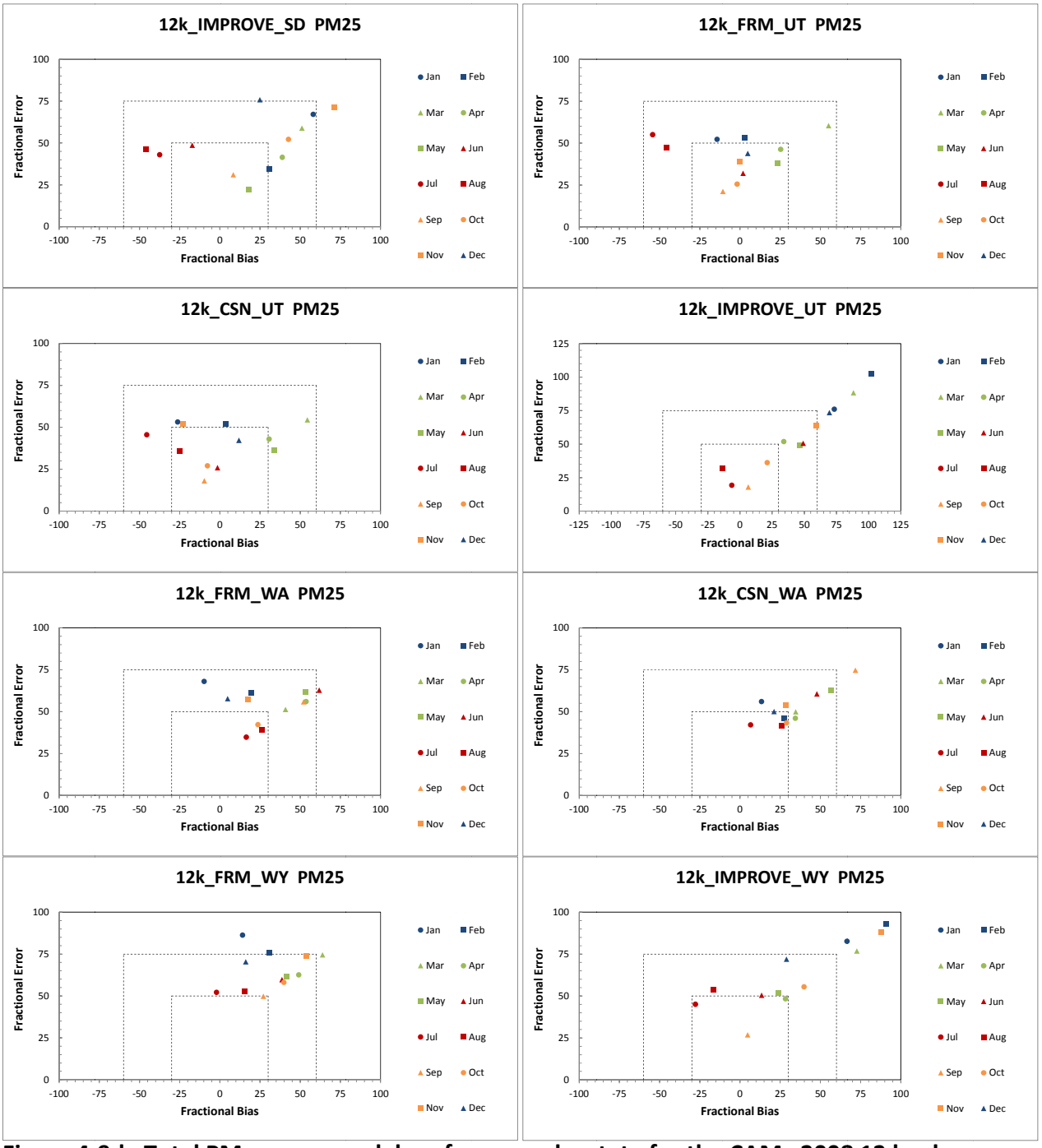


Figure 4-9d. Total $PM_{2.5}$ mass model performance by state for the CAMx 2008 12 km base case simulation and FRM, CSN and IMPROVE networks.

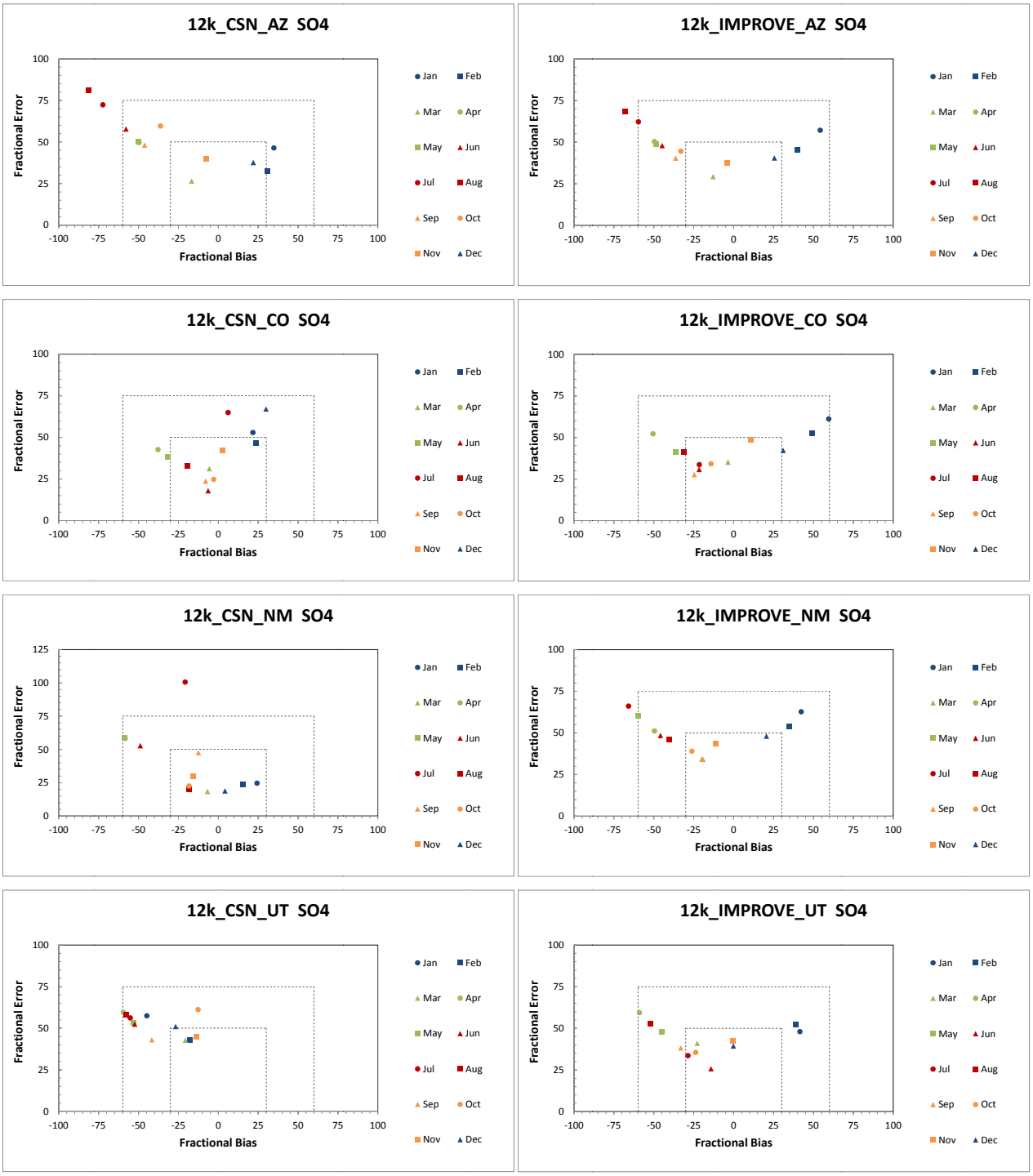


Figure 4-10. Sulfate (SO4) model performance across the CSN (left) and IMPROVE (right) monitoring networks in Arizona, Colorado, New Mexico and Utah.

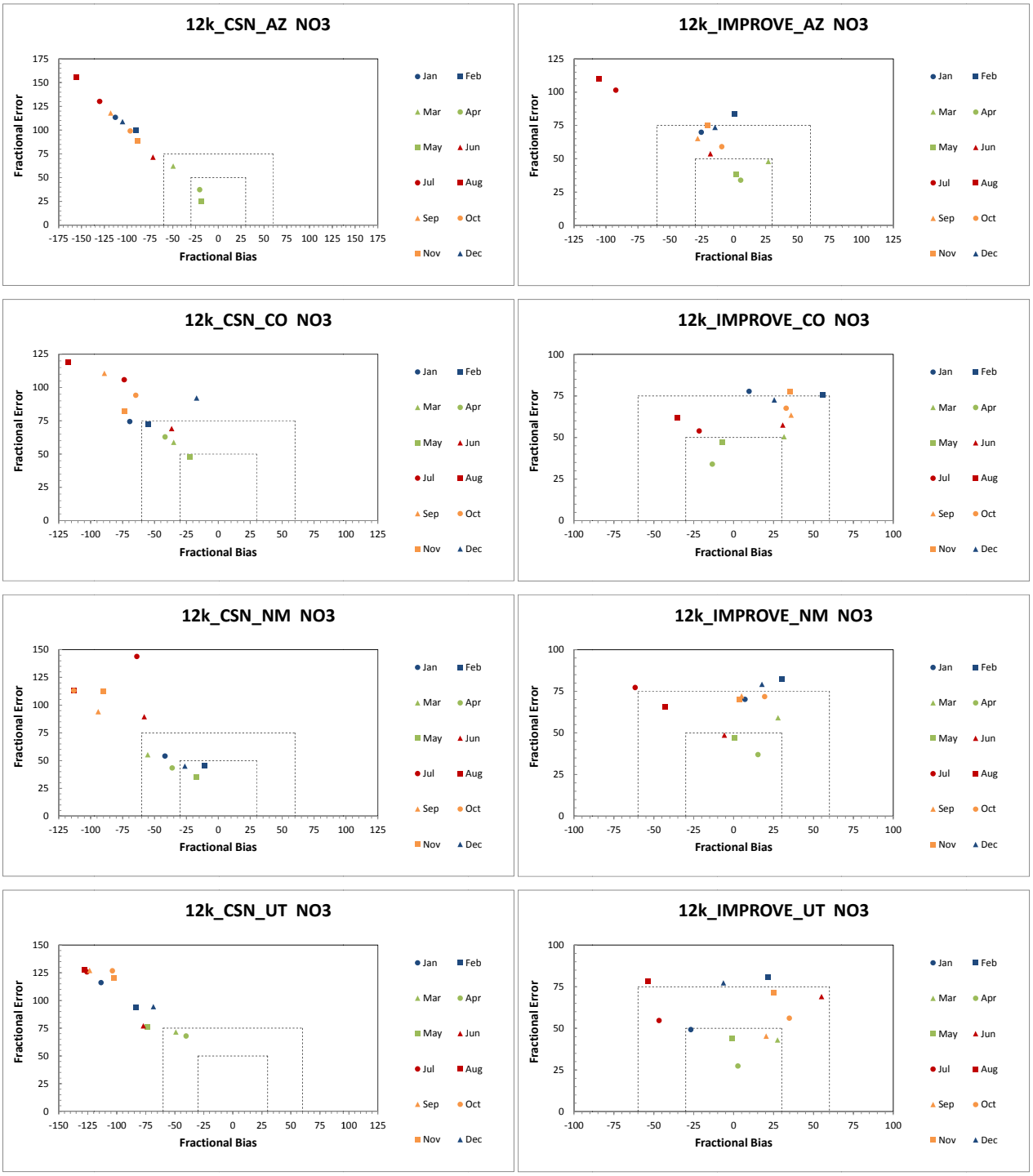


Figure 4-11. Nitrate (NO3) model performance across the CSN (left) and IMPROVE (right) monitoring networks in Arizona, Colorado, New Mexico and Utah.

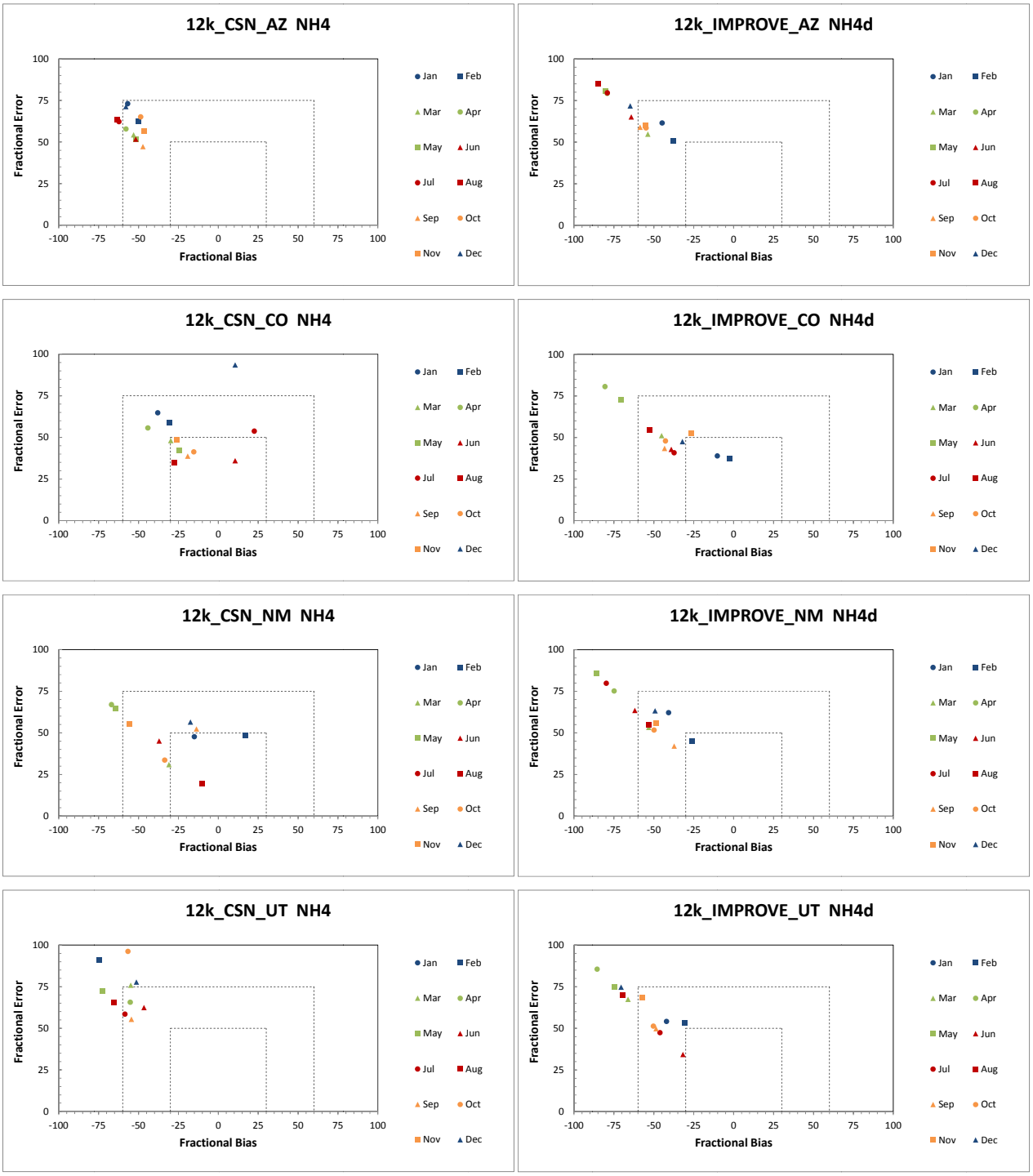


Figure 4-12. Ammonium (NH4) model performance across the CSN (left) and IMPROVE (right) monitoring networks in Arizona, Colorado, New Mexico and Utah (Note: NH4d for IMPROVE).

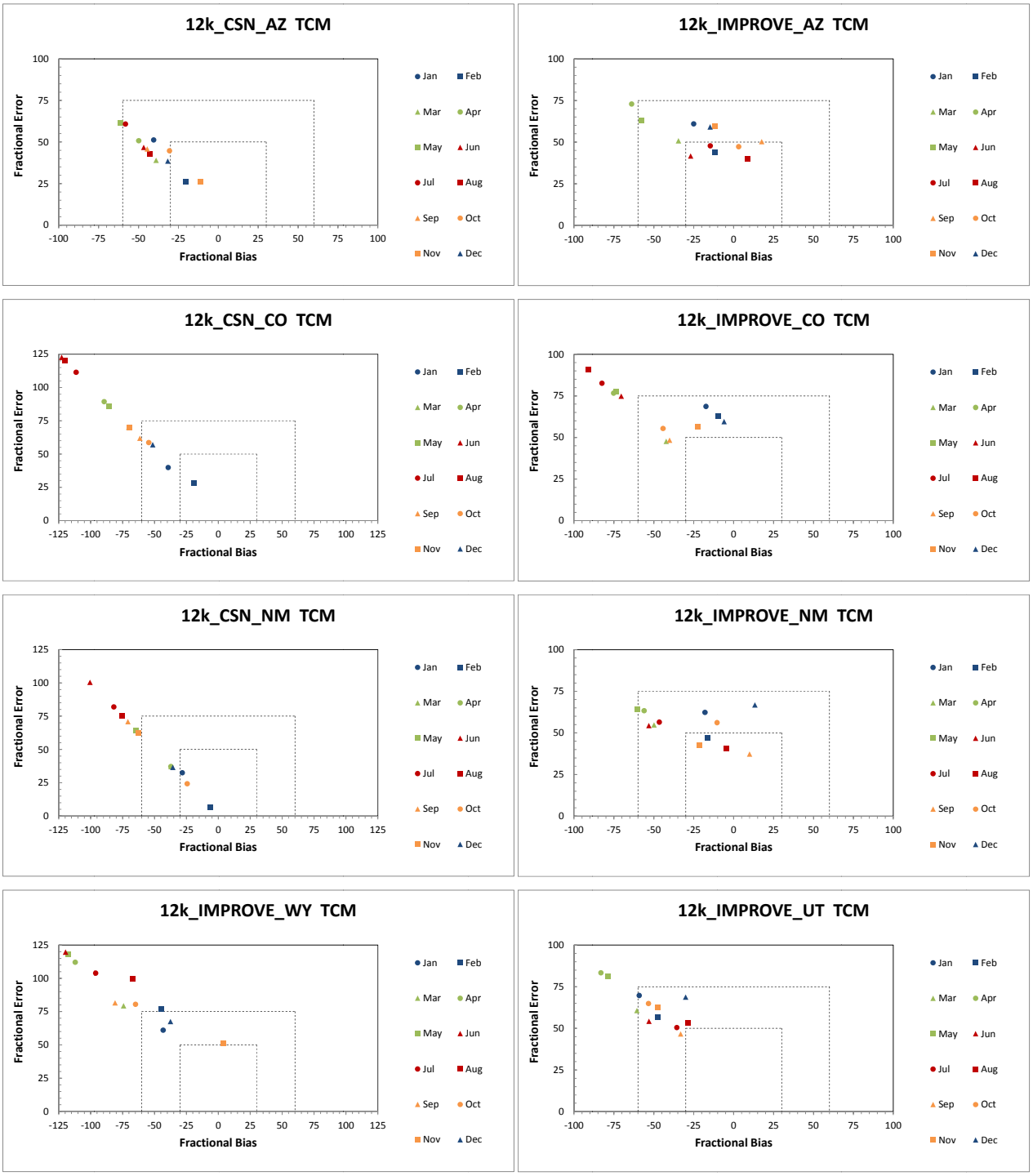


Figure 4-13. Total Carbon Mass (TCM) model performance across the CSN (left) and IMPROVE (right) monitoring networks in Arizona, Colorado, New Mexico and Utah.

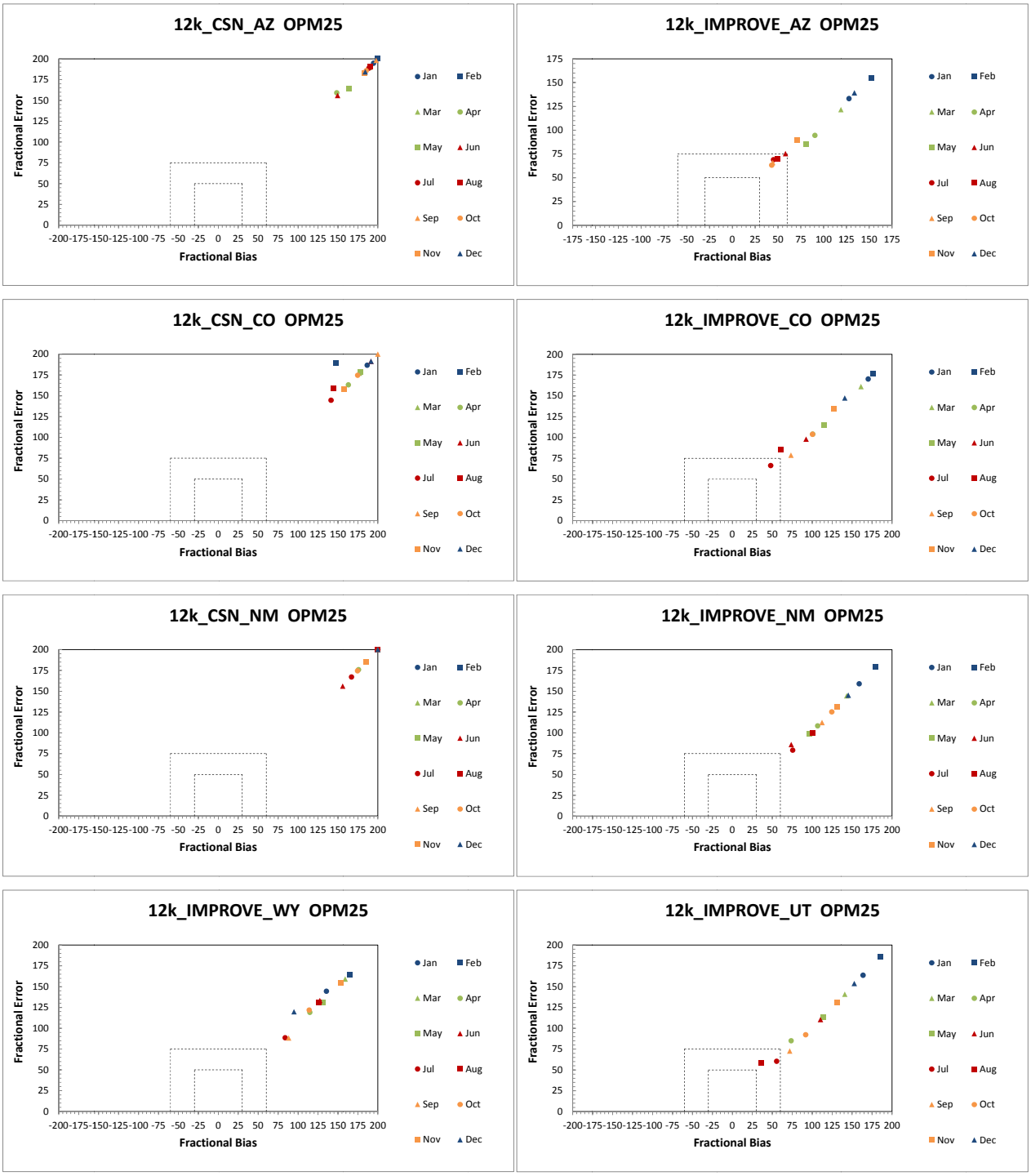


Figure 4-14. Other $PM_{2.5}$ (OPM2.5) model performance across the CSN (left) and IMPROVE (right) monitoring networks in Arizona, Colorado, New Mexico and Utah.

4.5.3 CAMx 4 km Model Performance within the IAD

A separate CAMx 4 km modeling database was developed for the 2008 annual period and the 4 km Impact Assessment Domain (IAD) for the Colorado Air Resource Management Modeling Study (CARMMS) depicted in Figure 1-5 that covers all of Colorado, the northern two-thirds of New Mexico as well as eastern Utah and northeastern Arizona. A separate model performance evaluation of the CARMMS 2008 CAMx 4 km base case simulation was conducted, which is discussed in this section.

Figure 4-15 displays the monthly and annual daily maximum 8-hour ozone CAMx 4 km model performance evaluation across CASTNet and AQS monitors within the CARMMS domain and compares them with the Ozone Performance Goals. The CAMx 4 km DMAX8 ozone bias is always within ±6% with an annual FB of less than 2% achieving the ozone ≤±15% goal by a wide margin. Similarly, the monthly Fractional Error tends to be between 5% and 12% so again achieves the Ozone Performance Goal of ≤35% by over a factor of 2. Some of the underestimation of the DMAX8 ozone at the Colorado CASTNet sites (e.g., in May) may be due in part to the model's inability to fully simulate stratospheric ozone intrusion events (e.g., at Gothic).

The CAMx 4 km total $PM_{2.5}$ mass performance across the FRM, IMPROVE and CSN sites in the 4 km CARMMS domain is shown in Figure 4-16. The model tends to overestimate $PM_{2.5}$ in the winter falling to a near zero bias in the summer. However, the overestimation bias is usually within the PM Performance Criteria with only 5 of the 36 monthly FBs (14% of the time) failing to achieve the PM Performance Criteria. 14 months achieve the PM Performance goal (~40% of the time), which occur in the summer and months adjacent to the summer.

Figures 4-17 and 4-18 display the CAMx 4 km model performance related to sulfur species that includes SO4 at IMPROVE, CSN and CASTNet monitoring networks, SO2 at CASTNet and wet SO4 deposition at NADP. SO4 tends to be overestimated in the winter and underestimated in the spring, summer and early fall. SO2 is also overestimated in the winter and fall with near zero bias to underestimating in the spring and summer, which indicates that the summer SO4 underestimation is not due to insufficient oxidation of available SO2 concentrations. The wet SO4 deposition also is overestimated in the winter and underestimated in the summer suggesting that too rapid wet depositions is not the cause of the summer SO4 underestimation tendency.

Figures 4-19 and 4-20 displays CAMx 4 km model performance statistics related to nitrogen species including NO3, HNO3 and combined NO3 plus HNO3. Monthly NO3 performance at the IMPROVE sites almost always achieves the PM Performance Goal, whereas it is generally underestimated across the CSN and CASTNet networks with the largest underestimation bias occurring in the summer. On the other hand, HNO3 tends to be overestimated by the CAMx 4 km CARMMS base case and the performance of total nitrate (HNO3+NO3) exhibits much better performance with near zero bias in the spring and summer that achieves the PM Performance Goals. These results suggest that some of the NO3 underestimation bias may be due to not enough conversion of the gaseous HNO3 to particulate NO3. This could be due to insufficient ammonia present to buffer the nitric acid or not fully accounting for other basic compounds that can neutralize nitric acid (e.g., Calcium, Sodium, etc.). Thermodynamic variables could also partly account for this if the temperatures were too hot or the atmosphere not moist enough.

NH4 model performance across he IMPROVE, CSN and NADP networks in the CARMMS 4 km domain is shown in Figure 4-21. NH4 is underestimated, which is consistent with the SO4 and NO3 underestimation bias, with the performance being better across the CSN network that always achieves the PM Performance Criteria and sometimes achieves the PM Performance Goal. The underestimation bias is greater across the IMPROVE network due to the use of derived NH4d in the evaluation that overestimates actual ambient NH4

concentrations. The NH4 wet deposition exhibits near zero or an underestimation bias indicating that the NH4 underestimation tendency is not due to overstated wet scavenging.

The CAMx 4 km model performance for gaseous NO_X and NO_Y across AQS and nonmethane organic compounds (NMOC) across PAMS monitoring sites are shown in Figure 4-22. NO_X is underestimated in the winter with near zero bias in the summer, whereas NO_Y is overestimated in the summer, underestimated in the winter and has near zero bias in the spring. Given that these measurements may have artifacts and picking up other reactive nitrogen species, it is hard to interpret the evaluation. NMOC is underestimated throughout the year, which may be due in part to the fact they tend to be sited in urban areas.

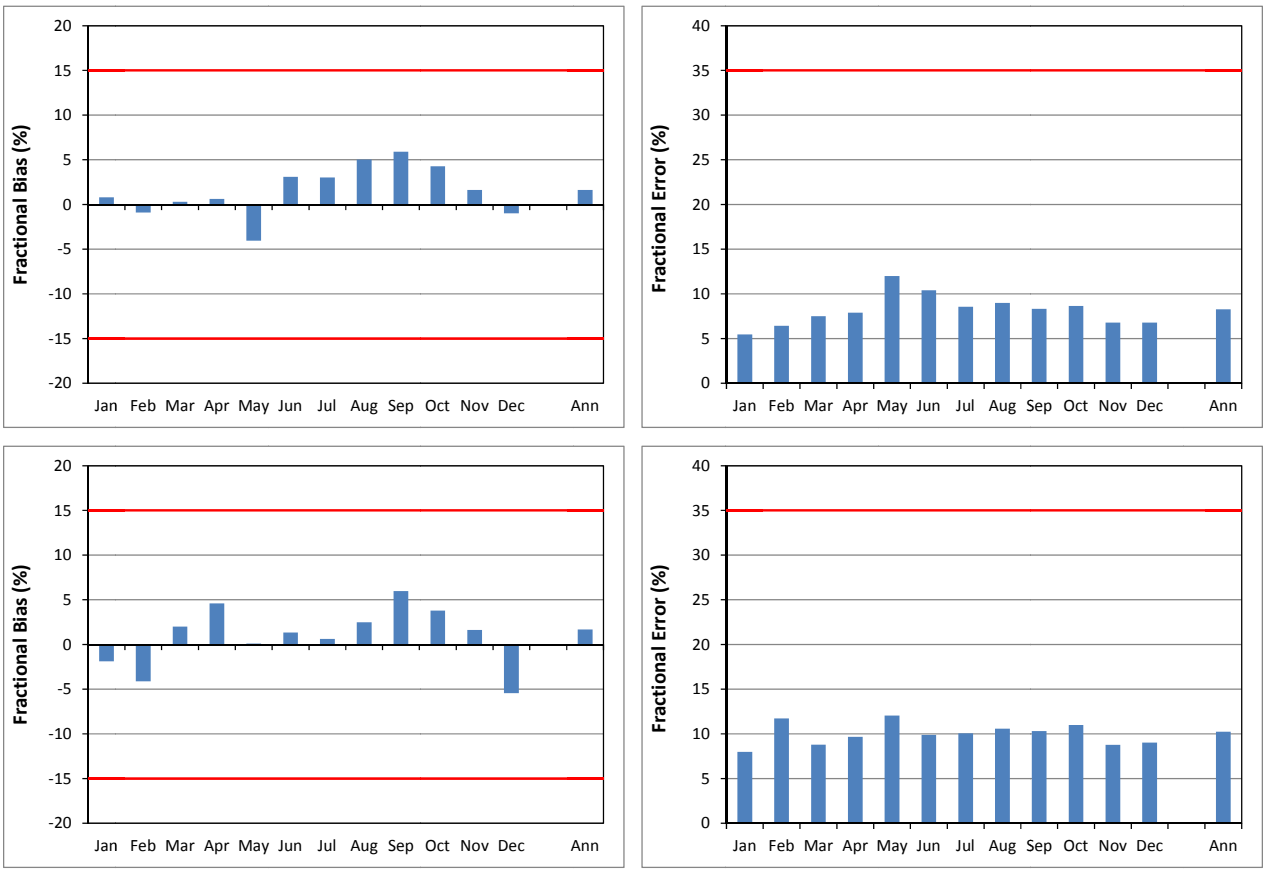


Figure 4-15. CAMx 4 km daily maximum 8-hour ozone model performance for FB (left) and FE (right) across CASTNet (top) and AQS (bottom) monitors within the CARMMS 4 km Impact Assessment Domain (IAD).

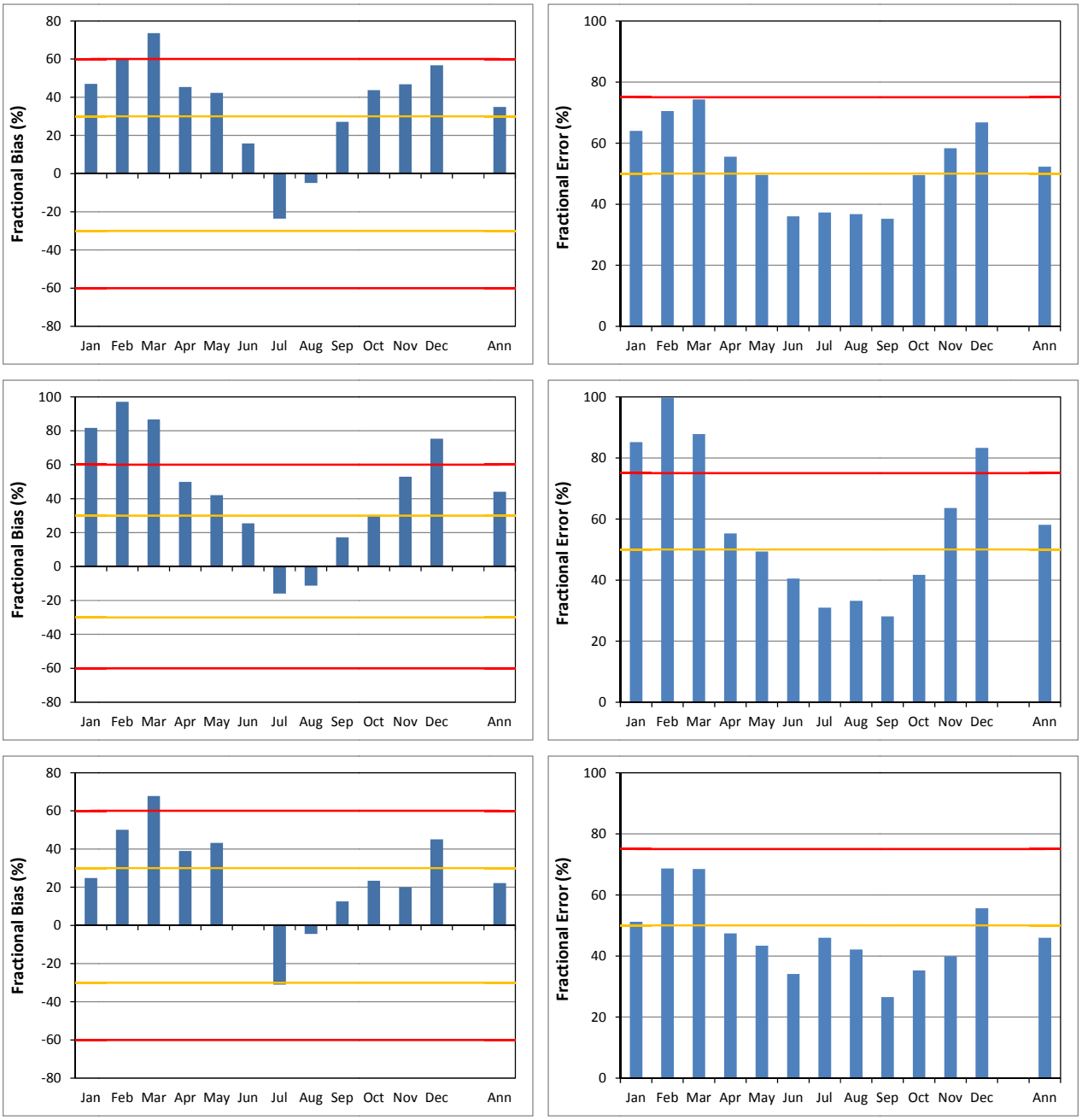


Figure 4-16. CAMx 4 km $PM_{2.5}$ model performance for FB (left) and FE (right) across FRM (top), IMPROVE (middle) and CSN (bottom) monitors within the CARMMS 4 km Impact Assessment Domain (IAD).

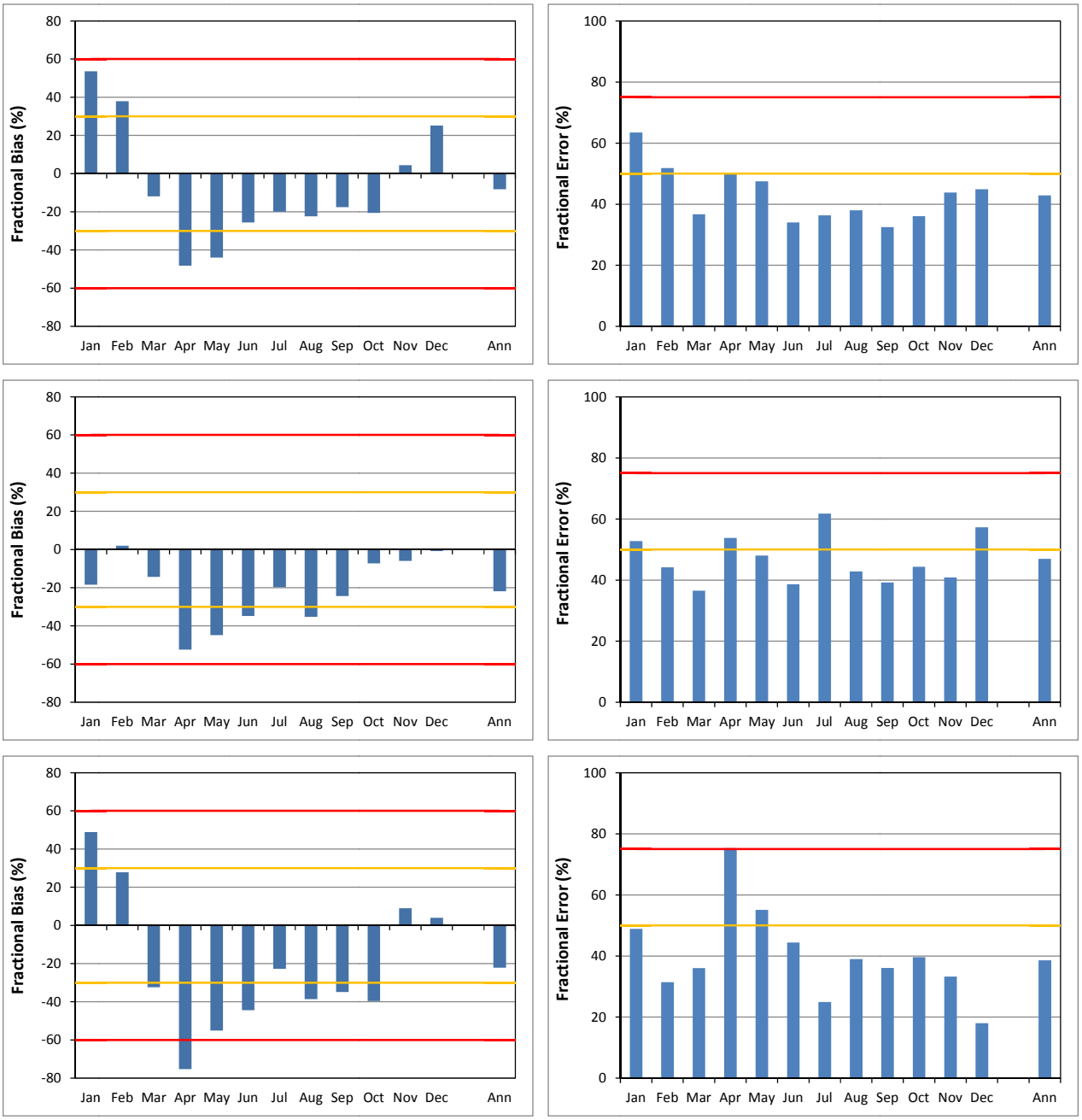


Figure 4-17. CAMx 4 km Sulfate (SO4) model performance for FB (left) and FE (right) across IMPROVE (top), CSN (middle) and CASTNet (bottom) monitors within the CARMMS 4 km Impact Assessment Domain (IAD).

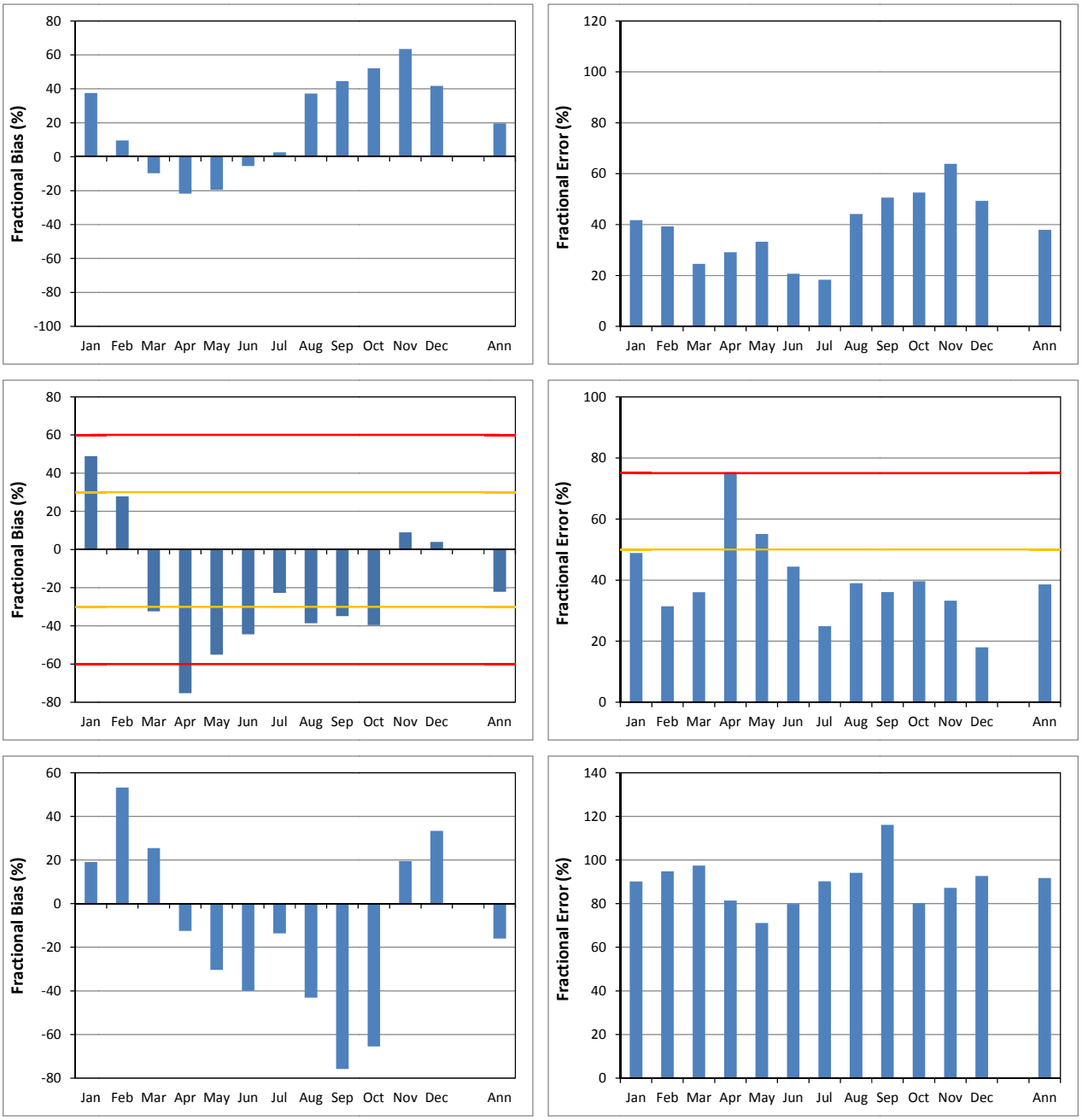


Figure 4-18. CAMx 4 km SO2 (top) and SO4 (middle) at CASTNet and SO4 Wet Deposition (bottom) at NADP model performance for FB (left) and FE (right) monitors within the CARMMS 4 km Impact Assessment Domain (IAD).

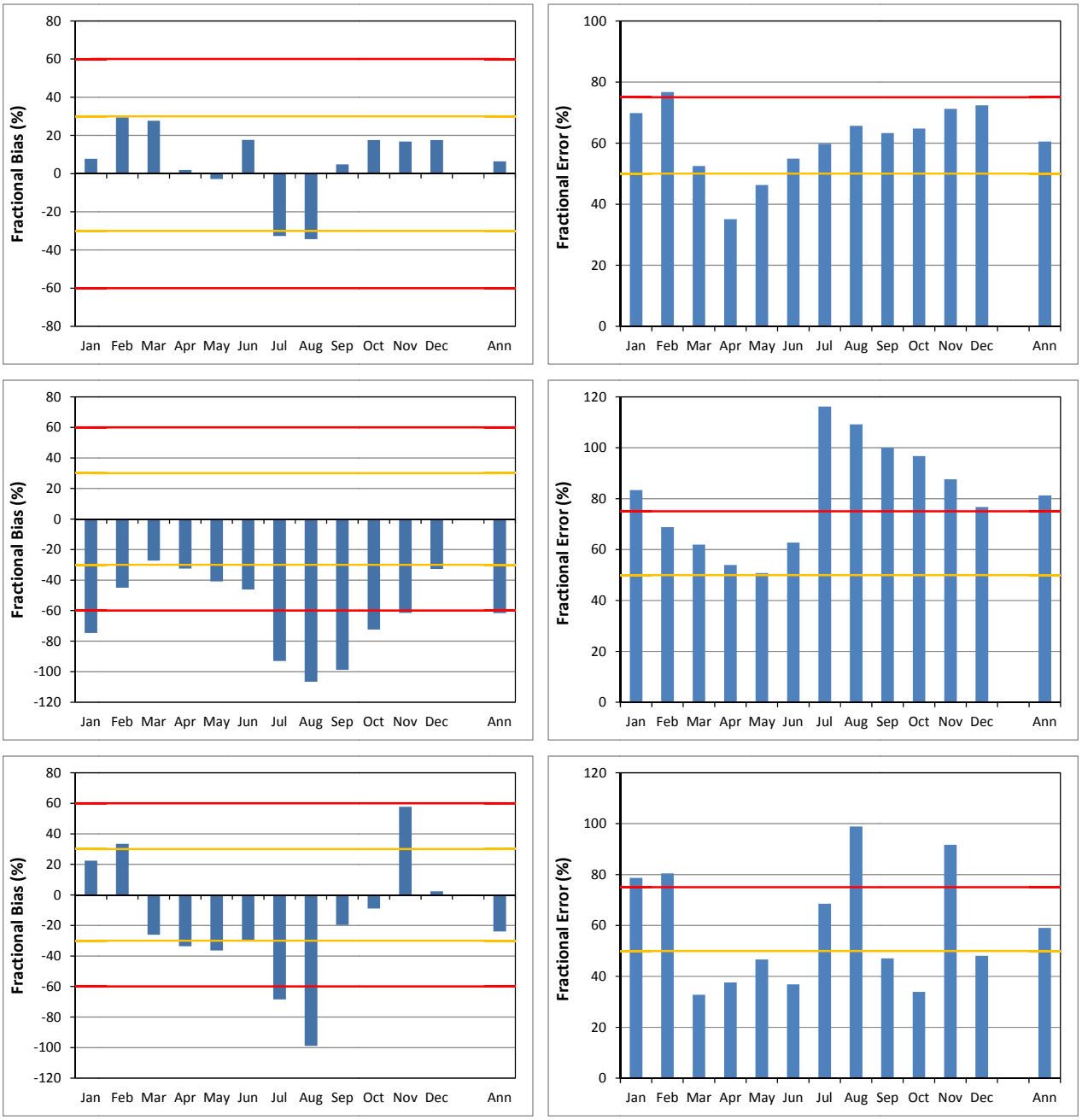


Figure 4-19. CAMx 4 km NO3 model performance for FB (left) and FE (right) across IMPROVE (top), CSN (middle) and CASTNet (bottom) monitors within the CARMMS 4 km Impact Assessment Domain (IAD).

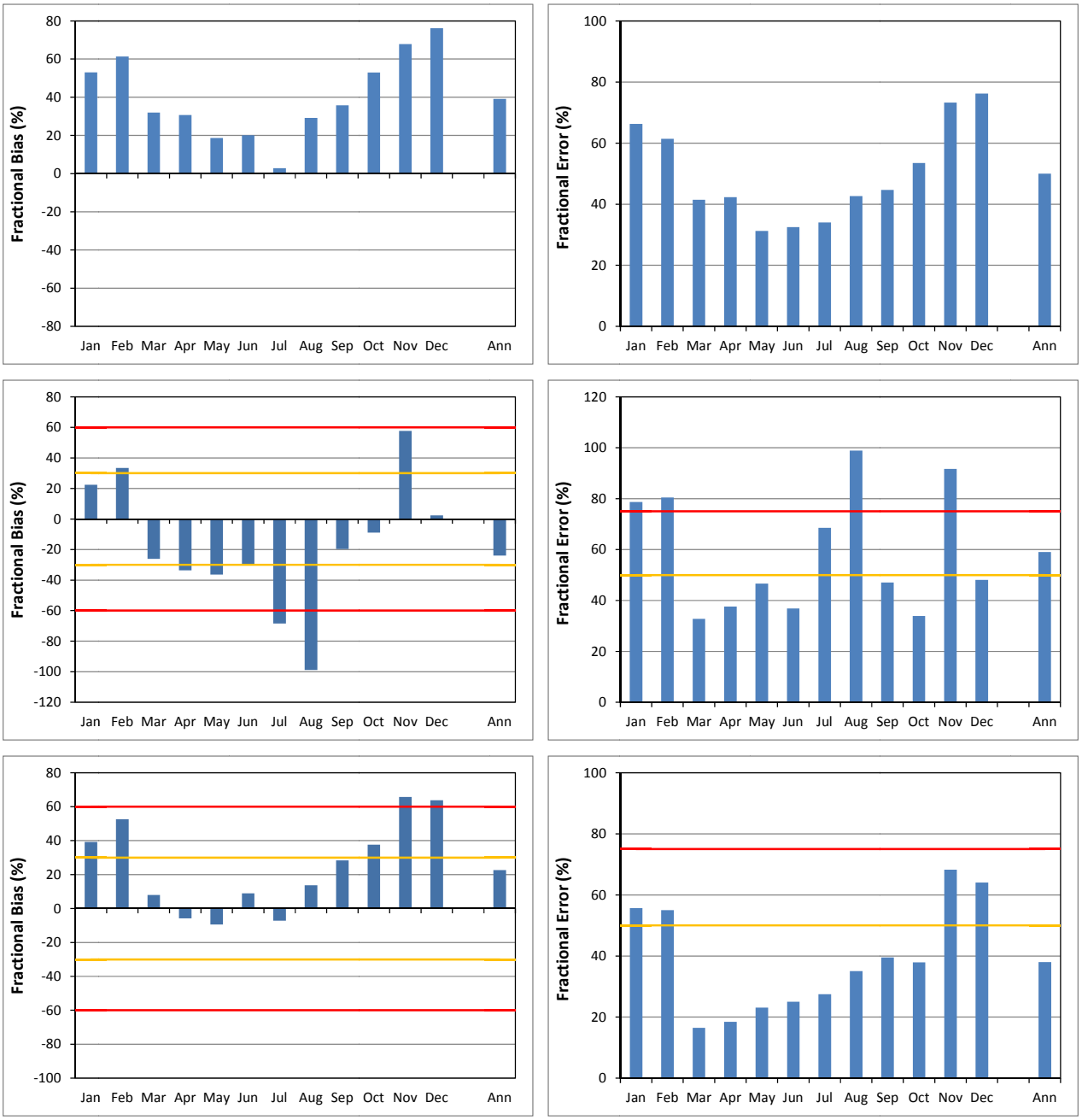


Figure 4-20. CAMx 4 km HNO3 (top), NO3 (middle) and tHNO3+NO3 (bottom) model performance for FB (left) and FE (right) across CASTNet monitors within the CARMMS 4 km Impact Assessment Domain (IAD).

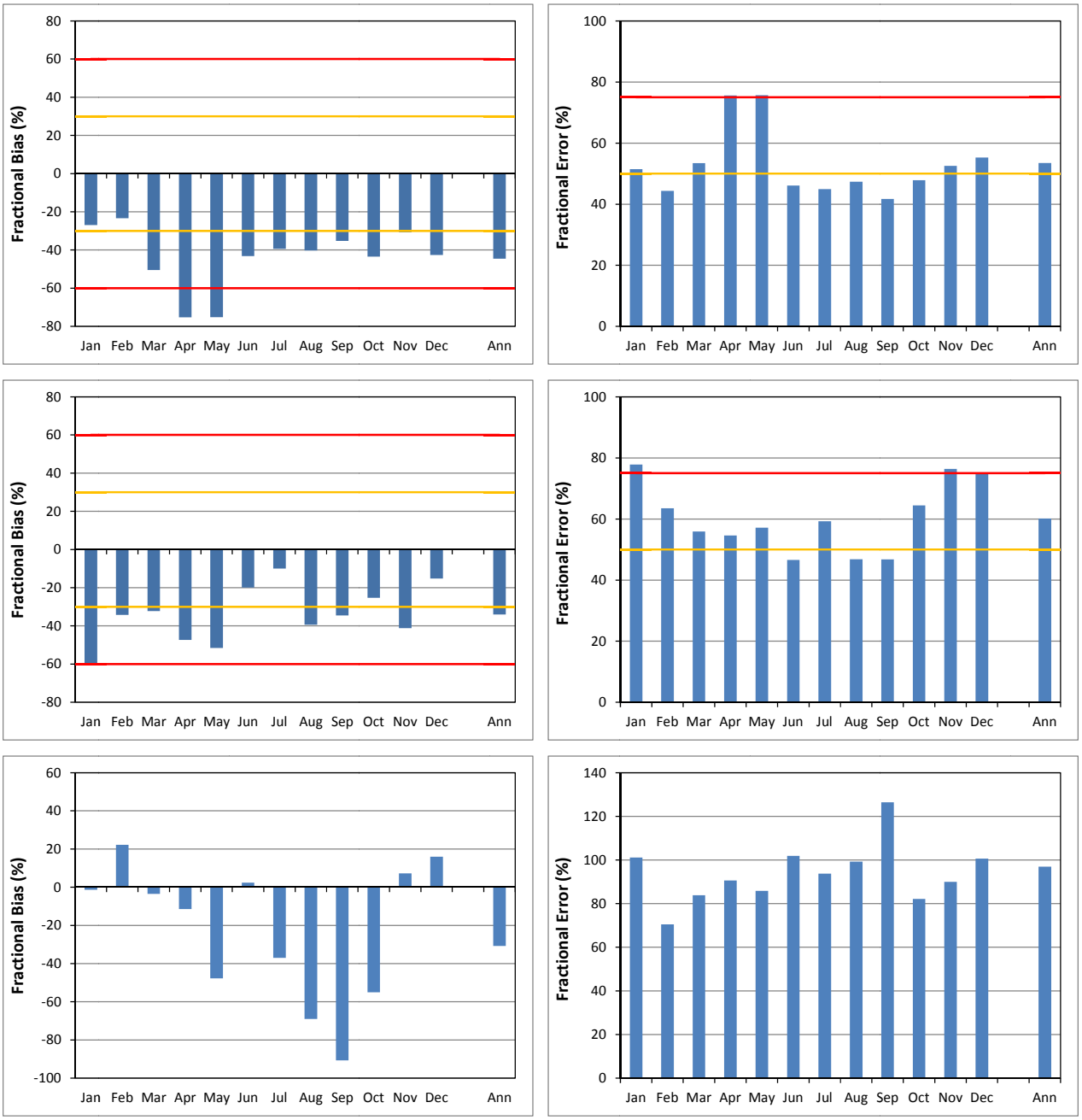


Figure 4-21. CAMx 4 km NH4 concentration and wet deposition model performance for FB (left) and FE (right) across IMPROVE (top), CSN (middle) and NADP (bottom) monitors within the CARMMS 4 km Impact Assessment Domain (IAD).

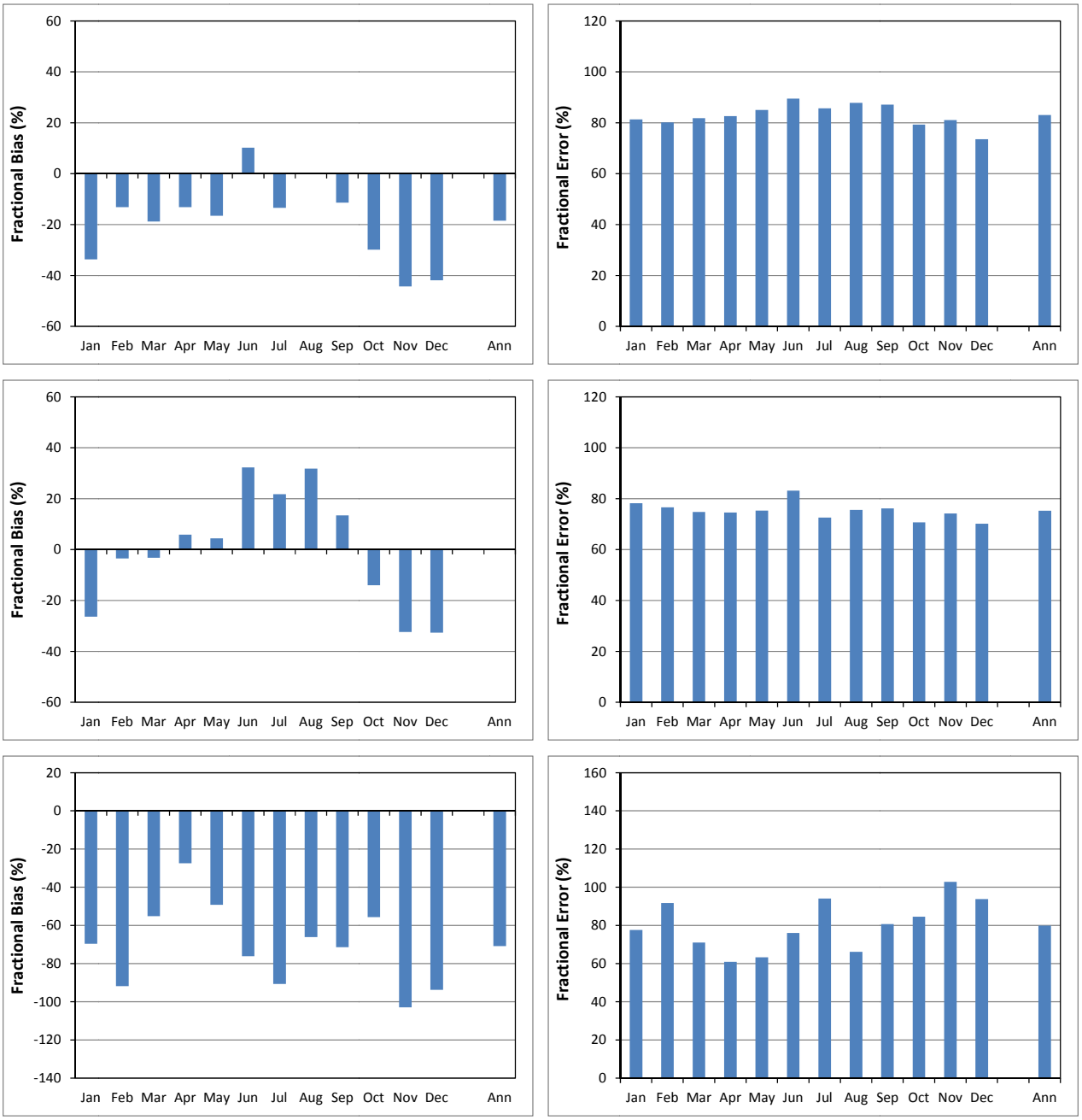


Figure 4-22. CAMx 4 km NO_X (top), NO_Y (middle) and NMOC (bottom) model performance for FB (left) and FE (right) across AQS and PAMS) monitors within the CARMMS 4 km Impact Assessment Domain (IAD).

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5.0 STATE-SPECIFIC OZONE SOURCE APPORTIONMENT MODELING

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

- State-Specific Source Apportionment that examined the contributions of an upwind state's anthropogenic emissions to downwind state's ozone and $PM_{2.5}$ concentrations and Design Values; and
- Source Category-Specific Source Apportionment that modeled the contributions of major source categories (e.g., oil and gas, point sources, mobile sources etc.) to ozone and $PM_{2.5}$ concentrations and Design Values.

In this Chapter we present the state-specific ozone source apportionment modeling with the state-specific PM source apportionment discussed in Chapter 6 and the source category-specific ozone and PM source apportionment discussed in Chapter 7. However, before presenting the state-specific ozone source apportionment modeling results, the different Probing Tools available in the CAMx/CMAQ photochemical grid models and what kinds of information they can provide are described below.

5.1 PROBING TOOLS

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

Brute Force Sensitivity: Brute Force Sensitivity modeling can be performed using any photochemical model and involves the application of the model for a base case and then for a sensitivity simulation that has a perturbation in the model or model inputs. The difference in concentrations between the base case and sensitivity simulation is the sensitivity of the model to the selected perturbation. Although a brute force sensitivity simulation can be performed for any model attribute, it is most frequently applied to changes in emissions. For example, multiple brute force simulations of across-the-board VOC and NO_X emission reductions can be performed to develop an ozone isopleth (EKMA) diagram that can be used to help identify a VOC/NO_X emissions control path toward ozone attainment. Another example of Brute Force Sensitivity applications is the sequence of control measures that are used to ultimately demonstrate attainment of the ozone or $PM_{2.5}$ standard as part of the development of a SIP control plan. Brute Force Sensitivity simulations have been used to completely eliminate (zero-out) emissions from a specific source sector (e.g., on-road mobile sources) and the differences between the base case and the specific source sector zero-out case has been interpreted as the contributions of that source sector. However, for reactive pollutants the zero-out approach is a sensitivity and not a source apportionment method. For example, the sum of the ozone contributions due to the zero-out modeling of all Source Groups does not add up to the base case ozone concentrations because the effect of altering the emissions in the zero-out runs

changes the chemistry in the photochemical model simulation thereby altering the source-receptor relationships from those in the base case.

CAMx Ozone and PM Source Apportionment: CAMx contains two versions of an ozone source apportionment tool, the Ozone Source Apportionment Technology (OSAT) and the Anthropogenic Precursor Culpability Assessment (APCA). CAMx also contains the Particulate Source Apportionment Technology (PSAT) that estimates source apportionment for particulate matter (PM) species. All three source apportionment techniques use reactive tracers (also called tagged species) that run in parallel to the host model to determine the contributions of ozone and PM to user selected Source Groups. A Source Group is typically defined as the intersection between geographic Source Regions (e.g., grid cell definitions of states) and user selected Source Categories (e.g., point, on-road mobile, etc.). The intersection of the Source Regions and the Source Categories defines the Source Groups (e.g., on-road mobile sources from California) for which individual source apportionment contributions are obtained. Source apportionment provides contributions of emissions within each Source Group to concentrations under the current model simulation conditions, but does not necessarily estimate what would be the effect that controls on a given Source Group would have on the concentrations, which is a sensitivity question.

- Ozone Source Apportionment: The OSAT method follows VOC and NO_X emissions from each Source Group and when ozone is formed in the host PGM, OSAT estimates whether ozone formation was more VOC-limited or NO_X-limited and then allocates the ozone formed to Source Groups based on their relative contributions of the limiting precursor. The APCA ozone source apportionment technique differs from OSAT in that it recognizes that some emissions are not controllable (e.g., biogenic emissions) so focuses ozone source apportionment on controllable emissions. In the case when ozone is formed due to the interaction of biogenic VOC and anthropogenic NO_X emissions under VOC-limited conditions, a case where OSAT would assign the ozone formed to the biogenic VOC emissions, APCA redirects the ozone formed to the controllable anthropogenic NO_X emissions. Thus, in APCA the only ozone attributable to biogenic emissions is when ozone is formed due to the interaction of biogenic VOC and biogenic NO_X emissions. Ozone and PM source apportionment techniques have also been implemented in CMAQ (OPTM, PPTM and ISAM), but the version of CMAQ with source apportionment is now out-of-date and a peer review of source apportionment techniques found the implementation in CAMx to be superior to CMAQ (Arunachalam, 2009). For each Source Group, OSAT/APCA uses four reactive tracers to track its ozone contribution: the Source Group's VOC and NO_X emissions and ozone attributed to the Source Group that is formed under VOC-limited or NO_X-limited conditions (O3V and O3N).

- Particulate Source Apportionment: The CAMx PSAT particulate source apportionment method has five different families of tracers that can be invoked separately or together to track source apportionment of the following particulate species: Sulfur (SO_4), Nitrogen (NO_3/NH_4), Primary PM, Secondary Organic Aerosol (SOA) and Mercury. Because PSAT needs to track the PM source apportionment from the PM precursor emissions to the PM species, the number of tracers needed to track a Source Group's source apportionment depends on the complexity of the chemistry and number of PM species involved. The Sulfur family requires only two reactive tracer species (SO_2 and SO_4) to track the formation of particulate sulfate from SO_2 emission source contributions for each Source Group. Whereas SOA family is the most expensive PSAT family with 18 reactive tracers needed for each

Source Group in order to track the four VOC precursors (aromatics, isoprene, terpenes and sesquiterpenes) and the 7 condensable gas (CG) and SOA pairs. The five families of PSAT PM source apportionment tracers are provided below along with the definitions of the reactive tracers used in each family.

Sulfur (2 Tracers)

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

Nitrogen (7 Tracers)

- RGN_i Reactive gaseous nitrogen including primary NOx ($NO + NO_2$) emissions plus nitrate radical (NO_3), nitrous acid (HONO) and dinitrogen pentoxide (N_2O_5).
- TPN_i Gaseous peroxyl acetyl nitrate (PAN) plus peroxy nitric acid (PNA)
- NTR_i Organic nitrates (RNO_3)
- $HN3_i$ Gaseous nitric acid (HNO_3)
- $PN3_i$ Particulate nitrate ion from primary emissions plus secondarily formed nitrate
- $NH3_i$ Gaseous ammonia (NH_3)
- $PN4_i$ Particulate ammonium (NH_4)

Secondary Organic Aerosol (18 Tracers)

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

- o $PO5_i$ Particulate organic aerosol associated with CG5
- o $PO6_i$ Particulate organic aerosol associated with CG6
- o $PO7_i$ Particulate organic aerosol associated with CG7

Mercury (3 Tracers)

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

Primary Particulate Matter (6 Tracers)

- o PEC_i Primary Elemental Carbon
- o POA_i Primary Organic Aerosol
- o PFC_i Fine Crustal PM
- o PFN_i Other Fine Particulate
- o PCC_i Coarse Crustal PM
- o PCS_i Other Coarse Particulate

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

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

5.2 STATE-SPECIFIC OZONE SOURCE APPORTIONMENT MODELING APPROACH

The WestJumpAQMS state-specific ozone source apportionment modeling used the APCA ozone source apportionment tool and the 2008 36/12 km CAMx model configuration to estimate the contributions of western state's anthropogenic emissions on downwind ozone concentrations and obtain an estimate of western U.S. ozone source-receptor relationships. The attributes of the CAMx 36/12 km state-specific APCA ozone source apportionment modeling are as follows:

- CAMx Version 5.41.
- APCA ozone source apportionment method.
- 36 km CONUS and 12 km WESTUS domains using two-way grid nesting.
- Source Regions (21):
  - Grid cell definitions of 17 individual western states, offshore shipping, Mexico, Canada and remainder eastern U.S. (21 Source Regions, see Figure 5-1):
- Source Categories (5):
  - Natural emissions (biogenic, lightning, sea salt and WBD);
  - Three types of fires (wildfires, prescribed burns and agricultural burning); and
  - Remainder anthropogenic emissions.
- Source Groups (107):
  - With 21 Source Regions and 5 Source Categories that results in 107 total Source Groups (=21 x 5 +2; 2 extra Source Groups for IC and BC) for which separate ozone contributions were obtained.
- Several procedures were used for post-processing the state-specific APCA ozone source apportionment modeling results to obtain:
  - Contributions of upwind state's anthropogenic emissions to 8-hour ozone Design Values in downwind states using the same procedures as used in the Cross State Air Pollution Rule (CSAPR);
  - Contributions to the ten highest modeled daily maximum 8-hour ozone concentrations at each monitoring site in the 12 km WESTUS modeling domain.
  - Spatial distribution of the contributions of state's anthropogenic emissions to the highest and fourth highest daily maximum 8-hour ozone concentrations greater or equal to 76 ppb (current NAAQS), 70, 65 and 60 ppb (range of possible future NAAQS) and 0 ppb (contributions everywhere).

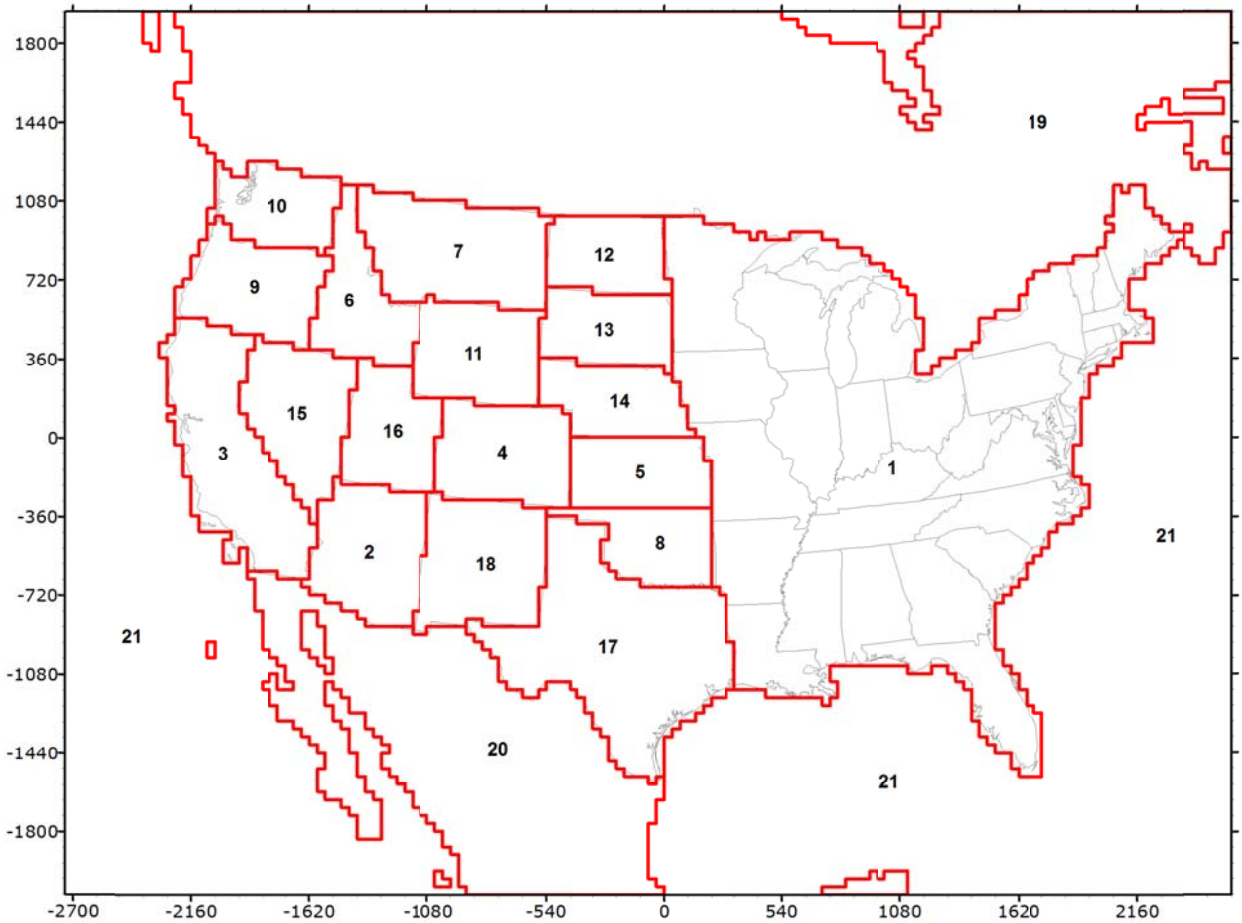


Figure 5-1. Source Regions used in the State-Specific APCA ozone and PSAT particulate matter 2008 source apportionment modeling for WestJumpAQMS.

5.3 CSAPR-TYPE POST-PROCESSING OF STATE-SPECIFIC OZONE SOURCE APPORTIONMENT RESULTS

EPA's procedures for projecting 8-hour ozone Design Values (EPA, 2007) that use the modeling results in a relative fashion were used to estimate an upwind state's anthropogenic emissions contribution to Design Values in a downwind state. These procedures use the modeling results in a relative fashion to scale a current year Design Value (DVC) to estimate a future year Design Value (DVF). The model derived scaling factors are called Relative Response Factors (RRFs) and are the ratio of future year to current year daily maximum 8-hour ozone modeling results near a monitor [DVF = DVC x RFF]. EPA has codified the recommended Design Value projection approach in the Modeled Attainment Test Software (MATS[79]) that was used in this study to calculate an upwind state's anthropogenic emissions contribution to downwind ozone nonattainment.

79 http://www.epa.gov/ttn/scram/modelingapps_mats.htm

MATS is generally applied using photochemical grid model output modeling results for a current year base case and a future year emission scenario to estimate ozone Design Values in the future year. However, in this application MATS was applied using the CAMx 2008 36/12 km base case modeling results and the CAMx base case modeling results with the ozone contributions from the APCA ozone source apportionment removed separately for each of the 17 state's anthropogenic emissions Source Groups. The difference in the base year Design Value (DVC) and the projected Design Value with the contributions of the state's anthropogenic emissions removed (i.e., the MATS future year DVF projection) is the state's contribution to current year Design Values (i.e., contribution to downwind ozone nonattainment). Specifics on the definitions of the MATS runs are as follows:

- State's anthropogenic emissions were defined as the usual anthropogenic emissions within a state's boundaries (Figure 5-1) plus prescribed burns and agricultural burning (i.e., planned fires).
- As was done in CSAPR, ozone projections were made starting with an average and maximum current year DVC (AvgDVC and MaxDVC) where the AvgDVC was the MATS default DVC that is based in an average of ozone Design Values over five years centered on the modeling year (i.e., average of Design Values from 2006-2008, 2007-2009 and 2008-2010) and the MaxDVC was defined as the maximum Design Value from the same five year period.
- Mostly default MATS projection parameters were specified that include:
    - For RRFs selected maximum 8-hour ozone concentrations within 3 x 3 array of 12 km grid cells centered on monitoring site.
    - Try to use at least 10 modeling days in constructing the RRFs:
        - Select modeling days with modeled 8-hour ozone concentrations above an 85 ppb threshold.
        - If don't obtain at least 10 days, reduce the threshold by 1 ppb until a 70 ppb floor is achieved.
        - If at the 70 ppb floor there are more than 5 days accept the RRF.
            - Note that we had to reduce this 5 day minimum requirement in some cases in the lowest ozone areas in the western states.

5.3.1 CSAPR-Type Ozone Modeling Results Under the Current Ozone NAAQS

In CSAPR, EPA defined a upwind state as having a significant contribution to nonattainment in downwind state if the contribution of its anthropogenic emissions to a downwind state's average Design Value (AvgDV) that was over the NAAQS was greater than or equal to one percent (1%) of the NAAQS. If an upwind state had over a 1% contribution to a maximum Design Value (MaxDV) that was over the NAAQS in a downwind state, but not for the AvgDV, then EPA determined that the upwind state was interfering with maintenance of the NAAQS. We applied the EPA CSAPR-type analysis to our CAMx 2008 36/12 km State-Specific ozone source apportionment modeling results to see which upwind states would have a significant contribution to ozone nonattainment in a downwind state using EPA's CSAPR definition of significance. Before presenting these results, there are several important differences and caveats related to our WestJumpAQMS CSAPR-type analysis of the CAMx 2008 state-specific source apportionment modeling results versus what EPA did in CSAPR:

- WestJumpAQMS included planned fires (Rx and Ag) in a state's anthropogenic emissions, in addition to traditional anthropogenic emissions.

- EPA's CSAPR analysis examined a state's contribution to downwind nonattainment for a future year (2012) for the purpose of imposing state-specific controls to reduce a state's significant ozone contribution and assist a downwind state in achieving the ozone NAAQS in the future.
    - WestJumpAQMS is examining an upwind state's contribution to ozone in a downwind state for an historical year (2008) for the purpose of having a better understanding of western U.S. ozone source-receptor relationships.
- EPA's CSAPR addressed attainment of the 1997 0.08 ppm 8-hour ozone NAAQS, whereas WestJumpAQMS examined contributions using the current (March 2008) 0.075 ppm (76 ppb) ozone NAAQS, as well as contributions under potential new (60-70 ppb) ozone NAAQS.

It is important to emphasize that the WestJumpAQMS CSAPR-type analysis is not tied to any rulemaking or regulatory decision making and is purely trying to generate more information on ozone source receptor relationships for the western states. In fact, because WestJumpAQMS only looked at a past year emissions scenario (2008), the results could not be used for any regulatory control actions.

Table 5-1 list upwind state contributions to downwind state nonattainment for the 17 western states (see Figure 5-1) under the current NAAQS (76 ppb) using the 2008 CAMx modeling results. Under the current NAAQS, the CSAPR-type analysis would implicate a state as having a significant contribution to or interfering with nonattainment in a downwind state if its contribution to the, respectively, AvgDV or MaxDV, was 0.76 ppb (1% of the NAAQS) or greater. Listed in Table 5-1a is the maximum contribution of an upwind state to the AvgDV in a downwind state when the AvgDV is 76 ppb or greater and the number of monitoring sites that the upwind state had a contribution of 1% or greater of the NAAQS in a downwind state when the AvgDV exceeds 76 ppb. Table 5-1b is the same as Table 5-1a only for the MaxDV. Of the 17 western states, five (CO, MT, ND, SD, NE) states did not have a significant contribution to a downwind state AvgDV. The largest significant contribution (17 ppb) was for California's contribution to Clark County, NV (Las Vegas). For MT and WA contributions to downwind nonattainment, care must be taken in the interpretation since it is indicating a maximum contribution to WY as the downwind state. The only AvgDV in WY that exceed the current NAAQS occur in Sublette County due to winter ozone cold pooling conditions. These are conditions of limited transport when emissions from MT and WA would likely have minimal contributions.

When using the MaxDV instead of the AvgDV there are more monitoring sites that exceed the NAAQS so there are more monitoring sites for the states to have significant contributions at. However, the same five states that did not have any significant contributions using AvgDV also did not have a significant contribution for the MaxDV. Probably the biggest difference between the AvgDV and MaxDV results is due to the introduction of the El Paso TX monitor where the AvgDV was below but MaxDV was above the NAAQS. This results in larger maximum contributions for several states using the MaxDV (e.g., AZ and NM).

Table 5-1a. Number of monitoring sites and maximum ozone contribution of an upwind state to average ozone Design Value (AvgDV)s in a downwind state.

Upwind State	# Monitors ≥ 0.76 ppb	Maximum Contribution (ppb)	State with Maximum	AvgDV at Site (ppb)
Arizona	23	1.15	NV	76.00
California	15	16.89	NV	76.00
Colorado	0	0.51	TX	80.00
Idaho	3	1.02	WY	78.67
Kansas	3	8.95	MO	76.00
Montana	0	0.39	WY	78.67
North Dakota	0	0.12	TX	77.67
Nebraska	0	0.28	MO	76.33
New Mexico	1	0.82	AZ	77.33
Nevada	20	1.28	CA	101.00
Oklahoma	18	6.52	MO	76.00
Oregon	26	1.13	CA	92.67
South Dakota	0	0.13	MO	76.33
Texas	4	11.55	OK	76.00
Utah	5	2.53	CO	82.0
Washington	1	1.03	WY	78.67
Wyoming	5	1.53	CO	78.00

Table 5-1b. Number of monitoring sites and maximum ozone contribution of an upwind state to maximum ozone Design Value (MaxDV)s in a downwind state.

Upwind State	# Monitors ≥ 0.76 ppb	Maximum Contribution (ppb)	State with Maximum	MaxDV at Site (ppb)
Arizona	34	3.46	TX	77.00
California	42	17.33	NV	78.00
Colorado	0	0.59	TX	77.00
Idaho	4	1.04	WY	80.00
Kansas	5	9.31	MO	79.00
Montana	0	0.39	WY	80.00
North Dakota	0	0.13	TX	81.00
Nebraska	0	0.39	MO	81.00
New Mexico	10	2.81	TX	77.0
Nevada	31	1.34	CA	81.00
Oklahoma	25	6.78	MO	79.00
Oregon	38	1.31	CA	76.00
South Dakota	0	0.14	MO	81.00
Texas	14	12.56	OK	76.00
Utah	9	2.66	CO	86.00
Washington	1	1.05	WY	80.00
Wyoming	9	1.61	CO	82.00

Appendix A is an interactive Excel spreadsheet that allows the examination of upwind state's contributions to nonattainment at up to five downwind states under various alternative NAAQS levels. Figure 5-2 shows example bar chart plots of state contributions under the current NAAQS for NM, NV and CA with the left panels showing the state contributions and the right panels displaying the AvgDV and MaxDV at the downwind monitoring sites. Under the current NAAQS, NM has a significant contribution to three downwind states: TX, AZ and CO. Note that the NM contribution to TX (2.81 ppb) is significant under the MaxDV (77.0 ppb) that is above the NAAQS but not significant under the AvgDV (73.67 ppb) because it is below the NAAQS. In CSAPR this condition would be known as interfering with the maintenance of the NAAQS. Under the current NAAQS, Nevada has a significant contribution to four downwind states (CA, UT, AZ and CO) with the largest contribution to a DV being 1.3 ppb at a site in Inyo County, CA. CA has a significant contribution to many downwind states (five listed in Figure 5-2) with the largest contribution of 17 ppb to Clark County (Las Vegas) NV. In fact, the CA contribution to Clark County is the largest seen in the modeling results. The CA significant contribution extends far downwind to El Paso TX (1.2 ppb) and Denver, CO (1.9 ppb). Under the current NAAQS, UT has a significant contribution to one downwind state (CO) with a maximum contribution of 2.5 ppb to the Rocky Flats North monitoring site in the Denver nonattainment area that has an 82 and 86 ppb AvgDV and MaxDV, respectively.

5.3.2 CSAPR-Type Ozone Modeling Results Under Alternative Ozone NAAQS

The Appendix A interactive spreadsheet also allows the user to perform CSAPR-type analysis using alternative levels of the NAAQS. Figure 5-3 displays the same information in Figure 5-2 only using a 65 ppb alternative NAAQS level. Using a lower NAAQS levels introduces many more monitoring sites that exceed the alternative NAAQS where a state can have a significant contributions to downwind nonattainment. For example, whereas using the current NAAQS there was only one state where UT had a significant contributions (CO), under the 65 ppb alternative NAAQS there are four states (CO, WY, AZ and NM). Of the five states that did not have a significant contributions under the current NAAQS, four would have a significant contributions under the 65 ppb alternative NAAQS with only South Dakota still not having a significant contribution.

Figure 5-2. CSAPR-type significant ozone contributions of upwind states to up to five downwind states under the current 0.075 ppb ozone NAAQS for NM, NV, CA and UT (from Appendix A).

Figure 5-3. CSAPR-type significant ozone contributions of upwind states to up to five downwind states under an alternative 65 ppb ozone NAAQS for NM, NV, CA and UT (from Appendix A).

5.4 OZONE CONTRIBUTIONS ON TEN HIGHEST MODELED OZONE DAYS

Appendix B is an interactive spreadsheet that displays ozone contributions to DMAX8 ozone on the ten highest modeled ozone days at every site in the U.S. using absolute modeling results from the CAMx 36/12 km state-specific ozone source apportionment simulation. There are drop down menus in cells B1 through B4 where the user must selects the data in the following order: (B1) State; (B2) County in State; (B3) Monitoring Site in County; and (B4) one of the 10 highest modeled DMAX8 ozone days.

Figure 5-4 displays ozone contributions for the six highest modeled DMAX8 ozone days at the Mesa Verde monitoring site in Colorado obtained from the Appendix B spreadsheet. The highest modeled ozone day at Mesa Verde (Figure 5-4, top left) was June 13, 2008 with a DMAX8 ozone value of 80.6 ppb of which 88% (71.2 ppb) is due to boundary conditions (BCs, i.e., the concentrations around the boundaries of the 36 km CONUS domain from the MOZART Global Chemistry Model). The pie chart displays the ozone contributions due to emissions within the 36/12 km domain separately for natural and three types of fires source categories and for the anthropogenic emissions by geographic region, including the 17 western states that makes up the non-BC portion of the modeled DMAX8 ozone (i.e., the remaining 9.4 ppb or 12% of the ozone on this day). On this day natural emissions (i.e., ozone due to biogenic and lightning from all source regions) and anthropogenic emission from Utah are the largest contributors.

On the second highest modeled ozone day at Mesa Verde (76.3 ppb on August 1, 2008; Figure 5-4, top right), BCs only contribute half of the DMAX8 ozone with anthropogenic emissions from New Mexico (20 ppb/26%) contributing about half of the remaining ozone not due to BCs. The third highest ozone day (74.9 ppb on July 9, 2008) has 82% of the modeled ozone due to BCs with Colorado contributing about half (5.7 ppb/7.6%) of the remaining non-BC ozone. BCs dominate (93%) the modeled DMAX8 ozone on the fourth highest ozone day at Mesa Verde (73.8 ppb on May 10, 2008) indicating that this is likely a modeled stratospheric ozone intrusion event. The 5th and 6th highest ozone days at Mesa Verde (72-73 ppb on May 2-3, 2008) are similar with BCs contributing most of the ozone (82-85%) and the remainder of the ozone coming from many different sources (Figure 5-4, bottom). Again, since this is a spring day with high BC ozone contribution, modeled stratospheric ozone contributions are likely contributing.

Results for other monitoring sites can be obtained using the Appendix B spreadsheet.

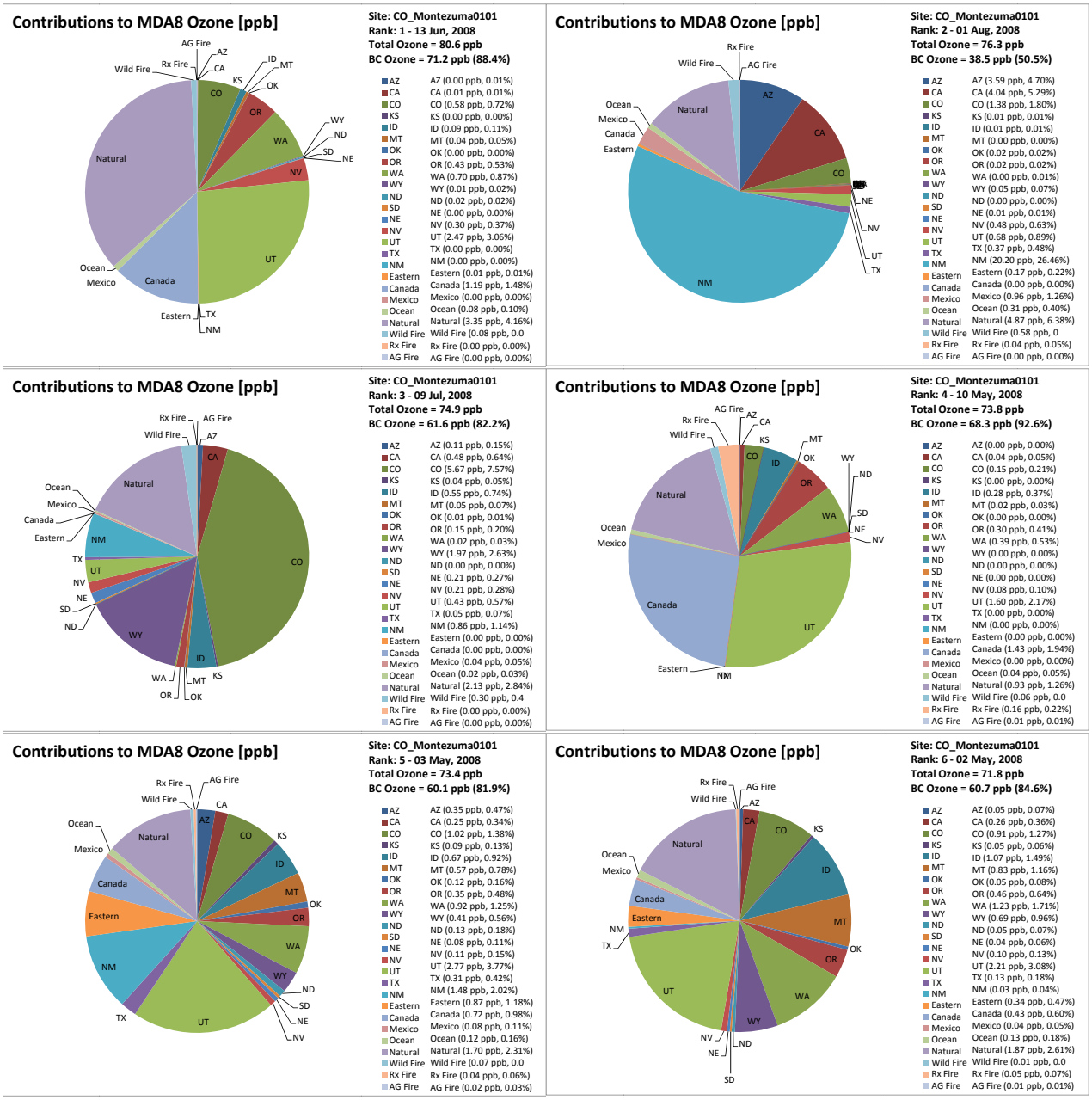


Figure 5-4. State-specific contributions to ten highest modeled daily maximum 8-hour ozone concentration days at Site 0101 in Montezuma County, Colorado (Mesa Verde National Park) using the absolute modeling results (from Appendix B).

5.5 SPATIAL DISTRIBUTION OF STATE OZONE CONTRIBUTIONS MODELING RESULTS

Appendix C contains spatial maps of the contributions of state anthropogenic emissions (defined as traditional anthropogenic emissions plus Rx and Ag fires) to the highest (1stmax) and fourth highest (4thmax) modeled DMAX8 ozone on days when the total DMAX8 ozone is greater than five thresholds: 76, 70, 65, 60 and 0 ppb. The 4thmax DMAX8 ozone corresponds to the form of the ozone NAAQS (three year average of 4thmax DMAX8 ozone) and 76 ppb corresponds to the current NAAQS, whereas 70, 65 and 60 ppb represent possible future NAAQS levels and the 0 ppb threshold will give contributions throughout the domain

Figure 5-5 displays the New Mexico state-specific spatial maps for the 4thmax DMAX8 ozone and the 0, 65, 70 and 76 ppb ozone thresholds that were obtained from Appendix C. The New Mexico contribution footprint to the 4thmax DMAX8 ozone in excess of 1 ppb extends out approximately one and a half states when the 0 ppb total ozone threshold is used (Figure 5-5, top left). Using the 60 ppb threshold, the New Mexico ozone footprint is similar to the 0 ppb threshold with only portions of Kansas and Nebraska dropping out; the grey areas in Figure 5-5 are areas where the modeled ozone is above the threshold but the New Mexico contribution is less than 1 ppb, whereas the clear areas are portions when the modeled DMAX8 ozone never gets above the threshold. Using the 70 and 76 ppb thresholds (Figure 5-5, bottom) there are less areas with modeled values above the threshold thereby limiting the New Mexico ozone footprint.

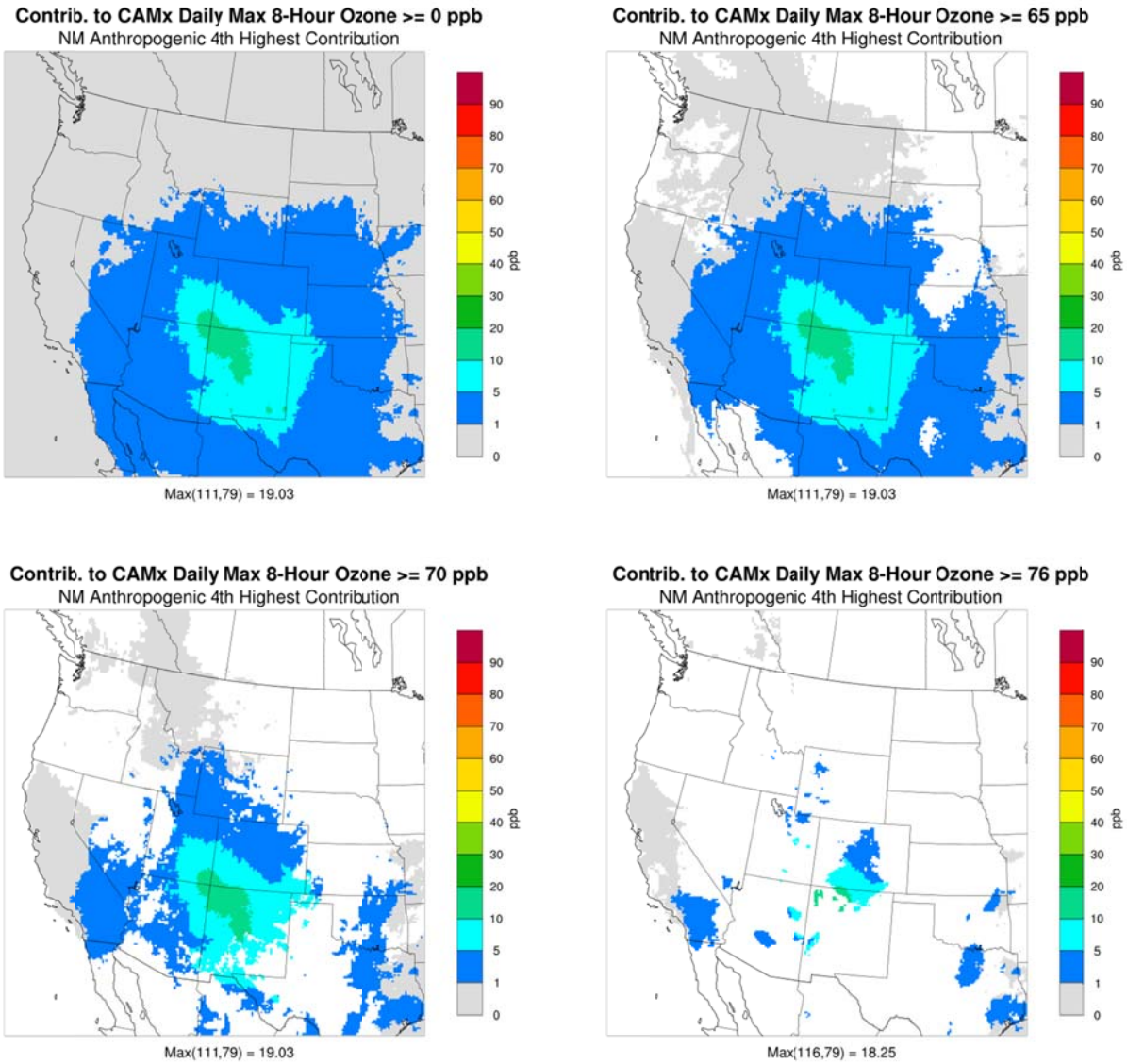


Figure 5-5. New Mexico state-specific 4thmax DMAX8 ozone contributions using 0, 65, 70 and 76 ozone thresholds (from Appendix C).

5.6 SPATIAL DISTRIBUTION OF SOURCE CATEGORY OZONE CONTRIBUTION MODELING RESULTS

Although the focus of the state-specific ozone source apportionment modeling was on state contributions to downwind ozone concentrations, it was performed so that we could also obtain the ozone contributions for several source categories:

- Natural emissions (biogenic, lightning, sea salt and windblown dust)
- Anthropogenic emissions (with and without Rx and Ag fires)
- Three types of fires (WF, Rx and Ag)
- Boundary Conditions: (BCs; i.e. contributions from international transport and stratospheric ozone that come into the 36 km CONUS domain through the day-specific BCs obtained from the MOZART GCM).

As was done for the state ozone footprint spatial maps, spatial maps of the contributions of the six source categories given above were generated for the highest (1stmax) and fourth highest (4thmax) daily maximum 8-hour ozone concentrations that were filtered by five thresholds of total ozone concentrations (76, 70, 65, 60 and 0 ppb). Spatial maps were made for both the 12 km WESTUS and 36 km CONUS domains. Note that the 1stmax and 4thmax DMAX8 ozone concentrations in each grid cell may occur on different days.

Figure 5-6 displays the source category contributions to the fourth highest DMAX8 ozone across the entire 12 km WESTUS domain (i.e., using a 0 ppb filter). As expected, the highest ozone contributions due to anthropogenic emissions (without Rx and Ag) occurs over the major urban areas, such as Los Angeles, San Francisco, Seattle, Houston, Dallas-Fort Worth and Phoenix where ozone contributions can exceed 40 ppb and a maximum contribution of 78 ppb occurs (Figure 5-6, top left). The contributions of natural emissions tends to range from 1 to 12 ppb over the western U.S. with the highest contributions occurring over KS and NE (Figure 5-6, top right). Recall that the state-specific ozone source apportionment modeling used the APCA version of the CAMx Ozone Source Apportionment technology (OSAT) probing tool that only allocates ozone formed to natural emissions when it is due to reactions between natural VOC and natural NO_X. In the case where ozone is formed due to reactions between biogenic VOC and anthropogenic NO_X under VOC-limited ozone formation conditions, a case that OSAT would assign to the biogenic emissions, APCA assigns to the anthropogenic NO_X recognizing that biogenic emissions are not controllable. The higher natural ozone over KS and NE is due to the higher biogenic NO_X emissions in this region.

BCs have widespread high contributions to ozone across the western U.S. ranging from 40 to 78 ppb (Figure 5-6, middle left). The highest contributions generally occur over higher terrain, where stratospheric ozone contributions are more common. 2008 was an intense wildfire year in northern California, which is reflected in the WF ozone contributions that can exceed 63 ppb (Figure 5-6, middle right). Away from northern California and its downwind influence, ozone due to WFs contributes 1-5 ppb to the fourth highest DMAX8 ozone in the western U.S. The contributions of Rx and Ag fires to ozone are smaller with maximum values of, respectively, 8 and 3 ppb. Relatively higher contributions of ozone due to Rx fires are seen in AZ-NM and WA-OR-ID-MT. Whereas higher ozone due to Ag burning is seen in KS due to the April Flint Hills burns and up in Alberta.

Figure 5-7 shows the same information as Figure 5-6 only for the 36 km CONUS domain. Anthropogenic emissions have a much more widespread and higher contribution in the eastern than western U.S. The natural emissions ozone contribution ranges from 1 to 12 ppb with the highest values occurring over NE where biogenic NO_X is greatest due to fertilizer application (e.g., corn). Boundary condition contribution is

widespread and ranges from 40 to 80 ppb and is highest over high terrain and in the Gulf of Mexico that is due to stratospheric ozone intrusion from tropospheric folding, which impacts high terrain features more, and large convective cells (e.g., AZ-NM) and the Gulf of Mexico and vicinity. In addition to high ozone due to the northern California WFs, high ozone is also seen in and off-shore of South Carolina due to the Evans Road fire in the Pocosin Lakes NWR in SC. The effects of prescribed burns in the southeast on ozone are also seen in Figure 5-7 (bottom left).

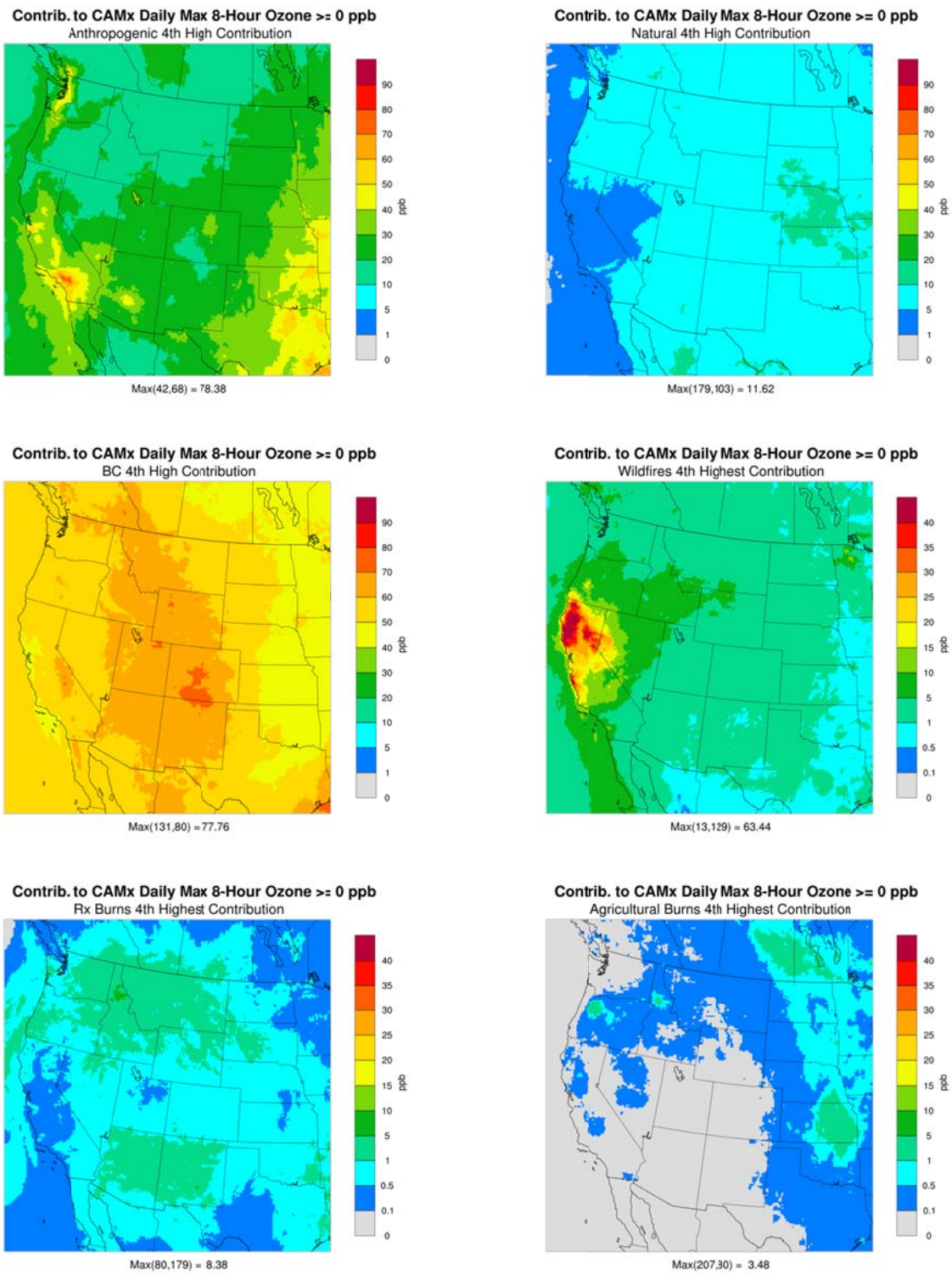


Figure 5-6. Source category contributions to fourth highest DMAX8 ozone (ppb) in the 12 km WESTUS domain.

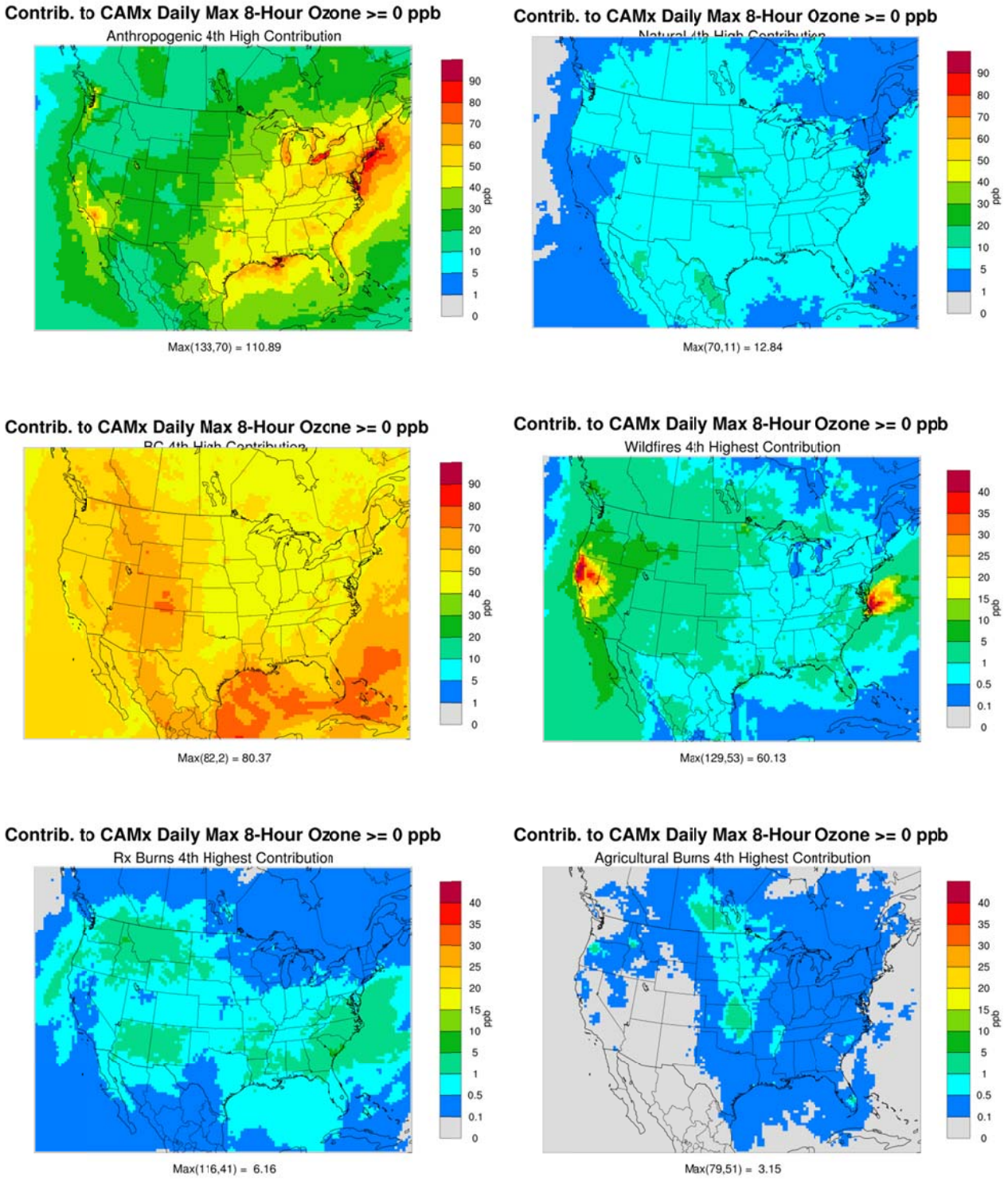


Figure 5-7. Source category contributions to fourth highest DMAX8 ozone (ppb) in the 36 km CONUS domain.

6.0 STATE-SPECIFIC PM SOURCE APPORTIONMENT MODELING

The State-Specific Particulate Matter (PM) source apportionment modeling used the exact same source apportionment configuration (21 Source Regions and 5 Source Categories, see Figure 5-1) as in the State-Specific ozone source apportionment modeling, only using the Particulate Source Apportionment Technology (PSAT) source apportionment tool Probing Tool that was described in Section 5.1. The State-Specific PSAT PM source apportionment used the Sulfate, Nitrogen and Primary PM PSAT source apportionment families of reactive tracers. Thus, the PM contributions of each Source Group were tracked using 15 extra reactive tracers, this compares to only 4 additional reactive tracers needed for each Source Group for the ozone source apportionment run. With 107 Source Groups, this means that the state-specific PM source apportionment simulation is adding 1,605 additional transported species to the CAMx simulation. The standard CAMx simulation with no source apportionment uses 73 transported species. Thus, the PM source apportionment run used ~23 times more transported species than a standard model simulation. This results in large computational requirements. In order to keep the WestJumpAQMS schedule, the state-specific PM source apportionment run was just run on the 36 km CONUS domain for the 2008 calendar year (with spin up days).

The PSAT SOA family of reactive tracers was not used in the state-specific PM source apportionment run. Although SOA can be an important component of $PM_{2.5}$, especially in the summer, we have found that a majority of the SOA in current version of CAMx is due to biogenic sources. SOA chemistry is fairly complex and in order to track source apportionment the PSAT algorithms requires 18 species to track SOA contributions for each Source Group, which is more than the 15 reactive species needed to track the SO4, NO3/NH3 and primary PM families of tracers combined. Given that the additional computational requirements of the SOA family of tracers and its small contribution to total $PM_{2.5}$ mass, we elected not to track state-specific SOA PM contributions. However, the standard CAMx model output have SOA as separate species so when looking at absolute model $PM_{2.5}$ predictions we can display the SOA contributions and see whether it is significant or not.

6.1 CSAPR-TYPE POST-PROCESSING OF STATE-SPECIFIC PM SOURCE APPORTIONMENT RESULTS

The State-Specific PM source apportionment modeling results were processed with MATS to obtain the contributions of upwind state anthropogenic emissions (including Rx and Ag fires) to annual and 24-hour $PM_{2.5}$ Design Values at monitoring sites in downwind states. MATS was run using current year $PM_{2.5}$ Design Values (DVC), 2008 base case modeling results and 2008 base case with a state's anthropogenic emissions contribution to PM concentrations removed to obtain a "future year" Design Value (DVF). A state's contribution to the $PM_{2.5}$ DVC was defined as the difference in the current year and "future year" Design Values (DVC – DVF). The state-specific PM source apportionment modeling results were only processed for the average current year Design Value (AvgDV) as the extra work in processing the MaxDV in the state-specific ozone analysis did not provide much additional information given the amount of additional work.

6.1.1 CSAPR-TYPE ANNUAL $PM_{2.5}$ RESULTS UNDER THE CURRENT $PM_{2.5}$ NAAQS

Table 6-1 lists the number of downwind monitoring sites with DVCs that exceed the current annual $PM_{2.5}$ NAAQS in downwind states that an upwind state has a contribution greater than or equal to 1% of the NAAQS for each of the 17 western states. Of the 17 states, 7 do not have a significant contribution to a downwind state's monitoring site for annual $PM_{2.5}$. Of the WRAP states that do contribute more than 1% of the NAAQS at a monitoring site that exceeds the annual NAAQS, there is only one downwind state

monitoring site where it occurs. This is because outside of California, there are very few current year annual $PM_{2.5}$ DVCs in the WRAP region that exceed the NAAQS, just one in Santa Cruz County AZ (12.88 µg/m^3) and another in Lincoln County, MT (12.52 µg/m^3). There are many more monitoring sites in the eastern U.S. whose DVC exceeds the current NAAQS resulting in more significant contributions for some of the 17 western states that are farthest east (e.g., TX, OK, KS and NE).

Table 6-1. Number of monitoring sites and maximum annual $PM_{2.5}$ contribution of an upwind state to an average annual $PM_{2.5}$ Design Value (AvgDV) in a downwind state.

Upwind State	# Monitors ≥ 0.12 (µg/m^3)	Maximum Contribution (µg/m^3)	State with Maximum	AvgDV at Site (µg/m^3)
Arizona	0	0.08	CA	15.05
California	1	0.24	AZ	12.88
Colorado	0	0.02	AZ	12.88
Idaho	1	2.56	MT	12.52
Kansas	17	0.18	IA	12.98
Montana	0	0.05	IA	12.98
North Dakota	1	0.12	IA	12.98
Nebraska	2	0.15	IA	12.98
New Mexico	1	0.12	AZ	12.88
Nevada	0	0.09	CA	12.43
Oklahoma	2	0.19	AR	12.21
Oregon	1	0.38	MT	12.52
South Dakota	0	0.04	IA	12.98
Texas	58	0.52	AR	12.21
Utah	0	0.03	AZ	12.88
Washington	1	1.65	MT	12.52
Wyoming	0	0.04	MO	12.27

Appendix D is an interactive spreadsheet that displays the current year annual $PM_{2.5}$ DVCs and upwind state contribution above the significance threshold at up to five downwind states for a user selected upwind state and NAAQS threshold. Figure 6-1 displays bar charts generated by Appendix D under the current annual $PM_{2.5}$ NAAQS (12.0 µg/m^3) and the upwind states of CA, OR, KS and NE. As noted in Table 6-1, there is only one monitoring site in Santa Cruz County, AZ where CA has a significant contribution under the current NAAQS (Figure 6-1, top). For OR, there is also only one monitoring site (Lincoln County, MT) where it has significant contribution. On the other hand, Figure 6-1 shows five downwind states where KS has a significant contribution to annual $PM_{2.5}$ under current (2008) conditions. Note that there could be more than five downwind states with significant contributions, the Appendix D spreadsheet is designed to list up to the five downwind states with the highest significant contributions from the upwind state. The bottom panel in Figure 6-1 is for NE and shows one site in Muscatine County, IA where NE has a significant contribution. Note that for this case the scale for the DVC in the NE plot has been adjusted so that state contributions can be viewed in the DVC bar chart (Figure 6-1, bottom right) illustrated the utility of using Excel as the data viewer so that custom displays can be made rather than using a flat figure that cannot be customized.

The Appendix D interactive spreadsheet also has the capability to provide the contributions of each of the species components of the annual $PM_{2.5}$ DVC when the total $PM_{2.5}$ DVC exceeds the selected threshold (not shown).

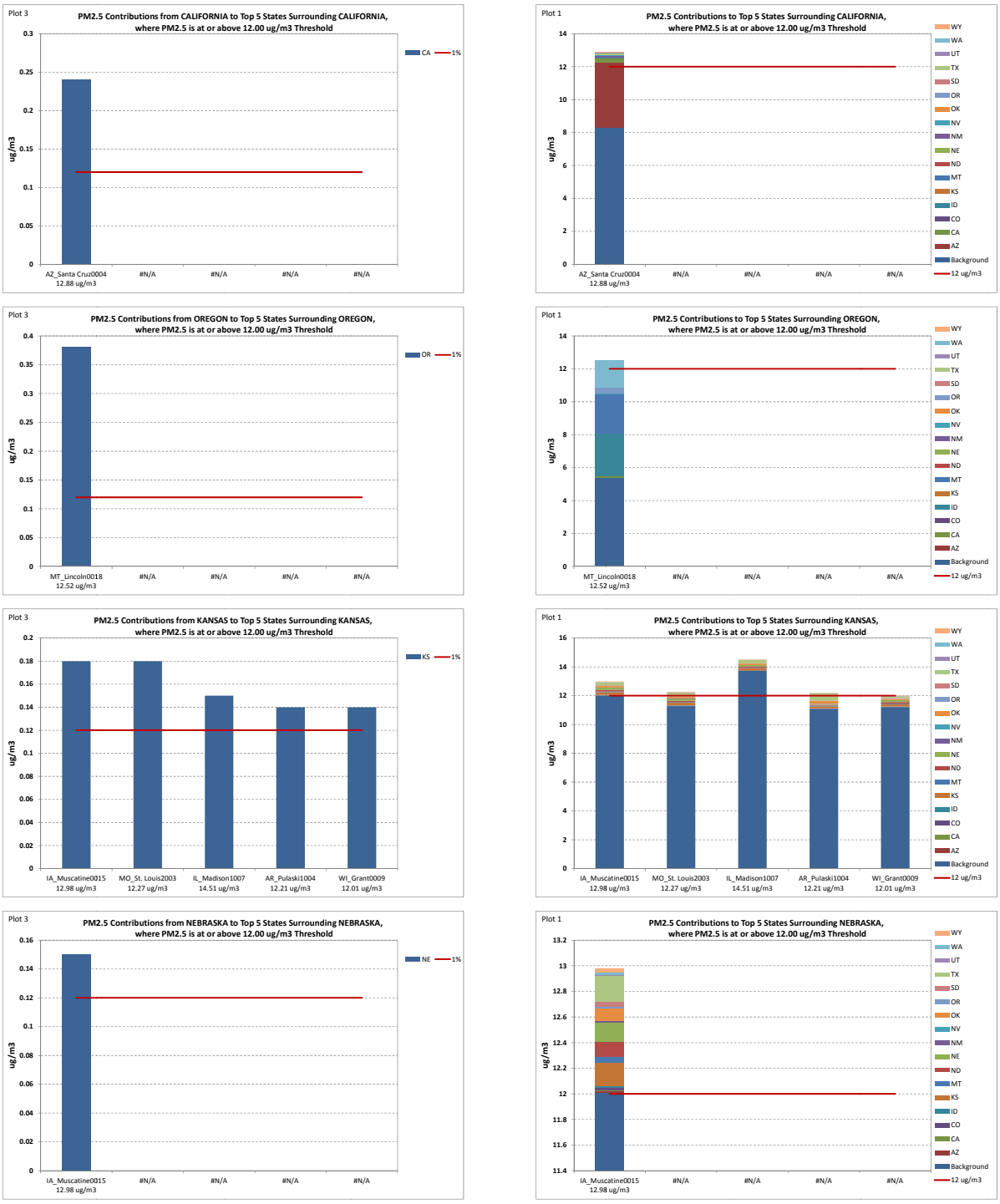


Figure 6-1. CSAPR-type significant annual $PM_{2.5}$ contributions of upwind states to up to five downwind states under the current 12.0 µg/m^3 annual $PM_{2.5}$ NAAQS for CA, OR, KS and NE (from Appendix D).

6.1.2 CSAPR-TYPE ANNUAL $PM_{2.5}$ RESULTS UNDER ALTERNATIVE NAAQS

Figure 6-2 displays the results from Appendix D for four upwind states using an alternative annual $PM_{2.5}$ NAAQS of 10 µg/m^3. It is similar to Figure 6-1, only using the lower alternative NAAQS and the states of NM and AZ are substituted for KS and NE in the bottom two sets of bar charts. Whereas CA only had contributions to one downwind state that were significant under the current NAAQS, there are four downwind states with significant contributions under the 10 µg/m^3 alternative NAAQS. Similar results are seen for OR where use of a lower NAAQS results in more downwind states where it has a significant contribution. For NM and AZ that had no significant contributions under the current annual $PM_{2.5}$ NAAQS, they would have two downwind states with significant contributions under a lower 10 µg/m^3 annual $PM_{2.5}$ NAAQS.

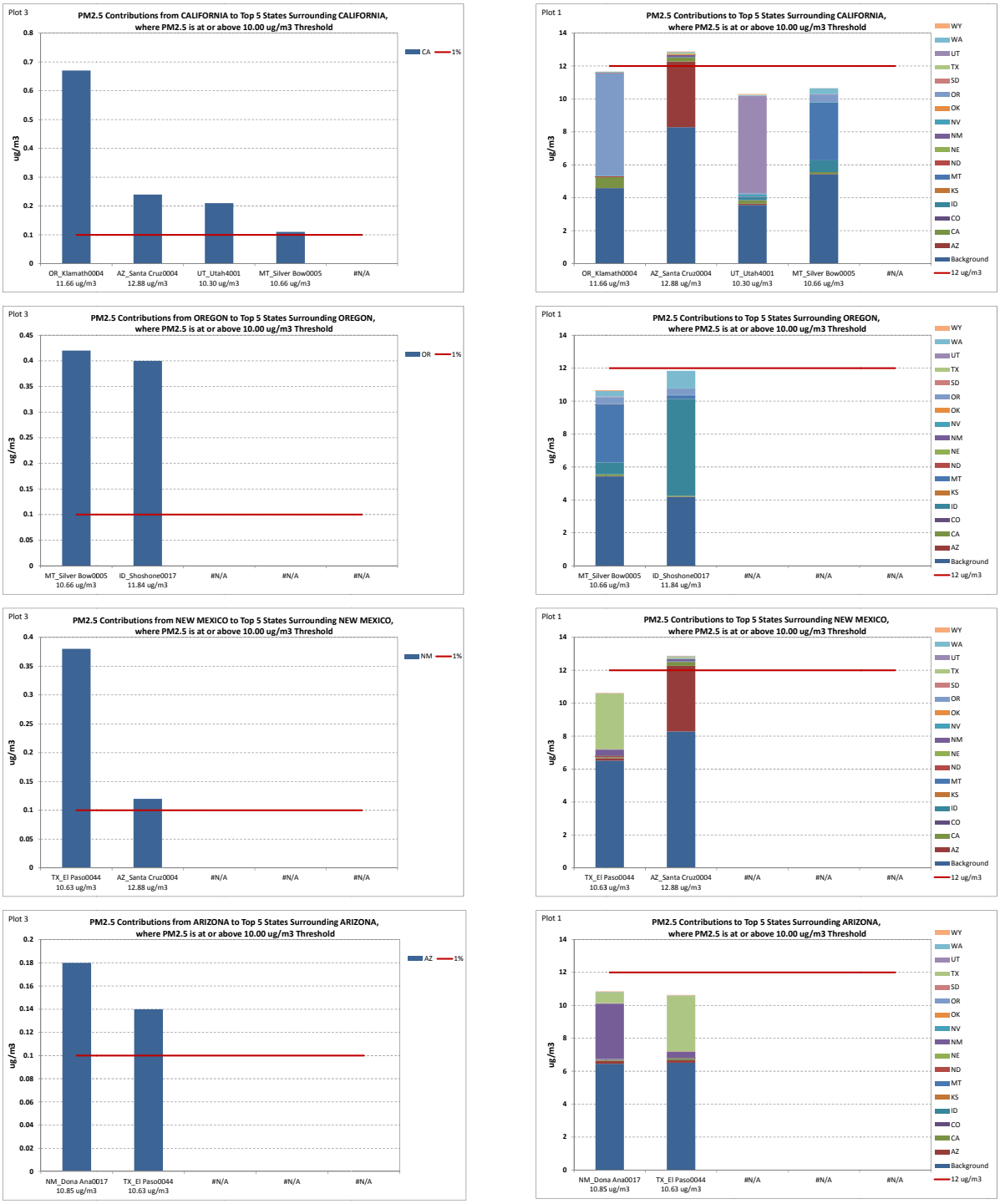


Figure 6-2. CSAPR-type significant annual $PM_{2.5}$ contributions of upwind states to up to five downwind states under an alternative 10.0 µg/m^3 annual $PM_{2.5}$ NAAQS for CA, OR, NM and AZ (from Appendix D).

6.1.3 CSAPR-TYPE 24-HOUR $PM_{2.5}$ RESULTS UNDER THE CURRENT $PM_{2.5}$ NAAQS

Table 6-2 summarizes the CSAPR-type analysis of the 2008 PM source apportionment modeling results for 24-hour $PM_{2.5}$ NAAQS (35 µg/m^3). Of the 17 western states, 5 do not have a significant contribution under the current 24-hour $PM_{2.5}$ NAAQS (CO, MT, ND, SD and WA). ID (12 sites) and CA (11 sites) have the most significant contributions to monitoring sites in downwind states and UT had the largest significant contribution (31.6 µg/m^3) to a site in a downwind state (ID).

Appendix F is an interactive spreadsheet that can display the 24-hour $PM_{2.5}$ DVCs and significant contributions for a user selected upwind state and NAAQS level. Figure 6-3 displays results from Appendix F for the upwind states of CA, ID, UT and WY and the current NAAQS. CA has significant contributions to 24-hour $PM_{2.5}$ DVCs at sites in five downwind states (OR, NV, AZ, UT and MT). ID has contributions to sites in MT, UT, OR and WA. The MT large 31.6 µg/m^3 contribution is to a site in Franklin County, ID that is within the Cache Valley that straddles the UT-ID state line. WY contributes significantly to sites in ID and UT.

Table 6-2. Number of monitoring sites and maximum 24-hour $PM_{2.5}$ contribution of an upwind state to average 24-hour $PM_{2.5}$ Design Value (AvgDV)s in a downwind state.

Upwind State	# Monitors ≥ 0.35 (µg/m^3)	Maximum Contribution (µg/m^3)	State with Maximum	AvgDV at Site (µg/m^3)
Arizona	7	2.00	CA	36.1
California	11	3.00	OR	46.0
Colorado	0	0.10	WI	36.3
Idaho	12	3.80	UT	39.5
Kansas	2	1.20	IA	36.4
Montana	0	0.20	IA	36.4
North Dakota	0	0.20	IA	36.4
Nebraska	2	0.80	IA	36.4
New Mexico	1	0.70	CA	36.1
Nevada	5	0.60	CA	41.6
Oklahoma	1	0.40	IA	36.4
Oregon	5	2.30	WA	42.5
South Dakota	0	0.10	WA	37.2
Texas	1	0.40	IA	36.4
Utah	1	31.6	ID	45.6
Washington	0	0.3	UT	40.4
Wyoming	5	1.50	ID	45.6

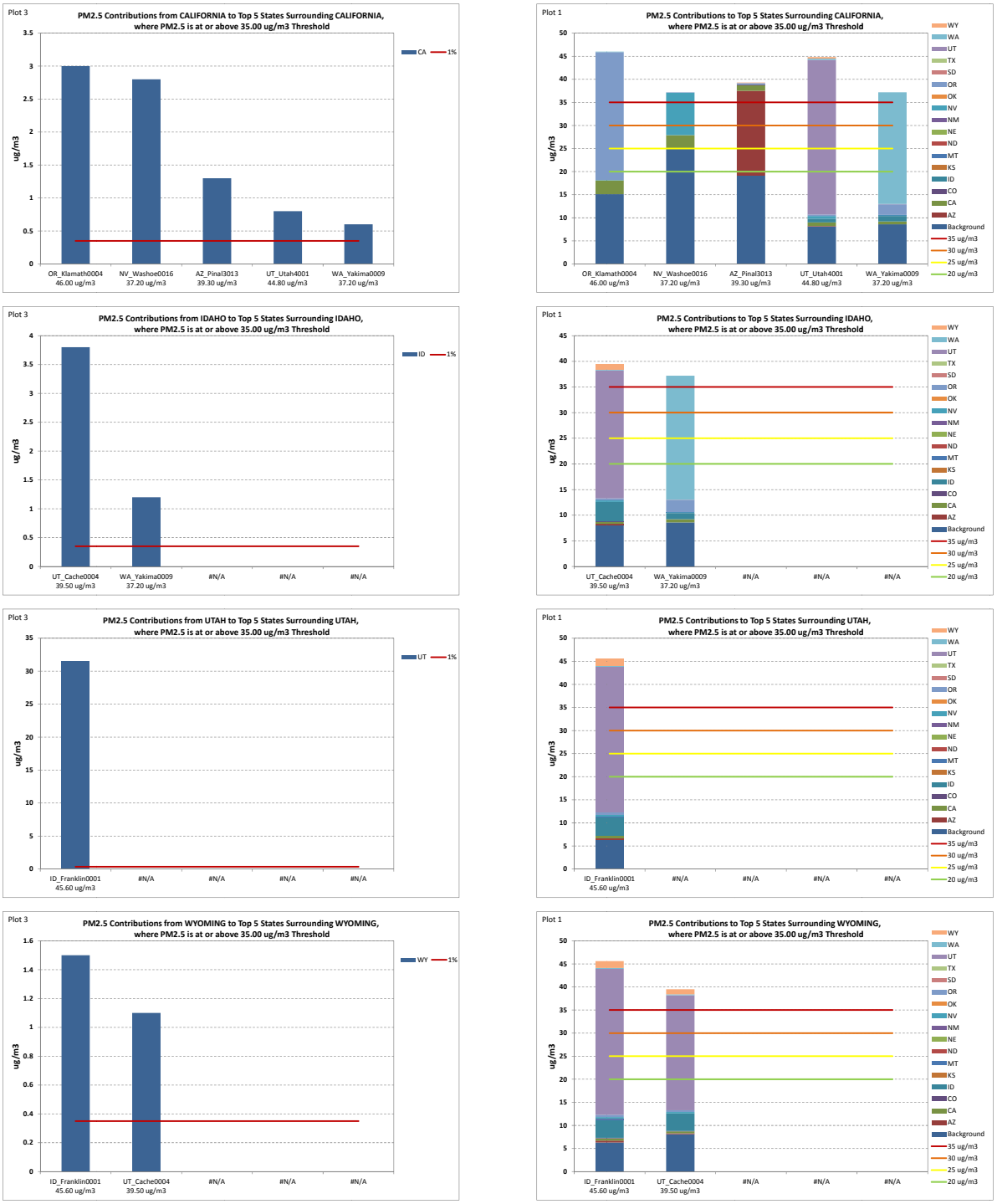


Figure 6-3. CSAPR-type significant 24-hour $PM_{2.5}$ contributions of upwind states to up to five downwind states under the current 35.0 µg/m^3 24-hour $PM_{2.5}$ NAAQS for CA, ID, UT and WY (from Appendix F).

6.1.4 CSAPR-TYPE 24-HOUR $PM_{2.5}$ RESULTS UNDER ALTERNATIVE NAAQS

An additional analysis was performed using the Appendix F spreadsheet for the same four upwind states as in Figure 6-3 only for a lower 30.0 µg/m^3 alternative 24-hour $PM_{2.5}$ NAAQS whose results are shown in Figure 6-4. At the lower NAAQS levels the results for CA are nearly identical as the current NAAQS with the same top four downwind state contribution monitoring sites (the fifth highest downwind state contribution for CA switches from WA to MT under the lower alternative NAAQS). The number of downwind states with contributions doubles from two to four for ID under the alternative NAAQS. MT adds two more states (CO and MT) under the lower NAAQS level to go with ID. There is no change in the state contributions for WY when lowering the NAAQS level.

Note that Appendix F also has the capability to provide contributions of each component species of 24-hour $PM_{2.5}$ to DVCs above the selected threshold and upwind state contributions (not shown).

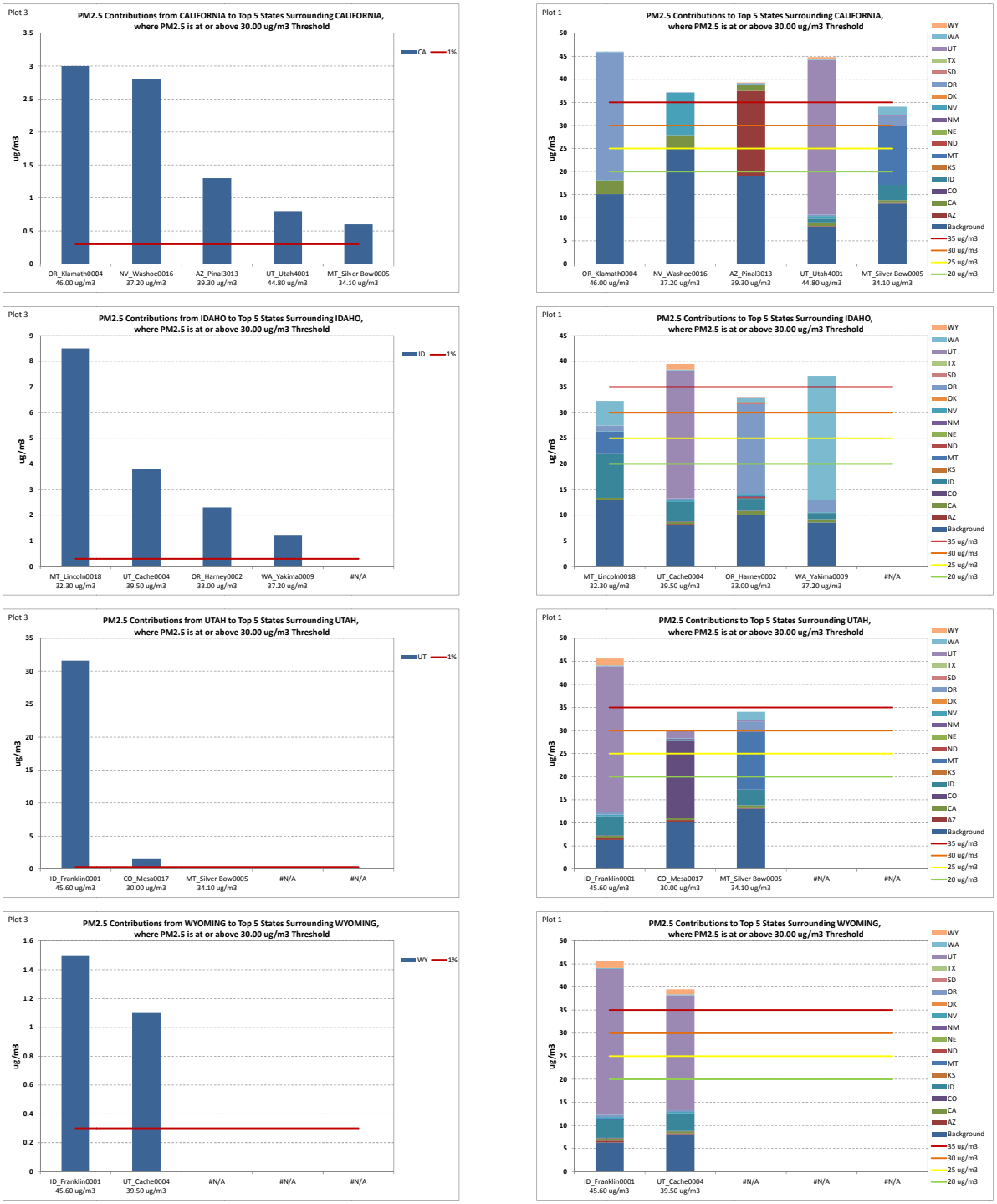


Figure 6-4. CSAPR-type significant 24-hour $PM_{2.5}$ contributions of upwind states to up to five downwind states under an alternative 30.0 µg/m^3 24-hour $PM_{2.5}$ NAAQS for CA, ID, UT and WY (from Appendix F).

6.2 MODELED STATE-SPECIFIC $PM_{2.5}$ CONTRIBUTIONS

In this section we analyze the contributions of the 17 western states to annual and 24-hour $PM_{2.5}$ concentrations using the absolute modeling results.

6.2.1 Modeled Contributions to Annual $PM_{2.5}$ Concentrations

Appendix E is an interactive spreadsheet that displays pie charts of the contributions of the 17 western states by source category to annual $PM_{2.5}$ concentrations at each monitoring site in the 36 km CONUS domain. Although the displays for the eastern U.S. monitoring sites are not very meaningful since the 17 western states have very small contributions. Figure 6-5 shows an example of the state-specific PM source apportionment annual $PM_{2.5}$ contribution pie chart for Mesa Verde. The pie chart shows the contributions of 17 states by 5 source categories, so there are 85 slices in the pie. The lower left corner displays the modeled total annual $PM_{2.5}$ at Mesa Verde (4.85 $\mu g/m^3$) along with the percent contribution of BCs (65.0%), off-shore (0.3%), Mexico (1.0%), Canada (0.2%), EUSA (0.1%) and other (6.2%). The pie chart displays the contributions of the 17 states that makes of 27.2% of the modeled annual $PM_{2.5}$ at Mesa Verde (1.32 $\mu g/m^3$). The largest contributions to annual $PM_{2.5}$ at Mesa Verde from the western states are anthropogenic (ANT) emissions from CO (9.6%), NM (5.7%), UT (2.2%), AZ (2.2%) and CA (1.6%). This kind of annual $PM_{2.5}$ contribution plot can be made for any site in the U.S. using the Appendix E spreadsheet. Note that because Appendix E is an Excel spreadsheet, plots can be customized if desired.

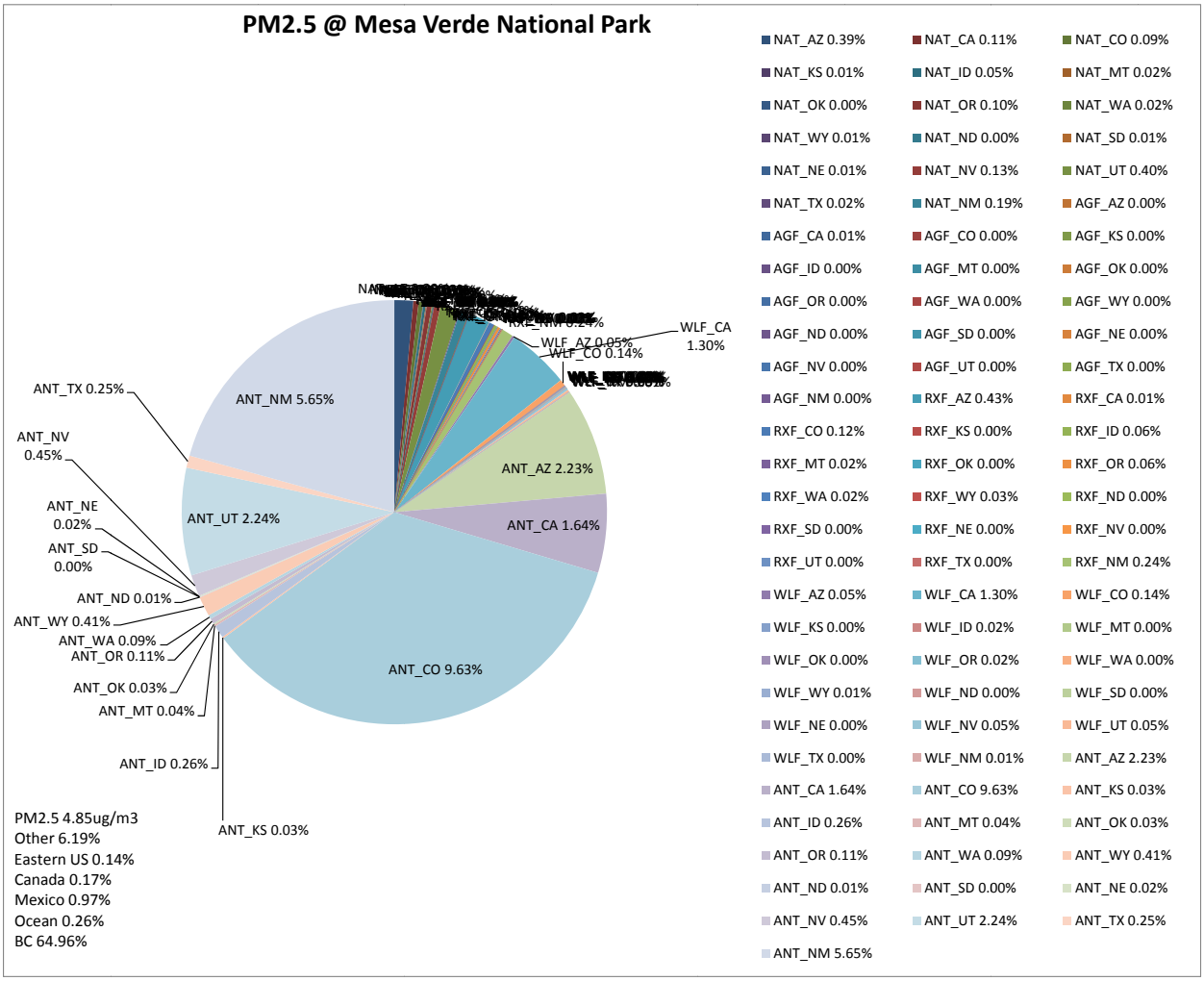


Figure 6-5. Modeled state and source category contributions to annual average $PM_{2.5}$ concentrations at Mesa Verde focusing on the contributions from the 17 western states (from Appendix E).

6.2.2 Spatial Distribution of State Contributions to 24-Hour $PM_{2.5}$ Concentrations

Appendix G is a zipped file of spatial maps of the contributions of state's anthropogenic plus planned (Rx and Ag) fire emissions contributions for the highest (1stmax) and 98th percentile (8thmax) 24-hour $PM_{2.5}$ concentrations for which the total daily $PM_{2.5}$ concentrations is filtered by five concentration thresholds: 35, 30, 25, 20 and 0 µg/m^3. Figure 6-6 contains example spatial maps of 24-hour $PM_{2.5}$ state footprint maps for the 98th percentile modeled 24-hour $PM_{2.5}$ concentrations and the states of AZ, CA, NM, UT, WA and WY with no threshold. Additional states and displays with concentration thresholds are provided in Appendix G.

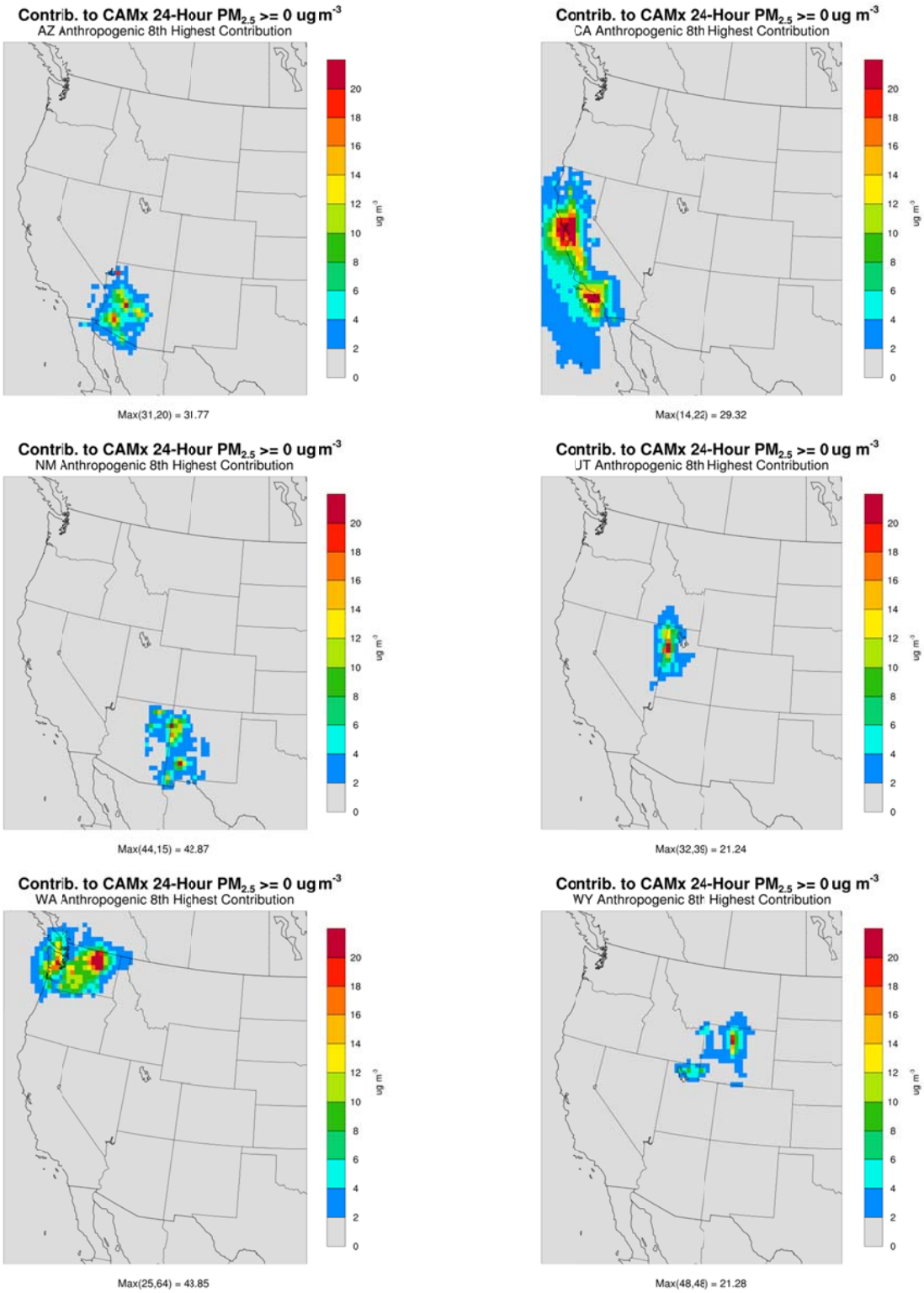


Figure 6-6. Example spatial maps of state's anthropogenic emissions contributions to modeled 98th percentile 24-hour $PM_{2.5}$ concentrations for AZ, CA, NM, UT, WA and WY (from Appendix G).

6.2.3 Spatial Distribution of Source Category Contributions to 24-Hour $PM_{2.5}$ Concentrations

Figure 6-7 displays example source category contributions to the 98th percentile (8th highest day) 24-hour $PM_{2.5}$ concentrations from the state-specific PM source apportionment simulation. The anthropogenic contribution has large contributions from the major urban areas in the western U.S. as well as entering from the eastern U.S with a maximum contribution of 39 µg/m^3. Natural emissions contribute very little to the 8th highest daily $PM_{2.5}$ concentrations with the largest contribution in the KS-NE area that is likely due to biogenic NO_X emissions. The contributions of BCs exhibit a south to north concentrations gradient with a range of 18 to 5 µg/m^3 that is likely due to biomass burning to the south of the domain (e.g., Mexico). Extremely high $PM_{2.5}$ contributions from wildfires are seen especially over northern CA. Contributions from Rx fires to 8th high daily $PM_{2.5}$ concentrations are seen in OR, WA and ID as well as AZ and NM. Ag fire contributions to the 8th high $PM_{2.5}$ concentrations are limited to Saskatchewan.

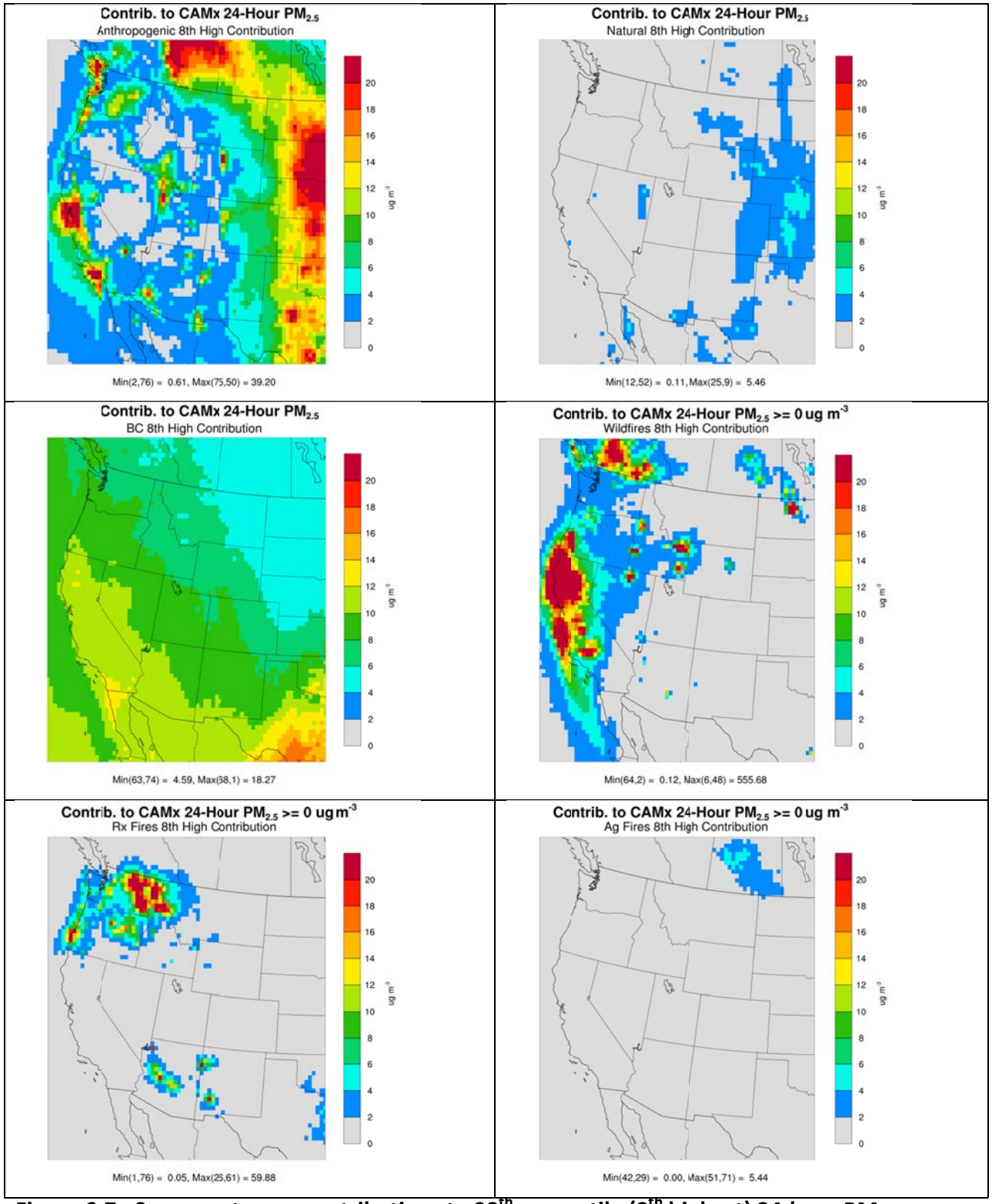


Figure 6-7. Source category contributions to 98th percentile (8th highest) 24-hour $PM_{2.5}$ concentrations (µg/m^3) in the western U.S. from state-specific PM apportionment simulation.

6.3 STATE CONTRIBUTIONS TO VISIBILITY IMPAIRMENT

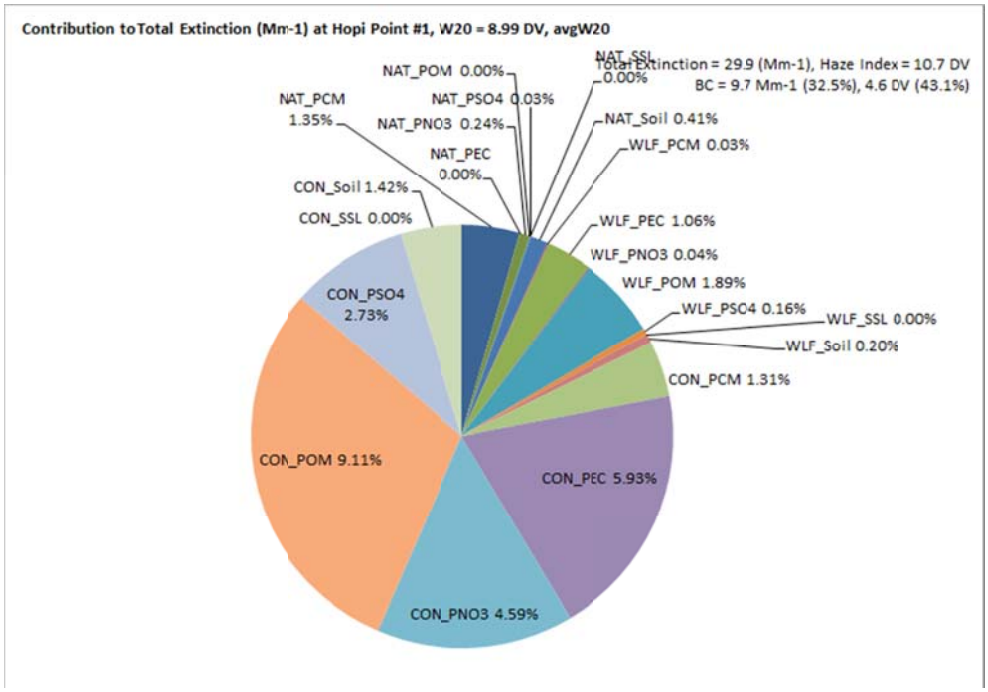
The state-specific PM source apportionment modeling results were extracted at the IMPROVE monitoring sites and processed using the updated IMPROVE equation follow the FLAG (2010) guidance document to generate daily visibility impairment metrics in inverse megameters (Mm^{-1}) and deciview (dv). Appendix O is an interactive spreadsheet that can generate visibility impairment displays for the modeled worst 20% and best 20% visibility days at IMPROVE sites from the CAMx 2006 36 km state-specific PM source apportionment modeling. To operate the Appendix O visibility spreadsheet, a state and monitoring site must first be selected. The user then needs to load in the data for that monitoring site by clicking on the pink "Import Data" button. The user then can select whether they want to examine the W20 and B20 days and then select a day from the W20 or B20 list, or an average of the W20 and B20 days. The Appendix O spreadsheet generates two types of pie charts of the contribution of the 17 western states to visibility impairment: (1) source category by species; and (2) state by species. The source categories are:

- CON = controllable emissions (anthropogenic and Rx and Ag fires)
- NAT = natural emissions (biogenic, lightning, sea salt and WBD)
- WLF = wildfires

Figure 6-8 displays example pie charts for the Hopi Point (Grand Canyon) monitoring site and average of the W20 days (AvgW20). There is much information within the Appendix O spreadsheet:

- The pie chart contributions are just for the 17 western states
- The total extinction without Rayleigh is in cell L8 (29.9 Mm^{-1} in the Hopi Point AvgW20 example)
- Background sources (i.e., EUSA, Mexico, Canada, off-shore and SOA) extinction is in cell L10 (11.1 Mm^{-1} in example)
- Boundary condition contribution is given in the plots (9.7 Mm^{-1} in example)

Figure 6-8 top displays the contributions of the 17 western states to visibility impairment at Hopi Point for the AvgW20 days by source category and species and indicates controllable emission are the largest contribution for OA (9.1%), EC (5.9%), NO3 (4.6%) and SO4 (2.7%). Figure 6-8 bottom displays contributions by the 17 western states to visibility impairment at Hopi Point for the AvgW20% days with AZ having the largest contribution follow by CA.



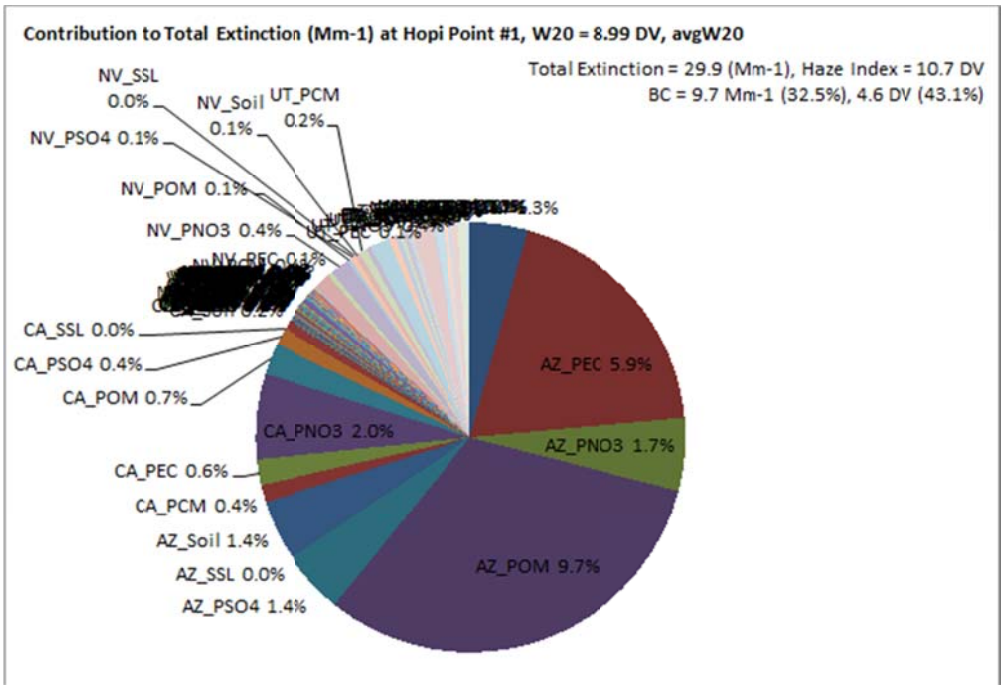


Figure 6-8. Source category and species contributions (top) and State and species contributions (bottom) from the 17 western states to visibility impairment at Hopi Point (Grand Canyon), AZ for the average of the 20% worst modeled visibility days (AvgW20) in 2008 (Appendix O).

7.0 2008 SOURCE CATEGORY-SPECIFIC SOURCE APPORTIONMENT MODELING

Source Category-Specific APCA ozone and PSAT PM source apportionment modeling was conducted to examine the contributions of major source categories to ozone and $PM_{2.5}$ concentrations in the western U.S. The source category-specific source apportionment modeling obtained contributions for the following six source categories from the U.S. portion of the modeling domain.:

- Natural Emissions (biogenic, lightning, sea salt and windblown dust).
- Fires (combined WF, Rx and Ag).
- Upstream Oil and Gas Development (point and area sources).
- All Point Sources (including all EGUs, CEM and non-CEM points sources except those associated with upstream oil and gas).
- Mobile Sources (Combined On-Road and Non-Road Mobile plus Off-Shore Marine).
- Remainder Area Sources (area sources, fugitive dust, livestock and agricultural).

The source category-specific source apportionment modeling also tracked Mexico, Canada and offshore as another source category.

7.1 OZONE SOURCE CATEGORY-SPECIFIC SOURCE APPORTIONMENT MODELING

The source category-specific ozone source apportionment modeling was performed using linked (i.e., two-way grid nesting) 36 km CONUS, 12 km WESTUS and 4 km Detailed Source Apportionment Domain (DSAD) as shown in Figure 1-2. Five Source Regions were used corresponding to the grid cell definitions of Wyoming, Utah, Colorado, New Mexico and remainder of the domain as shown in Figure 7-1. With five Source Regions and six Source Categories this results in 32 total Source Groups (32 = 5 x 6 + 2). The ozone source category-specific source apportionment simulation was run for May through August 2008. Note that the CAMx meteorological inputs for the 12 km WESTUS domain had to be re-generated for the 36/12/4 km source category-specific ozone source apportionment run. Because the WRF modeling was run on the much larger Intermountain West Processing Domain (IMWD; see Figure 1-1), there will be inconsistencies between the 12 and 4 km meteorological variables along the boundaries of the smaller 4 km DSAD. Thus, WRFCAMx was re-run using the WRF 12 and 4 km meteorological output to generate new 12 km WESTUS CAMx meteorological model inputs that blends the 4 km WRF data within the IMWD domain into the 12 km WESTUS meteorological fields.

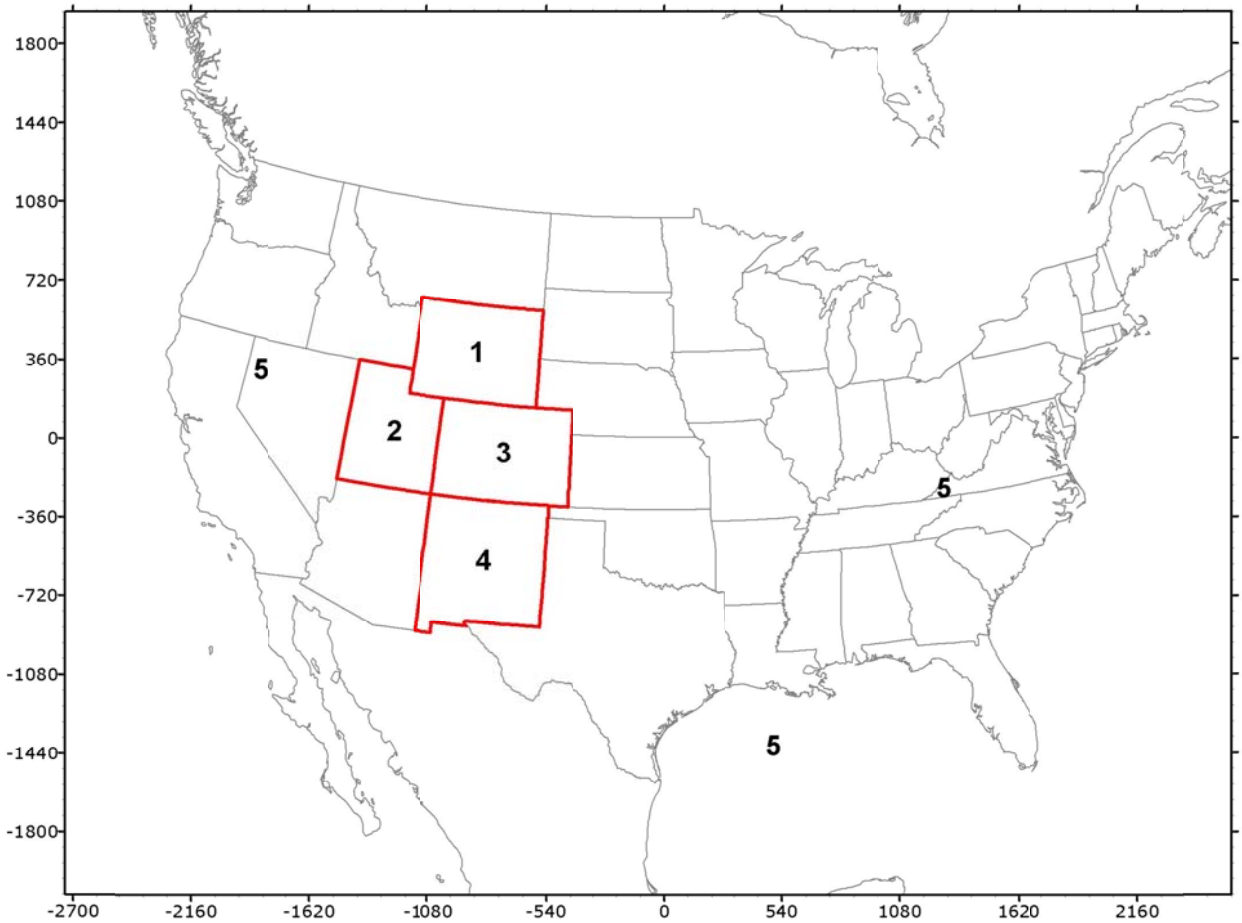


Figure 7-1. Five source regions used in the CAMx 36/12/4 km source category-specific ozone source apportionment simulation.

7.1.1 Source Category Contributions to Ozone Design Values using MATS

The Modeled Attainment Test Software (MATS) was used to obtain the contributions of the six major source categories, Canada/Mexico and boundary conditions (BCs) to the current year Design Values (DVC) in a similar fashion as was done for the state-specific ozone source apportionment MATS analysis. However, even though these eight portions of the ozone concentrations made up the total ozone concentrations, when separately run through MATS to get the separate contributions of each source category to the DVC the sum of the eight portions of the DVC did not equal the total DVC. This was due to the MATS selection of the maximum modeled ozone concentration from the 7 x 7 array of 4 km grid cells centered on the monitoring site for the 2008 base case and 2008 case with the source category ozone contributions removed. We have labeled the difference between the total DVC and the sum of the eight portions of the DVC from the source categories as "Unexplained." For ozone, the Unexplained portion of the DVC is typically very small. However, as will be described later, for $PM_{2.5}$, the Unexplained portion can be significant. In future analysis of ozone DVC source apportionment using MATS we should specify that MATS should just use the modeled ozone at the location of the monitoring site (i.e., 1 x 1 array of cells) rather than the MATS default (e.g., 7 x 7 array using a 4 km grid resolution), which should eliminate the Unexplained portion.

Appendix H is an interactive spreadsheet that can generate pie charts of the source category contributions to the ozone DVC at any monitoring site within the 4 km DSAD domain that covers portions of CO, NM, UT and WY. Figure 7-2 displays source category contributions to DVCs for six monitoring sites obtained from the Appendix H spreadsheet. The CO_Jefferson0006 monitor (Figure 7-2, top left) is the Rocky Flats North (RFNO) monitor that historically has had the highest ozone Design Values in the Denver/North Front Range ozone nonattainment area (NAA). As shown in Figure 7-2, the DVC at RFNO is 82.0 ppb with 41.9 ppb of that (51.1%) due to BCs. Note that since CAMx was run with the 36/12/4 km domains using two-way grid nesting the BCs represent the incoming concentrations through the boundaries of the 36 km CONUS domain even though we are analyzing monitoring sites within the 4 km DSAD. The contributions for the remainder of the ozone DVC (i.e., 40.1 ppb or 48.9%) is shown in the pie chart with half of the remainder of the DVC being due to mobile sources (25.1% of the total DVC), with point sources (8.0%), natural emissions (4.5%), oil and gas (4.0%) and area sources (2.8%) being next most important. The Unexplained portion represents 2.0% of the DVC at Rocky Flats North.

The CO_Weld009 monitor is also in the Denver/North Front range ozone NAA and has a similar source category contribution as RFNO only it has a larger oil and gas contribution (5.2%) since it lies within the Denver-Julesburg Basin oil and gas production area (Figure 7-2, top right). The more rural Mesa Verde monitoring site (CO_Montezuma0101) has a larger BC (49.6 ppb and 71.6%) and Unexplained (7.1%) contribution and lower mobile (6.5%) contribution. The ozone contribution at the Colorado Springs monitor (CO_El Paso0016) lies between the Denver and Mesa Verde contributions.

66.8% of the ozone DVC in Salt Lake City (UT_Salt Lake3006) is due to BCs (Figure 7-2, bottom left). Mobile sources contribute half of the remainder (16.9% of the DVC) with point sources (5.5%) and natural emissions (3.8%) being next most important. The San Juan County, NM monitor has 68.7% of its DVC due to BCs with point (9.7%) and mobile (8.4%) sources being the largest two source category contributors.

The Unexplained portion of the DVC tended to range from 1.3% to 7.1% (approximately 1 to 5 ppb) of the DVC. The reasons why it is much larger at Mesa Verde is not clear.

Note that the Appendix H spreadsheet also has the capability of making pie chart DVC contribution plots for the four monitoring sites in the four states that have the highest contribution of each of the six source categories (not shown).

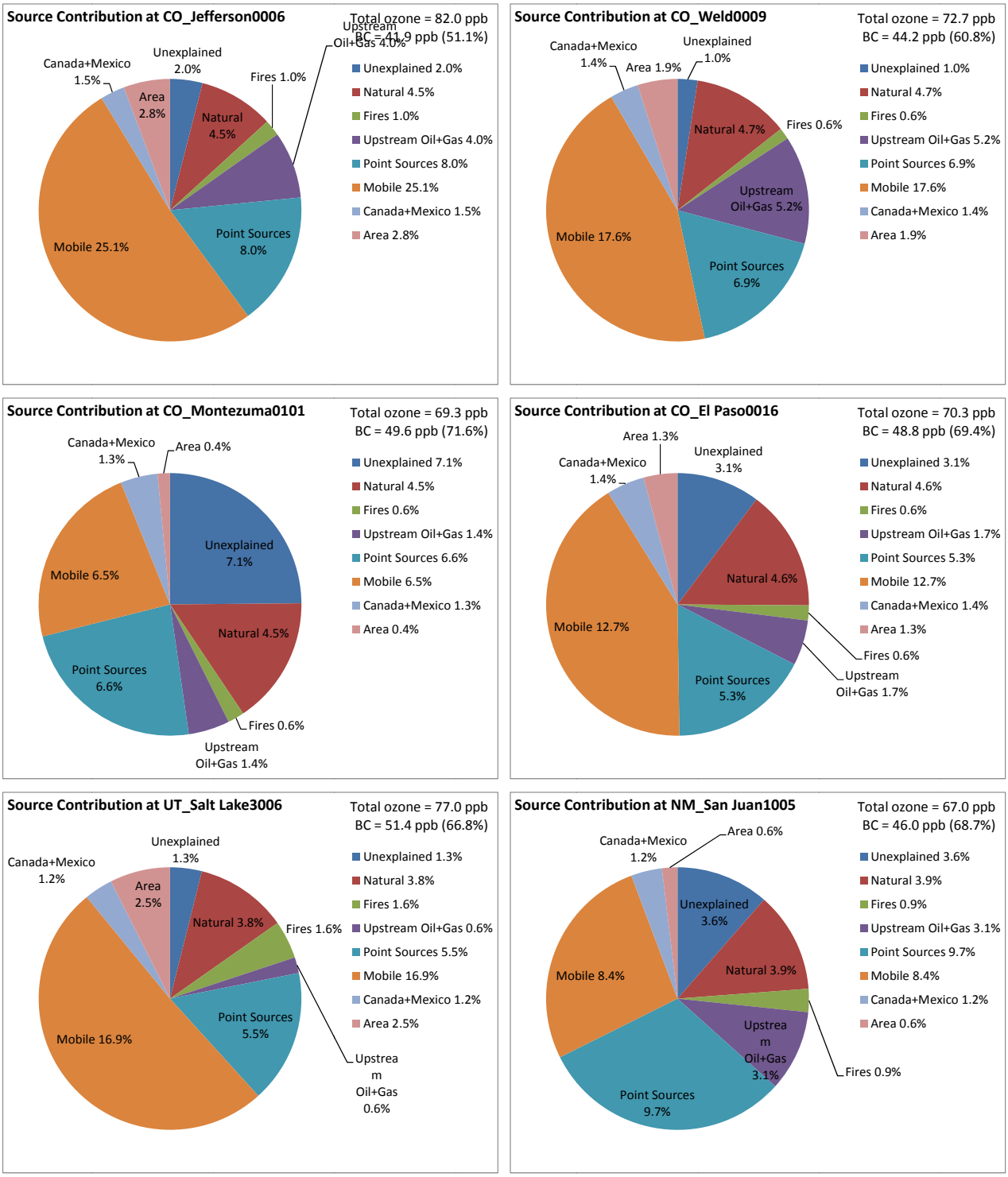


Figure 7-2. Source category contributions to current year ozone Design Values at six monitoring sites using MATS and 4 km DSAD source category-specific ozone source apportionment modeling results (from Appendix H).

7.1.2 Source Category Contributions to Ten Highest Modeled DMAX8 Ozone Days

Appendix I is an interactive spreadsheet that makes pie chart contribution plots for the ten highest modeled DMAX8 ozone days at each monitoring site within the 4 km DSAD domain. For example, Figure 7-3 displays the source category contributions for the six highest modeled DMAX8 ozone days at the RFNO monitoring site in the Denver area. These plots also include the observed DMAX8 ozone concentrations and the bias between the predicted and observed DMAX8 ozone so the user can obtain an assessment of the reliability of the modeling results. For example, on the highest modeled DMAX8 ozone day (83.5 ppb on May 7, 2013) the observed DMAX8 ozone is only 61.3 ppb resulting in a 36.3% overestimation bias indicating that the source apportionment may not be reliable. The 2nd through 5th highest modeled DMAX8 ozone days tend to have much better model performance with the bias ranging from -3.5% to +5.8%. The 6th highest modeled DMAX8 ozone day (73.7 ppb on June 13, 2008) has a very different source category contribution from the top five high days. The BC contribution (58 ppb) is 10 to 35 ppb higher than the other days suggesting it may be influenced by stratospheric ozone. The modeled ozone (73.7 ppb) is about 10 ppb higher than observed (62.6 ppb) on June 13, 2008.

The source category contributions on the modeled five highest DMAX ozone days tend to be similar with mobile sources from CO (MV_CO) being the largest source contribution with CO area, point and oil and gas also being important.

It should be pointed out that the MATS procedure for projecting future year ozone Design Values use ozone concentrations for constructing the Relative Response Factors (RRFs) from the (~10) highest modeled DMAX8 ozone modeling days. For RFNO site, the modeled highest DMAX8 ozone day (May 7, 2008) has fairly poor model performance (36% overestimation), yet MATS would use this day to make ozone projections. A model performance check should be added to MATS to assure poor performing modeled days are not used in the ozone projections. In this case since the source contributions on the highest modeled DMAX8 ozone day with poor model performance appears similar to the 2nd through 4th highest days with good model performance then the MATS ozone projections using that day would probably not provide an invalid signal.

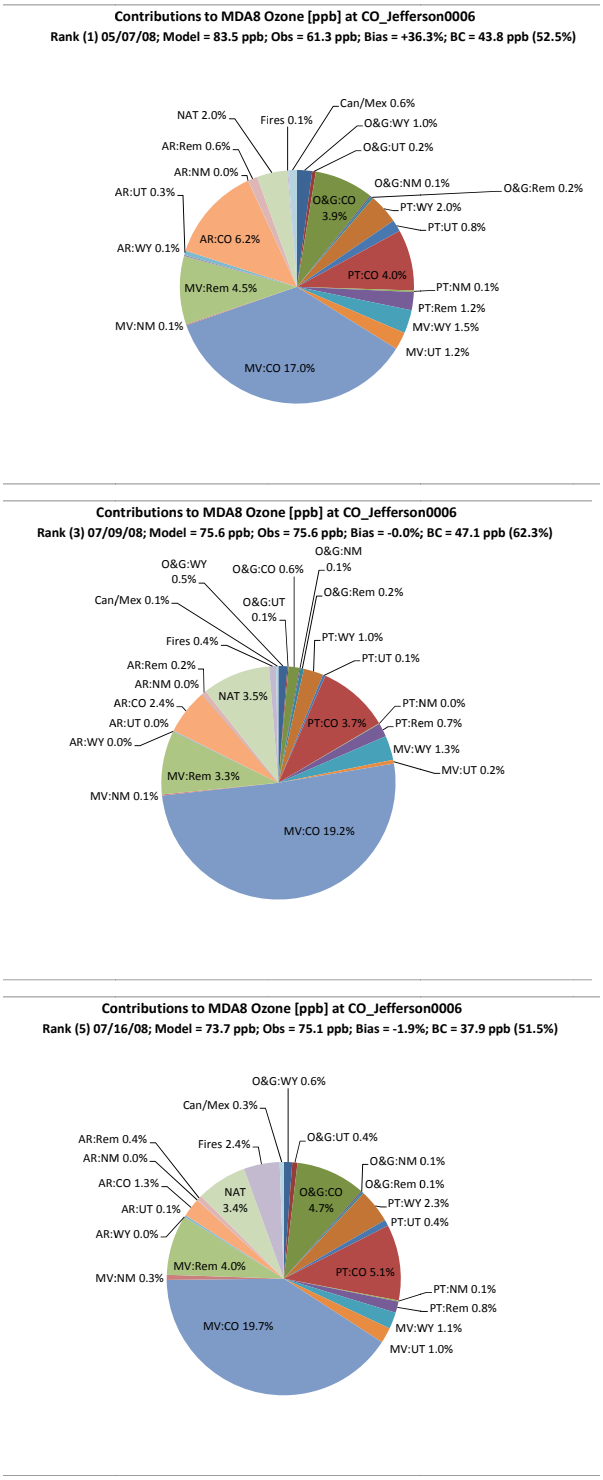


Figure 7-3. Source category contributions to DMAX8 ozone on the six highest modeled ozone days at the Rocky Flats North monitoring site (CO_Jefferson0006) in the Denver/Front Range ozone nonattainment area (from Appendix I).

7.2 PM SOURCE CATEGORY-SPECIFIC SOURCE APPORTIONMENT MODELING

The source category-specific PM source apportionment modeling was performed on the 36 km CONUS and 12 km WESTUS domains using two-way grid nesting for the 2008 calendar year. Original plans also intended to use the 4 km DSAD, but the memory requirements and run times would have been too long due to all the reactive tracers that need to be included for PM source apportionment. As another way to reduce the computer requirements of the PM source apportionment run was to run with one source region.

7.2.1 Source Category Contributions to Annual $PM_{2.5}$ Design Values

The 2008 36/12 source category-specific PM source apportionment modeling results were used with MATS to obtain the source category contributions to current year annual $PM_{2.5}$ Design Values (DVCs). As seen with the ozone DVC source apportionment analysis, the sum of the DVC contributions for all source categories does not equal the total DVC so we have labeled the extra portion of the DVC "Unexplained." However, unlike the ozone DVC source apportionment analysis where the ozone DVC Unexplained portion is typically small, the Unexplained portion of the $PM_{2.5}$ DVCs can be fairly large. Furthermore, since MATS uses the average concentration in an array of grid cells centered on the grid cell for constructing the PM RRFs rather than the maximum in an array as used for the ozone RRFs, the explanation for the Unexplained portion given for the ozone DVCs does not apply for the $PM_{2.5}$ DVCs.

The reasons for the Unexplained portion for the annual $PM_{2.5}$ are several fold and are due Secondary Organic Aerosol (SOA), blank mass, Particle Bound Water (PBW) and Sea Salt all of which were not modeled by the PSAT PM source apportionment tool. The SOA portion of the modeled OA was not modeled using PSAT by choice due to the extensive computer resources needed to track SOA contributions (see Section 5.1) and its typically small contribution to $PM_{2.5}$. The SANDWICH speciation approach (Frank, 2006a,b) used in MATS assumes that 0.5 $\mu g/m^3$ of the $PM_{2.5}$ is a blank correction mass to account for measurement artifacts, which should probably be removed from the Unexplained portion and labeled as blank mass. PBW is also not tracked by the PSAT source apportionment tool and instead is calculated internally in MATS using the current and future years SO4, NO3, NH4 and DON (degree of neutralization) values. In hind sight, we should have distributed the PBW DVC component across the SO4, NO3 and NH4 concentrations in each of the source categories based on relative contribution, which should be considered in future analysis of $PM_{2.5}$ DVCs using source apportionment. Sea Salt contributions tends to be small except near the coast and are held constant based on measurements so should probably be labeled as such rather than grouped with the Unexplained.

Appendix J is an interactive spreadsheet that displays pie charts of source category contributions to annual $PM_{2.5}$ DVCs for each FRM monitoring site in the 12 km WESTUS domain. Three options are available in the Appendix J spreadsheet: (1) monitoring site in the 12 km WESTUS domain; (2) source category; and (3) $PM_{2.5}$ species. Appendix J will then generate three pie charts of source contributions to the annual DVC at the selected site for: (1) total $PM_{2.5}$; (2) the species contribution to the $PM_{2.5}$ component of the DVC for the select source category; and (3) the source category contributions to the selected species component of the DVC. Figure 7-4 displays the DVC contribution pie charts generated by Appendix J for two sets of settings: (left) AZ_Maricopa9997 (Phoenix) monitoring site, mobile sources and organic aerosol; and (right) CA_Nevada0005 (northern California), fires and organic aerosol.

Area sources (40%) have the largest contribution to the annual $PM_{2.5}$ DVC in Phoenix followed by mobile sources (21%) and BC (17%) with the Unexplained portion accounting for 13% (Figure 7-4, top left). The mobile source contribution is dominated by OA (47%) and EC (42%) (Figure 7-4, middle left). The OA component comes mainly from area (60%) and mobile (22%) sources with 13% of the OA component of the Phoenix annual $PM_{2.5}$ DVC being Unexplained.

The Nevada County, CA monitoring site was selected for display in Figure 7-4 (right) because it is near the regions with extensive wildfires during June-August 2008. So not surprisingly, fires are a major component (30%) of the annual $PM_{2.5}$ DVC at this site along with area sources (30%) with BC (13%) and Unexplained (19%) being most of the rest. The fire contribution consists mainly of OA with most of the OA component coming from area sources and fires.

7.2.2 Source Category Contributions to Modeled Annual $PM_{2.5}$ Concentrations

Appendix K is an interactive spreadsheet that generates pie charts of source category and species contributions to modeled annual $PM_{2.5}$ concentrations at all FRM sites across the 36 km CONUS domain. The user selects a monitoring site, a species and a source category and Appendix K generates four pie charts of modeled annual $PM_{2.5}$ contributions for: annual $PM_{2.5}$ by source category; selected species by source category; selected source category by species and a combination pie chart that displays annual $PM_{2.5}$ contributions by source categories and species. Figure 7-5 shows example pie charts from Appendix K for a site in Bernalillo County, NM (Albuquerque) and Washoe County, NV (Reno). For these plots, the PM species selected was $PM_{2.5}$ so that we would obtain contribution plots of annual $PM_{2.5}$ by both PM species and source categories. The by source category and species combination plots shown in Figure 7-5b get complicated because it is plotting the seven source categories (NAT, Fire, O&G, MV, AR, BC and SOA) by 7 species (SO4, NO3, NH4, EC, OA, Crustal and Salt) so there are 49 slices in the pie.

7.2.3 Source Category Contributions to 24-Hour $PM_{2.5}$ Design Values

MATS was used to generate contributions to 24-hour $PM_{2.5}$ DVCs the same way it was used for ozone and annual $PM_{2.5}$ DVCs source contributions. However, we obtained a very large Unexplained portion for the MATS derived source category contributions to the 24-hour $PM_{2.5}$ DVCs that was much larger than seen for the annual $PM_{2.5}$ DVC Unexplained contributions. In addition to the SOA, blank correction, PRB and sea salt issues associated with the Unexplained portion of the annual $PM_{2.5}$ DVCs, the 24-hour $PM_{2.5}$ DVC has an additional issue associated with the form of the 24-hour $PM_{2.5}$ NAAQS. The form of the 24-hour $PM_{2.5}$ NAAQS is the three-year average of the 98th percentile 24-hour $PM_{2.5}$ concentration. When MATS makes a future year 24-hour $PM_{2.5}$ projection it projects many days to the future year and then re-calculates the 98th percentile by re-ordering the days. This means that we may be looking at different days when calculating source category contributions as the difference in the current and future year Design Values (DVC-DVF). Thus, this approach does not provide an accurate representation of a source categories contribution to the 24-hour $PM_{2.5}$ Design Values so no examples are presented here. Although, Appendix L is an interactive spreadsheet that uses the MATS approach to estimate source category contributions to 24-hour $PM_{2.5}$ DVCs if desired.

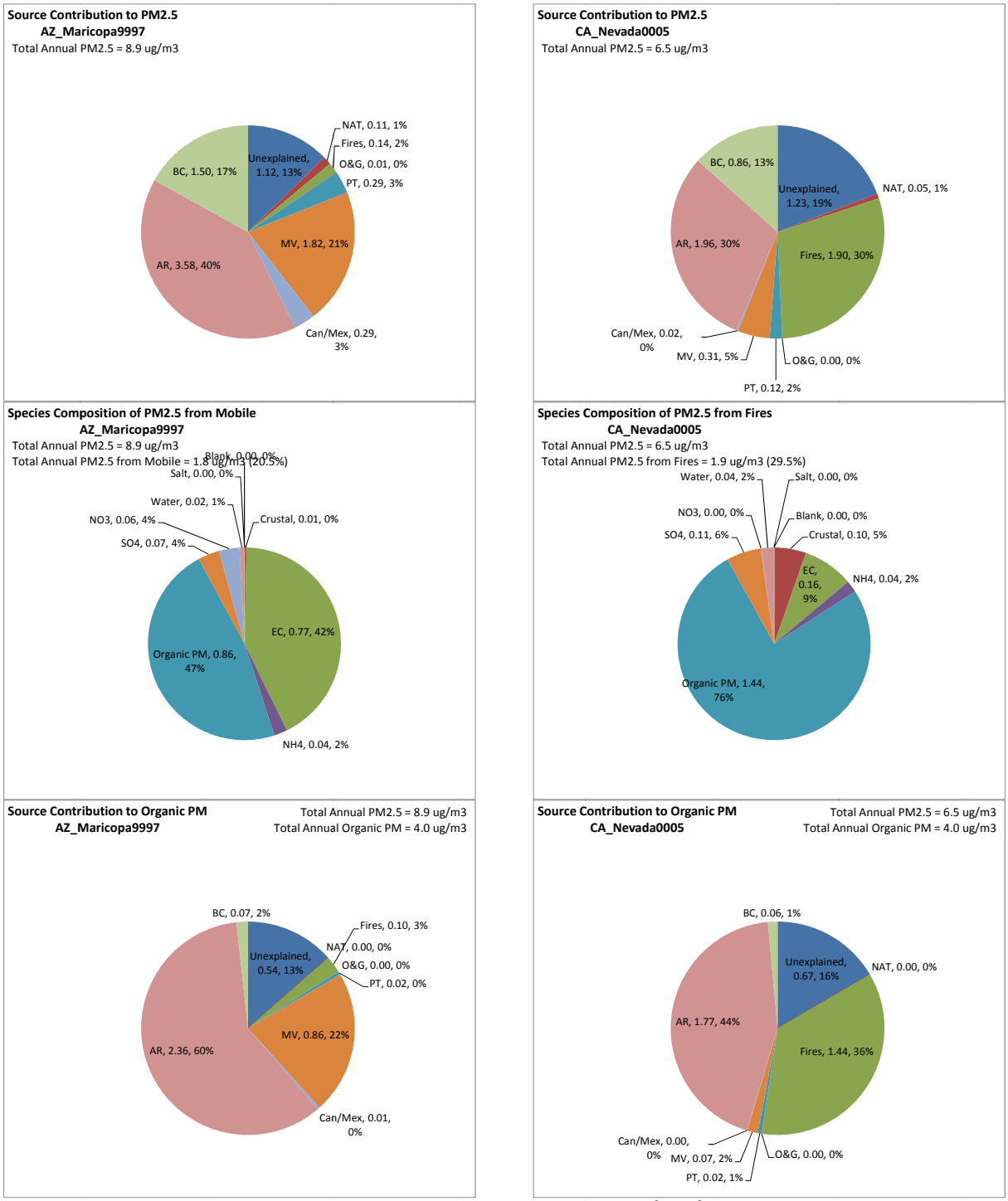


Figure 7-4. Annual $PM_{2.5}$ DVC source category contributions (top), species contribution to mobile component of the DVC (middle) and source category contributions to Organic Aerosol component of the DVC (bottom) for Maricopa County, AZ (left) and Nevada County, CA (right) using MATS and source category-specific PM source apportionment modeling results for 2008 (from Appendix J).

Figure 7-5a. Source category contributions to modeled annual $PM_{2.5}$ (top), species composition of annual modeled $PM_{2.5}$ (middle) and species composition of area source component of annual modeled $PM_{2.5}$ (bottom) concentrations at the NM_Bernalilo0029 (left) and NV_Washoe1005 (right) monitoring sites (from Appendix K).

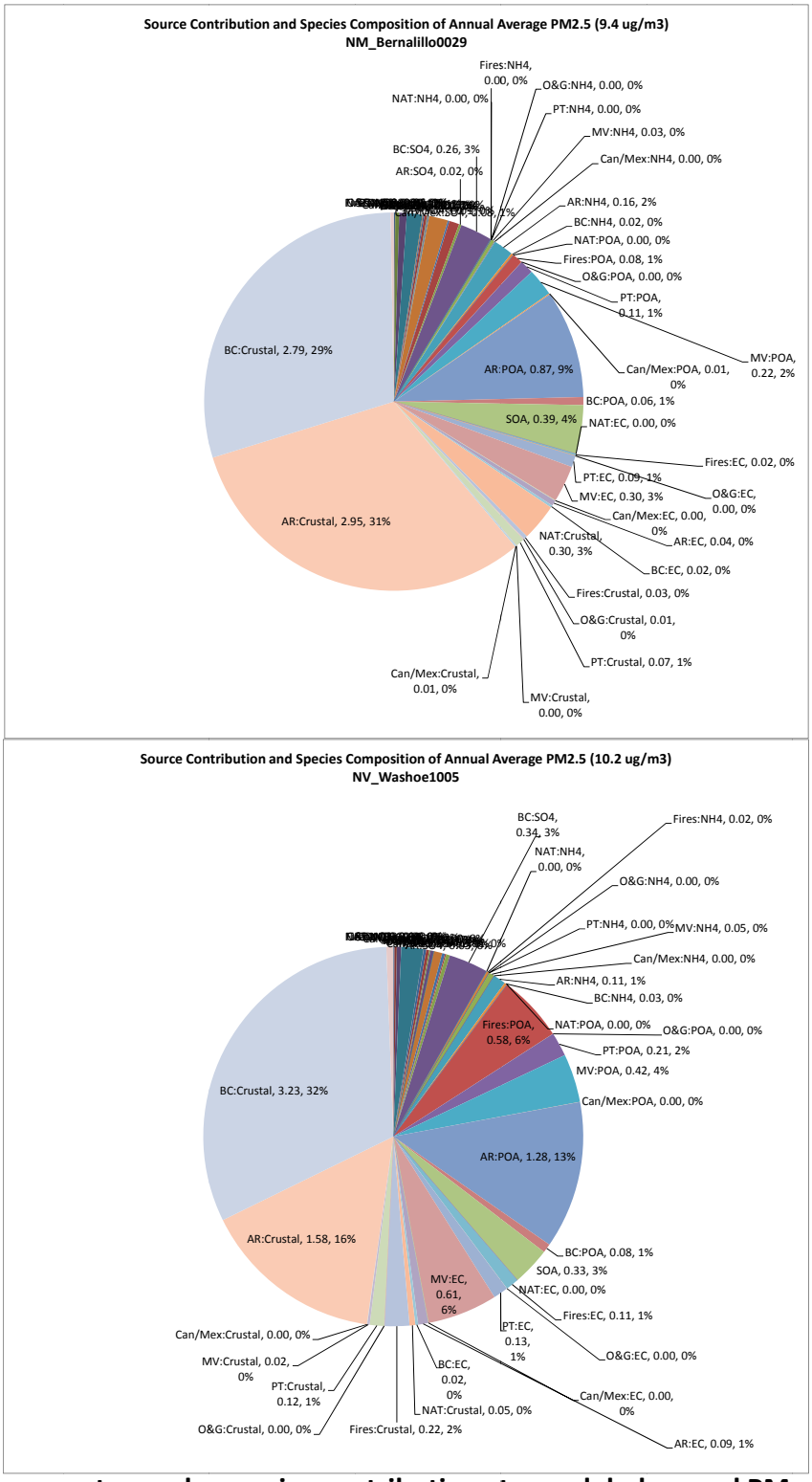


Figure 7-5b. Source category by species contributions to modeled annual $PM_{2.5}$ concentrations at the NM_Bernalilo0029 (top) and NV-Washoe1005 (bottom) monitoring sites (from Appendix K).

7.2.4 Source Category Contributions to Modeled 24-Hour $PM_{2.5}$ Concentrations

Appendix M is an interactive spreadsheet that generates several different types of pie charts (by source category and species) for the 10 highest modeled 24-hout $PM_{2.5}$ days at monitoring sites within the 12 km WESTUS modeling domain. The user selects a state, a monitoring site in a state, a species, a source category and one of the top 10 highest modeled 24-hour $PM_{2.5}$ days and the Appendix M spreadsheet will generate four different types of contribution pie charts for that site and day. For example, Figure 7-6 displays the source category contributions for the six highest modeled 24-hour $PM_{2.5}$ days at the Hopi Point monitoring site in the Grand Canyon (GRCA). These six modeled highest 24-hour $PM_{2.5}$ days at GRCA all occur in the spring (April and May) and have large BC contributions with some days also having a large fire contribution. An examination of the GRCA BC composition reveals it is mostly crustal component. This suggests that the highest modeled 24-hour $PM_{2.5}$ days at GRCA are due to either Asian dust transport (through the CONUS domain BCs derived from the Mozart GCM), fires or both.

7.2.5 Species Contributions to Annual Sulfur and Nitrogen Deposition

The CAMx PSAT PM source apportionment algorithm has an option to output wet and dry deposition amounts for its PSAT reactive tracer species. Unfortunately for the WestJumpAQMS source category-specific PM source apportionment run this option was not set to be on until the final two months of the simulation of two of the quarters. Thus, in this section we present annual sulfur and nitrogen deposition output from the standard model output.

Appendix N is an interactive spreadsheet that generates sulfur and nitrogen deposition by species and by wet, dry or total depositions at each IMPROVE monitoring site in the 36 km CONUS domain. We used the Appendix N spreadsheet to generate pie chart contribution plots for annual sulfur and nitrogen deposition by species and wet and dry deposition at Rocky Mountain National Park (ROMO) that are shown in Figure 7-7. The top left panel in Figure 7-7 shows the annual sulfur deposition at ROMO by species wet and dry deposition. For sulfur deposition, there are only three species (SO2, SO4 and SULF) with gaseous sulfuric acid mist (SULF) having insignificant mass so there are essentially only four slices in the pie chart so it is pretty easy to interpret that most of the sulfur deposition at ROMO is due to wet SO4 deposition with a little from dry depositions of SO2 (10%) and SO4 (9%). However, for the nitrogen total deposition plot by species and total (wet and dry combined) deposition (Figure 7-7, top right) there are 13 species so there would be 26 slices in the pie chart if we looked at wet and dry deposition together that can be difficult to interpret. The Appendix N spreadsheet also has the capability to generate pie charts separately by dry and wet deposition that for nitrogen is shown in the bottom panels of Figure 7-7. For nitrogen deposition at ROMO, a majority is from HNO3 as either dry (30%) or wet (15%) deposition. Wet deposition of NH4 is next most important (21%), followed by dry deposition of NO3 (11%) and wet deposition of NO3 (6%).

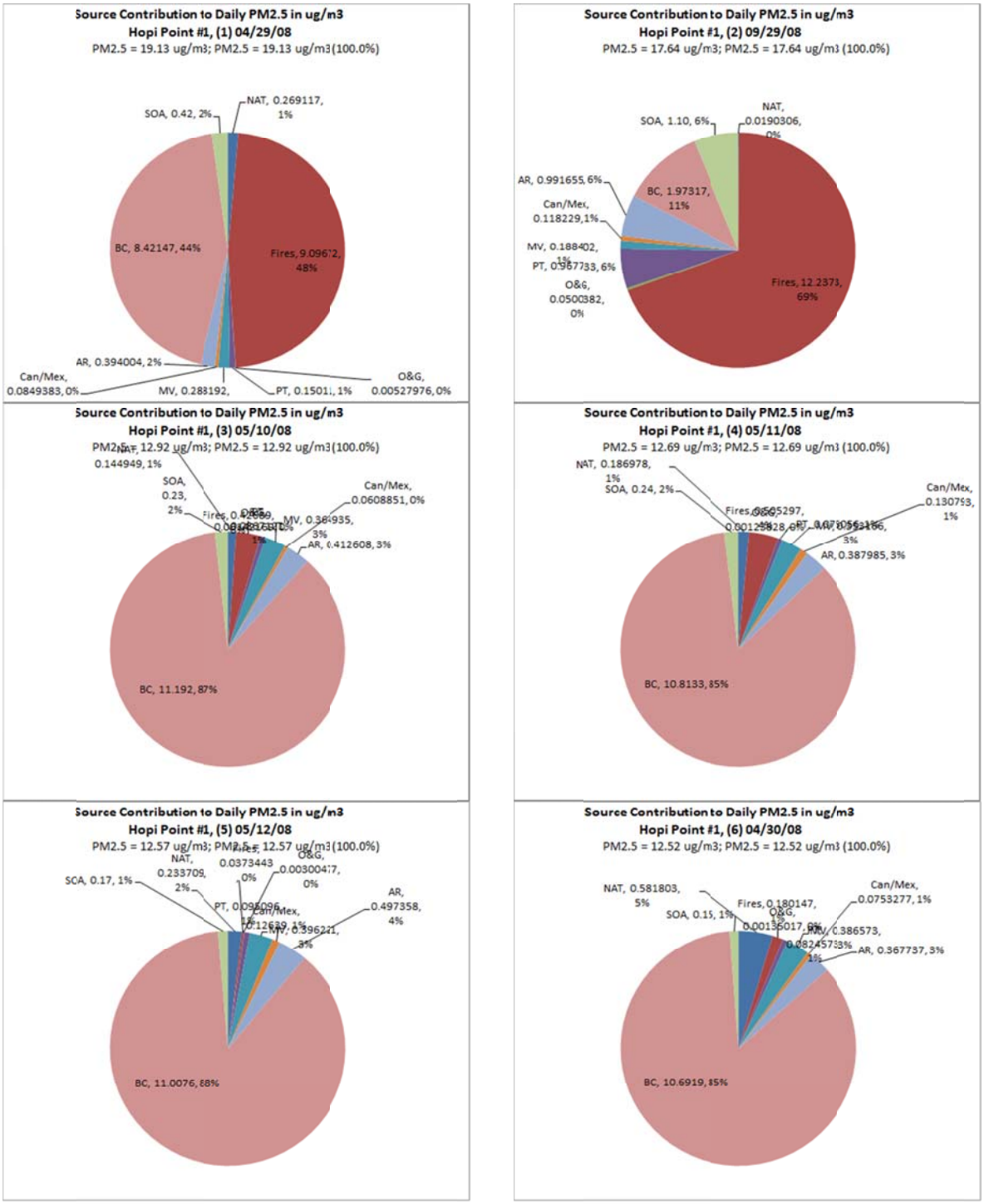


Figure 7-6. Source category contributions to the modeled 24-hour $PM_{2.5}$ concentrations for the six highest modeled 24-hour $PM_{2.5}$ concentration days at Hopi Point (Grand Canyon), AZ monitoring site (from Appendix M).

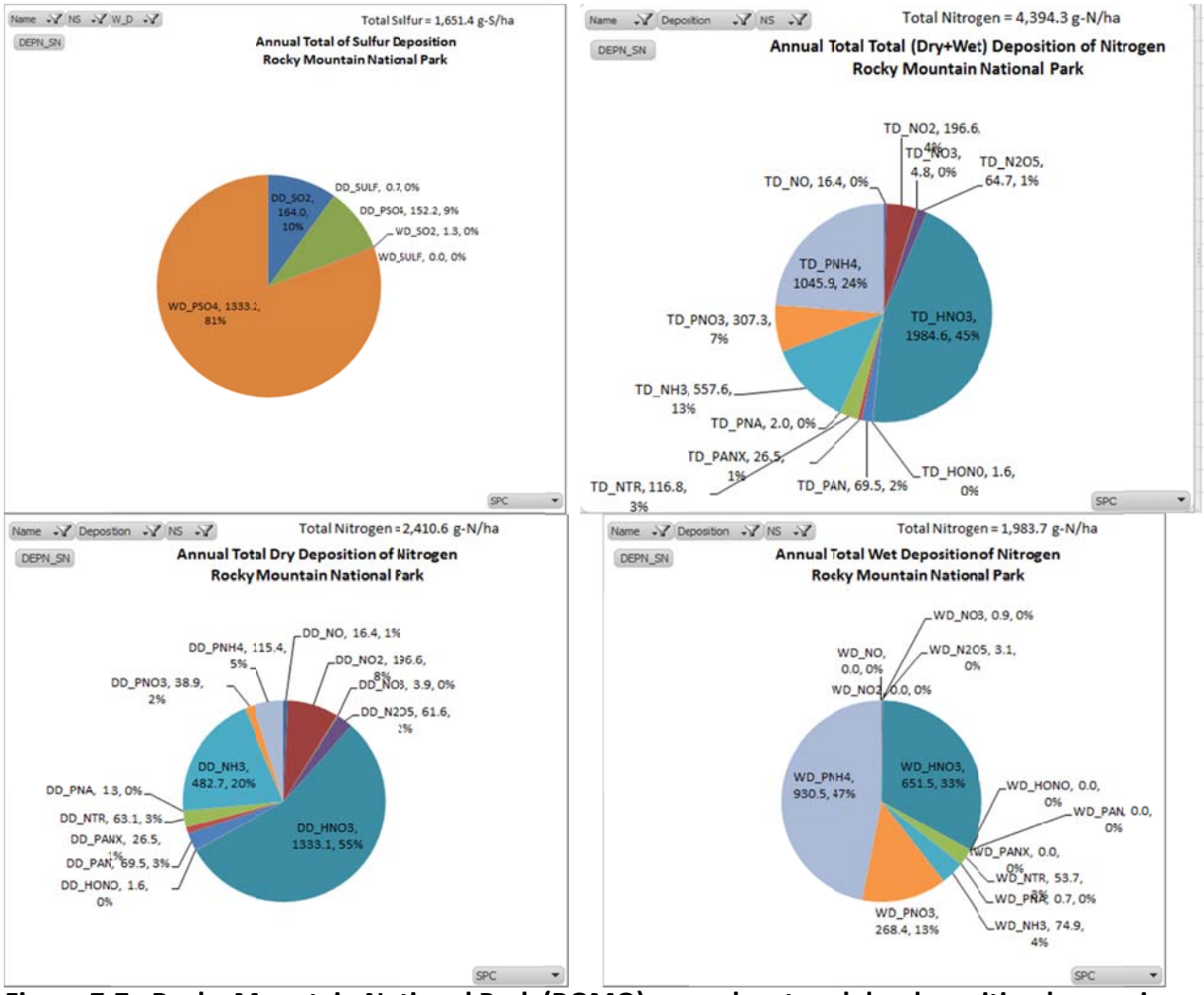


Figure 7-7. Rocky Mountain National Park (ROMO) annual wet and dry deposition by species for sulfur (top left), total deposition by species for nitrogen (top right), dry deposition by species for nitrogen (bottom left) and wet deposition by species for nitrogen (bottom right) in grams per hectare per year (g/ha/yr) (from Appendix N).

8.0 LESSONS LEARNED

The WestJumpAQMS was a very large photochemical grid modeling (PGM) study that involved activities and coordination among WRAP and the three modeling centers (ENVIRON, Alpine and UNC) as well as involvement of hundreds of stakeholders from federal, state and local governments, industry, and environmental and consulting groups. The 2008 PGM modeling platform developed by WestJumpAQMS will likely be used for years to come and will be archived in the Three-State Data Warehouse (3SDW). The Three-State Air Quality Study (3SAQS) is embarking on the development of a 2011 PGM platform for the western states. The WestJumpAQMS encountered numerous issues during the study that had to be addressed and overcome. In this Chapter we discuss the Lessons Learned from the WestJumpAQMS so that hopefully future PGM studies (e.g., 3SAQS) can benefit from the upfront identification of issues and potential resolutions to the issues.

8.1 EMISSIONS

Because there are many sources and components of an emissions inventory and emissions modeling is quite complex and data intensive, there are numerous opportunities for errors and other issues arising.

8.1.1 National Emissions Inventory (NEI)

The cornerstone of the WestJumpAQMS emissions database was version 2 of the 2008 NEI (2008 NEIv2) that was released in April 2012. The NEI is an extremely valuable resource for PGM studies and EPA should be commended for its development and the progress they have made in improving its quality and comprehensiveness. It has some limitations (see oil and gas discussion below), but generally is a high quality emissions data source for U.S. emissions. During the course of the WestJumpAQMS, EPA strongly advised us to not use the 2008 NEIv1.5 that was released in May 2011 and wait until the release of the 2008 NEIv2. As the emissions data source represents the start of the emissions modeling that requires many months to perform, waiting for the release of the 2008 NEIv2 resulted in delays in starting the WestJumpAQMS and seriously compromised the schedule that affected the detail in the source apportionment runs that also takes many months to perform. According to the 2008 NEI website, the major updates between 2008 NEIv1.5 and 2008 NEIv2.0 were as follows:

- *"Version 2 (April 10, 2012): Key updates are the use a draft version of the MOVES model for onroad mobile sources, a review and update of hazardous air pollutant emissions and additions of wildfires, prescribed burning and biogenic emissions."*[80]

As WestJumpAQMS performed their own MOVES on-road mobile source and MEGAN biogenic emissions modeling and used 2008 fire emissions from the DEASCO3 project, we question the benefits of waiting a year for the 2008 NEIv2.0 for key updates that were not even used. In hindsight, WestJumpAQMS probably should have proceeded with the 2008 NEIv1.5 so that the schedule would not have been compromised. EPA has implemented more automated procedures so that earlier versions of the NEI will likely be higher quality than seen in past years so that PGM studies can use these earlier versions and not compromise schedules. And it should be noted there are likely a lot of other updates between NEIv1.5 and NEIv2.0 so that by using NEIv2.0 WestJumpAQMS used a higher quality emissions database.

8.1.2 Oil and Gas Emissions

The WRAP Phase III oil and gas (O&G) emissions inventory represents one of the most comprehensive regional O&G emissions inventories ever assembled. However, the WRAP Phase III 2008 O&G only covered

80 http://www.epa.gov/ttnchie1/net/2008inventory.html

Basins in the inter-mountain west (and as part of WestJumpAQMS added the Permian Basin in southeast NM and northwest TX for 2008). In addition, at the time of the WestJumpAQMS emissions development, the Phase III O&G emissions were not yet available for the Williston and Great Plains Basins in MT and ND, although the O&G development in these two Basins in 2008 were nowhere near as high as they are today. Outside of the Phase III Basins (as well as in MT and ND), WestJumpAQMS used the 2008 NEIv2.0 O&G emissions that, for most states, only include large point sources that have high enough emissions to be reported (e.g., permitted sources). Consequently, we are missing a lot of O&G emissions outside of the Phase III Basins because each individual source's emissions is below the reporting threshold yet in total they represent a significant amount of emissions.

The WRAP Phase III O&G emissions were developed using, in part, surveys from the Operators for a 2006 baseline. Since 2006, the practice for developing O&G fields have changed including the regular and wide-spread use of fracing and the advent of shale oil and gas developments. New surveys focused on these un-surveyed O&G sources would be beneficial to characterize and quantify current and future O&G emissions. In addition, O&G surveys for the Paradox Basin (UT and CO) and Raton Basin (CO and NM) that was not covered in the original WRAP Phase III 2006 baseline development would also be useful.

Future studies should consider updating the WRAP Phase III surveys and emissions to capture current and potential future practices in O&G development and enhancing the unpermitted O&G emissions outside of the Phase III Basins.

For tribal emission sources, the WRAP Phase III and NEI use different locational identifiers. The WRAP Phase III uses county and state identifiers, whereas the NEI uses tribal land identifiers. Initially we used the Phase III county identifiers to remove O&G emissions from the NEI to be replaced by the WRAP Phase III O&G emissions without accounting for the NEI O&G sources with tribal identifiers. This resulted in a double counting of O&G emissions from the Southern Ute Indian Tribe (SUIT) in the North San Juan Basin (southern CO) in early emissions inventories that was corrected in later versions of the 2008 emissions that were used in the modeling.

8.1.3 On-Road Mobile Sources

For WestJumpAQMS on-road mobile source emissions, the MOVES2010a model was run in the inventory mode to generate monthly average diurnally varying on-road mobile source emissions for each county in the U.S. The SMOKE emissions model was then used to spatially allocate the monthly diurnally varying emissions to the modeling grids using appropriate spatial surrogates (e.g., road-ways) as well as perform chemical speciation. Since WestJumpAQMS developed its 2008 on-road mobile emission inputs, EPA released MOVES2010b as well as the SMOKE-MOVES tool that uses hourly gridded meteorological data (e.g., from WRF) and emissions factors lookup table generated by running MOVES multiple times for representative counties to generate hourly day-specific gridded speciated on-road mobile source emissions for PGM applications. At the time of the WestJumpAQMS mobile source emissions modeling, SMOKE-MOVES was not fully developed and tested. Running MOVES in the emissions inventory mode for each month and county in the U.S. is quite labor intensive. Now that SMOKE-MOVES is fully operational, we recommend using it for on-road mobile sources to generate day-specific inventories that reflect the day-specific hourly meteorological conditions (e.g., temperature). Although SMOKE-MOVES is more computer intensive than running MOVES in inventory mode, it is probably less labor intensive so actually might save time.

In running MOVES in inventory mode to generate monthly county-level emissions, we noticed some unexpected variations in monthly emissions. We traced this to an assumption in MOVES concerning the fraction of weekdays and weekend days that all months in a year did not meet. This issue was corrected

using a simple scaling analysis for the offending months. This issue can be alleviated in future applications by running MOVES in emissions factor mode and using SMOKE-MOVES as discussed above.

8.1.4 EGU Point Sources

Emissions for Electrical Generating Units (EGUs) with Continuous Emissions Monitors (CEMs) were based on hourly emissions (SO2 and NO_X) or annual emission allocated to each hour using hourly heat input (other species). These emissions are available on the EPA Clean Air Markets Division (CAMD) website.[81] However, the hourly CEM emissions on the CAMD website were not developed for modeling, but rather they were developed to demonstrate compliance with emission limits as part of the acid rain emissions trading program. Consequently, when a CEM device is not operating correctly so that the hourly emissions are not reported, the hourly emissions are replaced by maximum emissions in order to assure compliance with emissions limits. For PGM applications, WestJumpAQMS replaced the hours with the substituted maximum emissions rates (i.e., missing CEMs data) using typical emission rates for the EGU in question.

8.1.5 Non-EGU Point, Non-Road and Non-Point Emissions

With some exceptions as indicated in this Chapter (e.g., oil and gas and ammonia), the 2008 NEIv2.0 non-EGU point, non-road and non-point (area) emissions were used with the SMOKE emissions modeling system using default spatial and temporal allocation and chemical speciation without any issues encountered.

8.1.6 Ammonia Emissions

The WestJumpAQMS convened an ammonia emissions workgroup to identify approaches for improving ammonia emission inventories in future modeling studies. The results of the workgroup findings are documented in a Technical Memorandum (Adelman and Morris, 2013[82]). Although ammonia emission factors are uncertain, the workgroup identified improvement in spatial allocation as the low hanging fruit that could improve ammonia emission inputs for PGM studies. As livestock and fertilizer make up 86% of the annual ammonia emissions in 2008, procedures for improving the spatial distribution of these two ammonia source categories have been identified. In particular, obtaining data on locations and number of animals in Concentrated Animal Feeding Operations (CAFOs) from states and other sources was identified. More details can be found in the ammonia workgroup Technical Memorandum cited above.

8.1.7 Fire Emissions

Emissions from fires were based on a detailed inventory for 2008 emissions from WF, Rx and Ag fires from the DEASCO3 study. Early on in the WestJumpAQMS study, 2008 fire emissions from the Fire INventory from NCAR (FINN) and the SMARTFIRE emissions available on the 2008 NEI website using the Bluesky framework were evaluated. WestJumpAQMS selected the 2008 FINN fire emissions for initial 2008 modeling because it was more complete (e.g., included Canada) and better documented.[83] For the final PGM applications, the DEASCO3 2008 fire emissions inventory was used.

The DEASCO3 fire emissions specified the lower and top heights of the fire emissions (i.e., plume rise), as was done with the WRAP 2002 fires. In the past, in order to get the fire emissions in the correct vertical layers in CAMx and CMAQ, several virtually point source stacks were define with heights at the center of each vertical layer that required fire emissions. This resulted in using many point sources within each grid cell where a fire occurred in order to inject the emissions into the correct vertical layers. Starting with the WestJumpAQMS 2008 database, a new feature in CAMx was used whereby the top and bottom of the fire plume was defined

81 http://www.epa.gov/airmarkets/
82 http://www.wrapair2.org/pdf/Memo_NH3_Modeling_NextSteps_Sep30_2013.pdf
83 http://www.wrapair2.org/pdf/Memo_5_Fires_Apr27_2012_Final.pdf

and CAMx internally calculates fraction of mass needed to be injected in each vertical layer to obtain a uniform distribution from the bottom to top of the fire plume. This greatly reduced the number of point sources needed as input to represent fires.

8.1.8 Biogenic Emissions

The WestJumpAQMS biogenic emissions were based on a version of MEGAN updated by WRAP to use more representative biomass data for the western U.S. using day-specific satellite Photosynthetically Active Radiation (PAR) and 8-day average Leaf Area Index (LAI) from MODIS satellite measurements.[84] Although biogenic emissions are uncertain, the WestJumpAQMS 2008 biogenic emissions used the best science algorithms and data available. Note that satellite PAR data are no longer archived so that future PGM studies would have to use an alternative source of PAR data, such as from WRF. The WRAP biogenic emissions study found significant differences between the satellite observed PAR and WRF PAR estimates that affect biogenic emissions. However, without anyone processing the satellite data to obtain PAR, there isn't another source of PAR data.

8.1.9 Canada

Canada emissions were based on a 2006 Province level emissions inventory for Criteria Air Contaminant (CAC) from Environment Canada. No process information was provided for point sources so we could not use the usual SMOKE default chemical speciation profiles and temporal allocation schemes by SCC. However, the VOC emissions were speciated into the CB05 chemical classes that were used in WestJumpAQMS. According to the documentation in the 2006 EC emissions files, a 0.25 fugitive dust transport factor (FDTF) was applied to dust emissions (e.g., construction, road dust etc.) to reduce dust emissions by 75% to account for dust emissions that fall out locally to the source and are not transported downwind. However, when working with the 2006 EC inventory in Alberta we discovered that the FDTF was not applied in the 2006 EC inventory so that dust emissions in Canada are overstated by approximately a factor of 4 in the WestJumpAQMS modeling. If used in future modeling studies, the 2008 EC dust emissions should be reduced using FDTFs.

Alberta Environment and Sustainable Research Development (AESRD) has performed or is performing several studies to update the Alberta Provincial emissions inventory to 2010. Other Provinces may be doing similar updates. Future PGM studies should contact the regulatory agencies in Canada to obtain the latest emission inventories.

8.1.10 Mexico Emissions

The WestJumpAQMS used a 2008 emissions inventory that was projected off of a 1999 inventory that was first available in 2006. This inventory is now rather dated and there are likely incremental updates for some locations. Future PGM studies should investigate the availability of updated emissions for Mexico.

8.1.11 Other Emissions

Other emissions include lightning, sea salt and windblown dust (WBD). Lightning NO_X emissions were based on an annual emission estimate for North America allocated to locations and days using the WRF convective activity. This is a simple approach for including lightning NO_X emissions in the modeling and there are more complicated approaches that use lightning ground detect networks and ratios of cloud-to-cloud to cloud-to-ground lightning strikes. However, currently anthropogenic NO_X emissions overwhelm lightning NO_X so the lightning NO_X has little effect on the current year modeling results, especially during high ozone events. Thus, it is questionable whether spending significant extra efforts on lightning emissions is worth the reward since

84 http://www.wrapair2.org/pdf/Memo_9_Biogenics_May9_2012_Final.pdf

even the more detailed approaches are highly uncertain. Lightning emissions will become more important in future years as anthropogenic emissions are reduced or when looking at issues like the North America Background (NAB) that is defined as the level of ozone in the absence of anthropogenic emissions in North America.

Sea salt emissions have a small effect mainly in coastal areas. The pre-processor used for CAMx uses current algorithms and is likely adequate for this emissions parameter. It should be pointed out that when making $PM_{2.5}$ projections the PGM sea salt predictions are not used and instead the future year sea salt concentrations are assumed to be the same as observed in the current year.

WBD emissions in WestJumpAQMS were based on the WRAP WBD model using the 2008 WRF meteorology. The WRAP WBD model is now rather dated and very dependent on the meteorological inputs. The WRAP WBD emissions estimates using the 2008 WRF data produced results that were very different and inconsistent with the 2002 dust emissions based on the WRAP MM5 meteorological modeling. Some of the assumptions in the WRAP WBD model also appear to be questionable, such as no disturbed land in an urban area resulting in no urban WBD emissions. New procedures for developing WBD emissions should be investigated in future PGM studies.

8.2 EMISSIONS MODELING

SMOKE was the primary emissions modeling tool in WestJumpAQMS, although MOVES and MEGAN models were used for on-road mobile and biogenic sources, respectively. There were also several specialty emissions models for sea salt, lightning, fires and WBD that are mentioned above.

8.2.1 Emissions Processing Streams

The processing of the 2008 emissions was split into many emissions processing streams by source category and even subsets of source categories (see Chapter 3). This facilitated the QA/QC of the emissions as it was easier to identify misplaced emissions on a category-by-category basis. It also facilitated the use of source apportionment later in the study as the emissions were already split by source categories so SMOKE reruns were not necessary.

8.2.2 Merging of Emissions

Performing SMOKE emissions modeling with many processing streams results in many model-ready "pre-merged" emission files by source category that need to be merged together to get the final model-ready emission inputs for all source categories. The emissions merging step can take a long time (e.g., a week or more) that needs to be taken into account when estimating model run times.

8.2.3 Quality Assurance/Quality Control

Quality Assurance/Quality Control (QA/QC) is an important and necessary component of emissions modeling. Splitting into multiple processing streams facilitates QA/QC. WestJumpAQMS adapted the WRAP QA/QC approach that includes generating spatial and temporal plots by source category and posting the plots to a website where they can be examined by multiple members of the project team. This approach was used to identify obvious problems, like the MOVES monthly weekend day to weekday fraction issue discussed above. The spatial maps also helped identify an O&G emissions county swapping issues in New Mexico involving San Juan and Sandoval Counties. Since these two counties are adjacent to each other with a lot of the O&G emissions at their intersection, the swapping of the O&G emissions between these two counties was a subtle error to catch. The O&G emissions in these two counties were swapped due to different alphabetical sorting algorithms, where some sorting algorithms treat the space in "San Juan" as a character putting it in front of Sandoval, whereas others ignore the space putting San Juan behind Sandoval in the alphabet.

8.3 METEOROLOGICAL MODELING

The WestJumpAQMS performed 2008 WRF modeling using a 36/12/4 km grid structure with a very large 4 km IMWD that required extensive computational time.

8.3.1 WRF Modeling Domain

In the end, the WestJumpAQMS only used a fraction of the WRF data from the 4 km IMWD for the 4 km DSAD source apportionment modeling and development of the 4 km CARMMS database. Part of the reason for this was the compressed schedule due to waiting for the availability of the 2008 NEIv2 emissions so the size of the source apportionment modeling domains had to be reduced to accommodate the schedule. Future studies should be careful not to define modeling domains bigger than will be used.

8.3.2 Quality Assurance/Quality Control

It is important that the QA/QC process involve multiple people using different tools. Early on in the WestJumpAQMS, a post-processing program was adding up the precipitation incorrectly giving indication that WRF was grossly overestimating precipitation. After several sensitivity tests were performed to try and address this seemingly performance issue, the error in post-processing was discovered. It could have been discovered earlier if more people were examining the results using multiple sets of post-processing tools. In the end it did not affect the schedule for WestJumpAQMS, but it did use up resources unnecessarily.

8.4 MODEL PERFORMANCE EVALUATION

The model performance evaluation was mixed with the model performing better for some species and locations and worse for others.

8.4.1 Model vs. Measurement Incompatibility

There are fundamental differences in some of the measured and modeled species that need to be accounted for in the interpretation of the model performance evaluation. The SANDWICH technique for applying the CSN speciated $PM_{2.5}$ data to the FRM $PM_{2.5}$ mass measurements taking into account measurement artifacts in both technologies introduces the concept of blank mass correction, Particle Bound Water (PRB) and not using the CSN OC measurement but instead obtaining Organic Aerosol (OA) by mass balance difference. Analogous procedures are needed for mappings between the modeled species and the different measurement technologies. For example, where does the blank mass correction fit in with the modeled species? The poorer model performance for OA and other $PM_{2.5}$ (OPM2.5) is partly related to a mismatch in the definitions of the modeled and measured species.

8.4.2 Diagnostic Sensitivity Tests

Performing diagnostic sensitivity simulation to improve model performance has been part of PGM studies for over thirty years. WestJumpAQMS performed numerous WRF sensitivity tests to determine a better performing WRF configuration.[85] Early WestJumpAQMS CAMx simulations using the CNB6 chemical mechanism encountered an ozone overestimation bias in the eastern U.S. so the CB05 chemical mechanism was adopted that alleviated this issue somewhat. WestJumpAQMS also performed a PGM BC sensitivity test using the MOZART and GEOS-Chem Global Chemistry Model (GCM) that is documented in Morris, Jung and Koo (2013[86]). The sensitivity of the model predictions to fires were also investigated (FINN vs. DEASCO3). However, time and resource constraints limited the more thorough investigation of model issues to improve the modeling database.

85 http://www.wrapair2.org/pdf/WestJumpAQMS_2008_Annual_WRF_Final_Report_February29_2012.pdf
86 http://www.wrapair2.org/pdf/Morris_MOZART-GEOS_WestJumpAQMS_Jul10_2013_Draft1.pdf

8.5 SOURCE APPORTIONMENT MODELING

The WestJumpAQMS source apportionment modeling have shown it to be a valuable tool for examining the role of transport in the western U.S. for ozone and PM and related issues (e.g., visibility and deposition). The CSAPR-type analysis suggests that the western U.S. also has ozone transport issues that should not be ignored and transport will become even more important at lower levels of the NAAQS.

8.5.1 Computational Requirements

The computational requirements of the source apportionment algorithms limit the scope and detail of its application, especially for the PSAT PM source apportionment tool. Although there were never any plans to use the PSAT source apportionment for SOA, the compressed schedule for the source apportionment modeling and its computational requirements resulted in some simplifications in the PSAT PM source apportionment modeling: (1) the state-specific PM source apportionment modeling was just performed on 36 km CONUS domain, rather than also using the 12 km WESTUS domain as originally planned; and (2) the source category-specific PM source apportionment just used the 36/12 km domains without the 4 km DSAD as originally planned.

8.5.2 Role of Transport

With the exception of some of the highest urban ozone events, and possibly the winter ozone events that were not studied in WestJumpAQMS, the largest contributor to ozone concentrations in the western U.S. were the boundary conditions (BCs) coming through the boundaries of the 36 km CONUS domain that represent international transport and stratospheric ozone. State-to-state ozone transport was also important in the western U.S. If the ozone NAAQS is lowered, transport will be even more important.

Transport is also important for $PM_{2.5}$, although it tended to be not as important as for ozone. At some of the more pristine locations, the BCs are also important. For example, the top modeled 24-hour $PM_{2.5}$ concentration days at the Grand Canyon were dominated by spring transport of Asian dust through the BCs and fires.

One of the approaches for reducing the computational time that was considered was to perform the source apportionment on just the 12 km or 12/4 km domains without the 36 km CONUS domain. However, this would have severely compromised the interpretation of the results as the BC contributions would have included U.S., Canada and Mexico emission sources. Use of the 36 km CONUS domain in the source apportionment modeling results in a more cleaner interpretation of the role of BCs as mainly due to international transport and stratospheric ozone.

8.5.3 Use of MATS to Source Apportionment Design Values

The use of MATS with the CSAPR-type analysis was straight forward and provided a way to assess state contributions to downwind ozone and $PM_{2.5}$ nonattainment in a manner consistent with CSAPR that was used for the eastern U.S. WestJumpAQMS assessed the ozone and $PM_{2.5}$ contributions for historical conditions (2008) rather than a future year as done in CSAPR so does not provide the forward looking view as needed for a regulatory action. Since WestJumpAQMS is an information gathering exercise, rather than a regulatory rulemaking, this is not a deficiency in the analysis.

Using the source apportionment modeling results to apportion the contributions to an ozone or $PM_{2.5}$ Design Value using the MATS created issues when we tried to bring closure to all the contributions of a current year Design Value (DVC). The sum of all the DVC components from all of the Source Group contributions obtained using MATS did not match the total DVC. There was always an “Unexplained” component when combining the components of the DVC from all of Source Groups using MATS.

For ozone, the Unexplained component was small and was traced to using the MATS default procedure to select the maximum modeled DMAX8 ozone concentrations from an array of grid cells centered on the monitoring site (7 x 7 for 4 km grid resolution) in the 2008 base case and 2008 base case with the ozone contribution from the Source Group removed. The ozone DVC Unexplained portion should be resolved by limiting the MATS analysis to calculate RRFs using just the single grid cell containing the monitoring site (i.e., 1 x 1 array of grid cells).

For annual $PM_{2.5}$, the Unexplained portion of the DVC is larger and is due to four issues: SOA, blank correction, sea salt and PBW. The blank correction and sea salt are held constant based on the components in the observed DVC so should be labeled as such when projecting the source apportionment modeling results on the DVC. Particle Bound Water (PBW) should be allocated to the DVC using the source apportionment SO4, NO3, NH4 and OA contributions following the MATS PBW algorithms. The SOA contribution should also be run through in MATS and the contribution labeled as SOA. This should greatly reduce if not eliminate the Unexplained portion of the annual $PM_{2.5}$ DVC.

For 24-hour $PM_{2.5}$ DVCs, the Unexplained portion has all the issues as described above for the annual $PM_{2.5}$ DVC, but is further complicated by the form of the NAAQS: the three year average of the 98th percentile (i.e., 8th highest with every day data) of 24-hour $PM_{2.5}$ concentrations. When MATS calculates the "future year" 24-hour $PM_{2.5}$ DVF (i.e., with the Source Group's PM contribution removed) it reorders the days that can result in a different day being the 98th percentile 24-hour $PM_{2.5}$ concentration in the DVF than in the DVC. This can result in a large Unexplained portion when summing up the DVC components from all of the Source Groups (DVC-DVF), especially when looking at large emission changes that will more likely result in a re-ordering of the days to recalculate the 98th percentile (e.g., source category source apportionment modeling). To address this issue in future studies, we analyzed how MATS is using the modeling results to project "future year" 24-hour $PM_{2.5}$ DVFs. MATS uses quarterly average RRFs to project 24-hour $PM_{2.5}$ days within each quarter to obtain a new distribution of 24-hour $PM_{2.5}$ days for the "future year" from which the 98th percentile day is calculated. Thus to project the source apportionment modeling results onto the current year 24-hour $PM_{2.5}$ DVC, we should calculate source apportionment for quarterly averages and then weight them by the number of days within the top 2% of the observed 24-hour $PM_{2.5}$ distribution. So instead of source apportionment of the single day that ends up being the 98th percentile day, this provides source apportionment for the top 2% of days, which should be a more robust metric and a better indication of the upper distribution of the daily $PM_{2.5}$ concentrations than focusing on a single day that could be very different from the rest of the high 24-hour $PM_{2.5}$ days.

8.5.4 Source Apportionment Visualization

One of the difficulties in reporting results from ozone and PM source apportionment modeling is that the source apportionment generates so much information that it is impossible to present all of it in a report. This is especially true for the PSAT PM source apportionment. For the State-Specific PM source apportionment we contributions from 107 Source Groups for total PM2.5 mas as well as the six components of PM (SO4, NO3, NH4, EC, OA and OPM2.5) for multiple averaging times (annual and 24-hour) as well as for visibility. In the WestJumpAQMS we adopted the development of interactive spreadsheet Appendices that will allow the user to drill down into the source apportionment results for sites or other parameters of interest. This concept could be further expended to having interactive websites so that the user doesn't have to be bothered by downloading files and the data can be updated more easily.

8.5.5 Data Archiving

The size of the source apportionment simulations outputs make them difficult to archive. The WestJumpAQMS results will be archived by the Three-State Data Warehouse (3SDW). 3SDW has already performed test transfer and independent benchmarks. The remainder of the WestJumpAQMS data will be transferred to the 3SDW in September 2013.

9.0 ACRONYMS

ACHD	Allegheny County Health Department
ACM	Asymmetric Convective Mixing
AES	Applied Envirosolutions
AMET	Atmospheric Model Evaluation Tool
APCA	Anthropogenic Precursor Culpability Assessment
APU	Auxiliary Power Units
AQ	Air Quality
AQRV	Air Quality Related Value
AQS	Air Quality System
BC	Boundary Condition
BEIS	Biogenic Emissions Information System
BLM	Bureau of Land Management
CAFOS	Concentrated Animal Feeding Operations
CAMD	Clean Air Markets Division
CAMx	Comprehensive Air-quality Model with extensions
CARMMS	Colorado Air Resource Management Modeling Study
CASTNet	Clean Air Status and Trends Network
CAVR	Clean Air Visibility Rule
CB05	Carbon Bond mechanism version 5
CB6	Carbon Bond mechanism version 6
CD-C	Continental Divide-Creston
CDPHE	Colorado Department of Health and Environment
CE	Capture Efficiency
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
COSO	BLM Colorado State Office
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
FDTF	Fugitive Dust Transport Factor
FE	Fractional Error
FINN	Fire INventory from NCAR
FLM	Federal Land Manager
FRM	Federal Reference Method
FWS	Fish and Wildlife Service
GCM	Global Chemistry Model
GEOS-Chem	Goddard Earth Observing System (GEOS) global chemistry model
GSE	Ground Support Equipment
HDDM	Higher order Decoupled Direct Method
IAD	Impact Assessment Domain
IMPROVE	Interagency Monitoring of Protected Visual Environments
IMWD	Inter-Mountains West Processing Domain
IPAMS	Independent Petroleum Association of the Mountain States
JSFP	Joint Science Fire Program
LCP	Lambert Conformal Projection
LTO	Landing and Takeoff Operations
LSM	Lane Surface Model
MADIS	Meteorological Assimilation Data Ingest System
MATS	Mercury and Air Toxics Standards
MATS	Modeled Attainment Test Software
MCIP	Meteorology-Chemistry Interface Processor
MEGAN	Model of Emissions of Gases and Aerosols in Nature
MM	Meteorological Model
MM5	Version 5 of the Mesoscale Model
MNGE	Mean Normalized Gross Error
MNB	Mean Normalized Bias
MOVES	Motor Vehicle Emissions Simulator
MOZART	Model for OZone And Related chemical Tracers
NAAQS	National Ambient Air Quality Standard
NAB	North American Background ozone
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
PBW	Particle Bound Water
PGM	Photochemical Grid Model
PiG	Plume-in-Grid
PM	Particulate Matter
PPM	Piecewise Parabolic Method
PSAT	Particulate Source Apportionment Technology
QA	Quality Assurance
QC	Quality Control
RAQC	Regional Air Quality Council
RMC	Regional Modeling Center
RMNP	Rocky Mountain National Park
RMP	Resource Management Plan
ROMANS	Rocky Mountain Atmospheric Nitrogen and Sulfur Study
RPO	Regional Planning Organization
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
TDM	Travel Demand Model
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
WESTUS	Western United States
WRAP	Western Regional Air Partnership
WGA	Western Governors' Association
WRF	Weather Research Forecasting model

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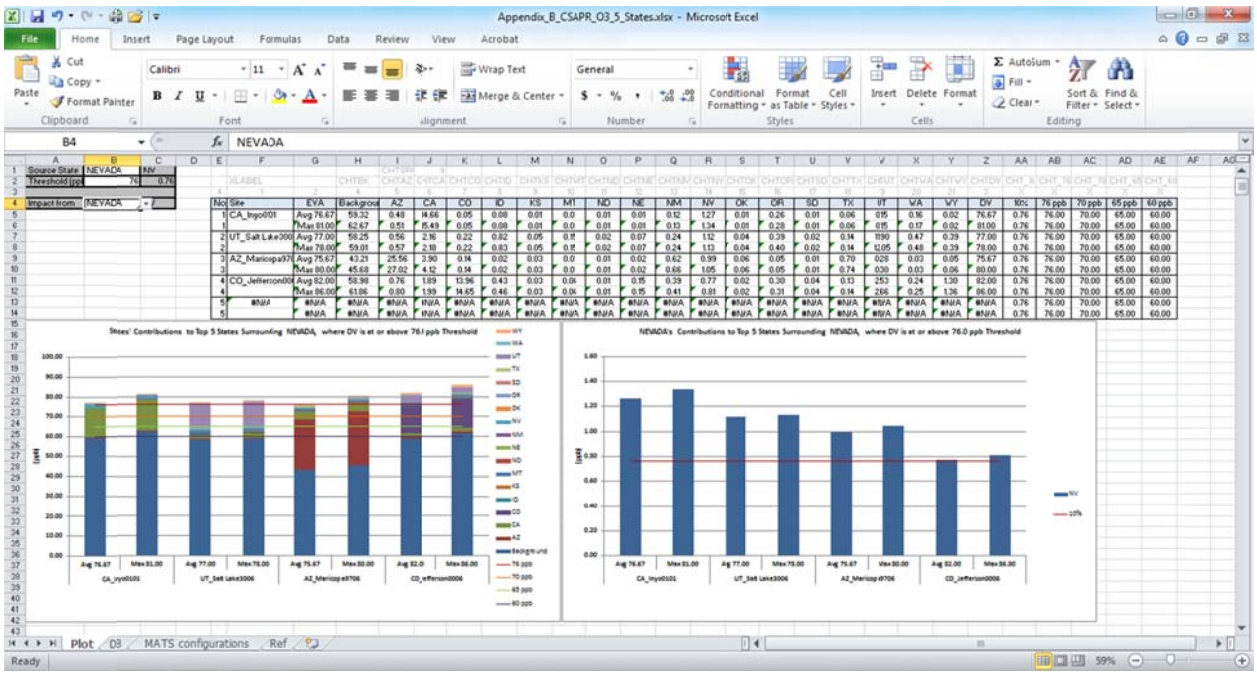
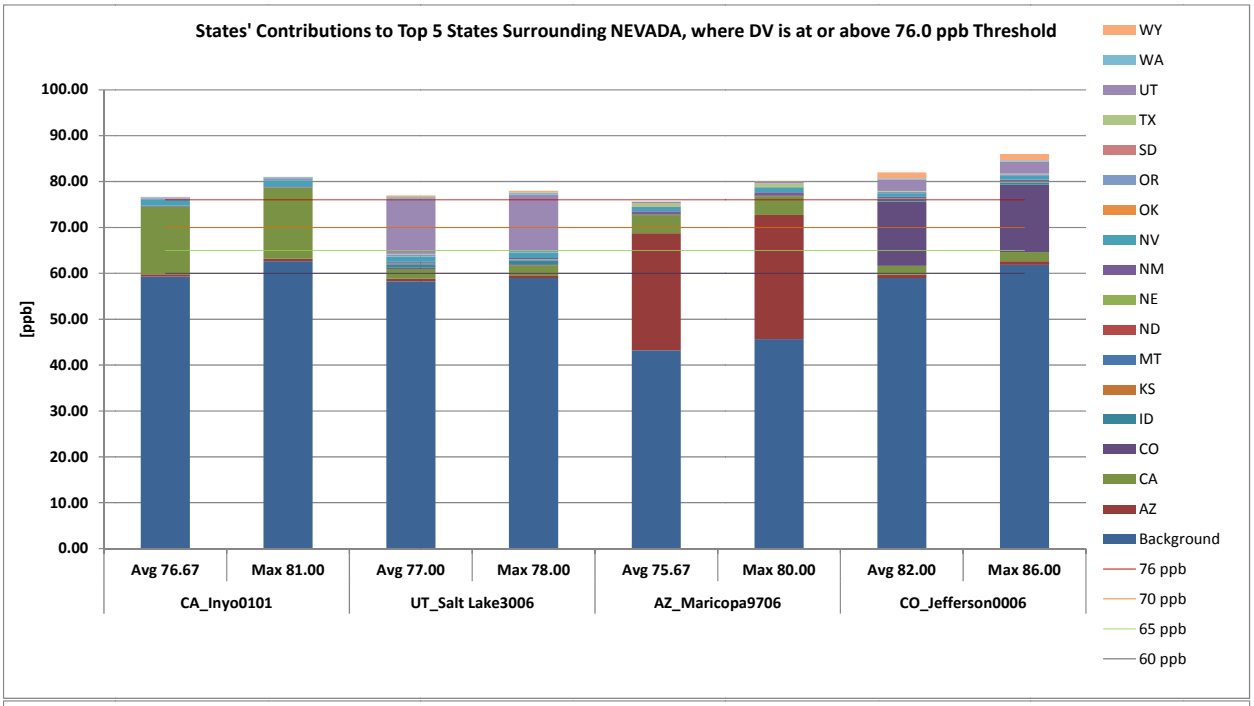
Appendix A

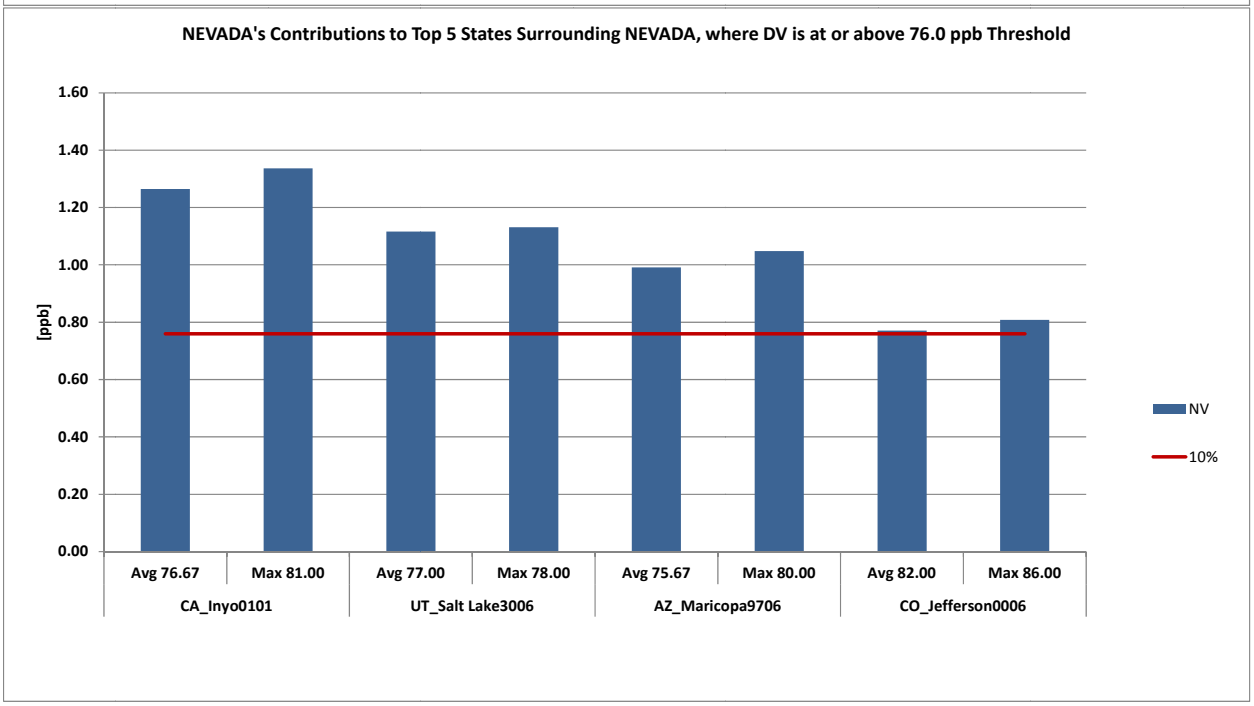
CSAPR-Type Analysis for 2008 Upwind State Highest Contribution to Average and Maximum Ozone Design Values at any Monitoring Site in up to 5 Downwind States using MATS

"Appendix_A_CSAPR_DVO3_5_States.xlsx" (0.4 Mb)

Cell B1 = Select Upwind State (Example for Nevada)
Cell B2 = Select NAAQS Threshold for Analysis (76 ppb for current NAAQS in example)
Cell B4 = Select Upwind State for Contributions (usually same as Cell B1)




States' Contributions to Top 5 States Surrounding NEVADA, where DV is at or above 76.0 ppb Threshold
[ppb]
100.00
90.00
80.00
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00
Avg 76.67
Max 81.00
Avg 77.00
Max 78.00
Avg 75.67
Max 80.00
Avg 82.00
Max 86.00
CA_Inyo0101
UT_Salt Lake3006
AZ_Maricopa9706
CO_Jefferson0006
WY
WA
UT
TX
SD
OR
OK
NV
NM
NE
ND
MT
KS
ID
CO
CA
AZ
Background
76 ppb
70 ppb
65 ppb
60 ppb

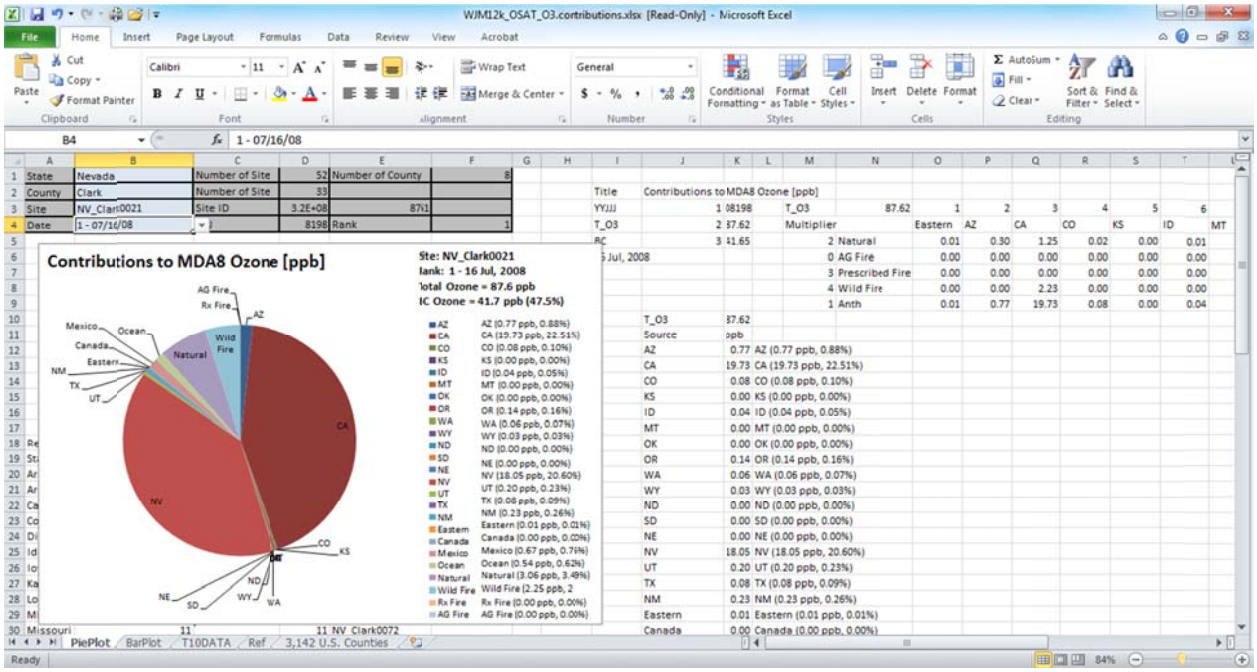

NEVADA's Contributions to Top 5 States Surrounding NEVADA, where DV is at or above 76.0 ppb Threshold
[ppb]
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
Avg 76.67
Max 81.00
Avg 77.00
Max 78.00
Avg 75.67
Max 80.00
Avg 82.00
Max 86.00
CA_Inyo0101
UT_Salt Lake3006
AZ_Maricopa9706
CO_Jefferson0006
NV
10%

Appendix B

State Contributions to Daily Maximum 8-Hour Ozone Concentrations on 10 Highest Modeled Ozone Days in 2008 by Monitoring Site

"Appendix_B_O3_10hi_Model_Days.xlsx" (20.0 Mb)

<u>Sheet#1 = Pie Plot</u>
Cell B1 = State (Example for Nevada)
Cell B2 = County (Example for Clark County)
Cell B3 = Monitoring Site (Example for NV_Clark0021)
Cell B4 = Date of 10 Highest Modeled Ozone Days (Ranked 1 on 7/16/13 in example)

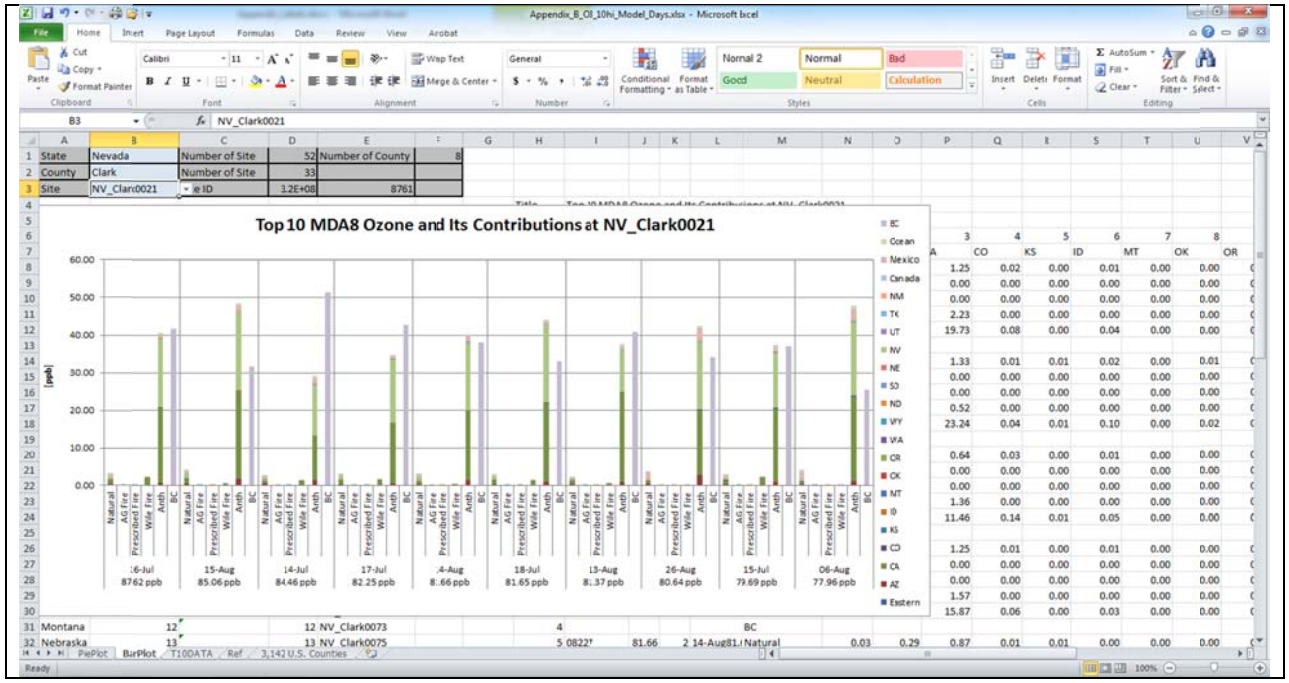


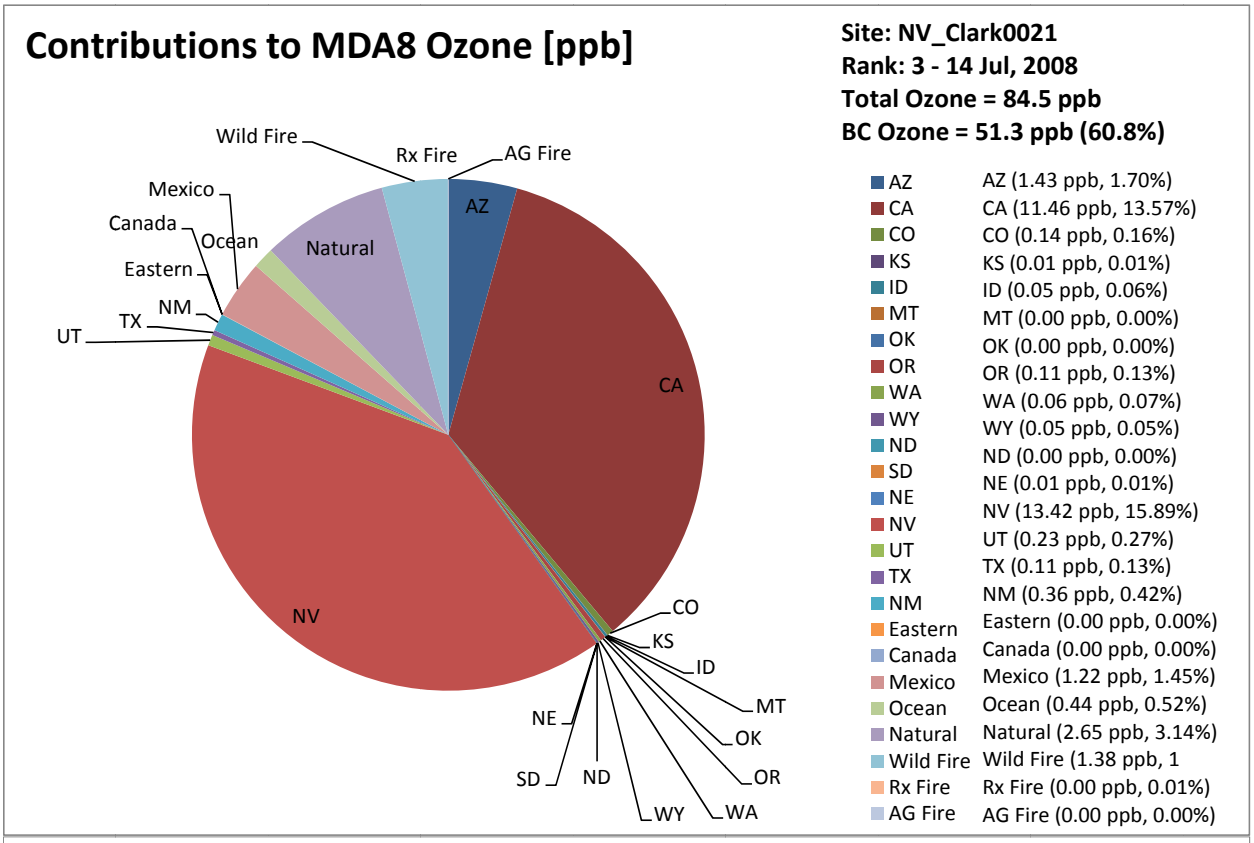
<u>Sheet #2 = Bar Plot</u>

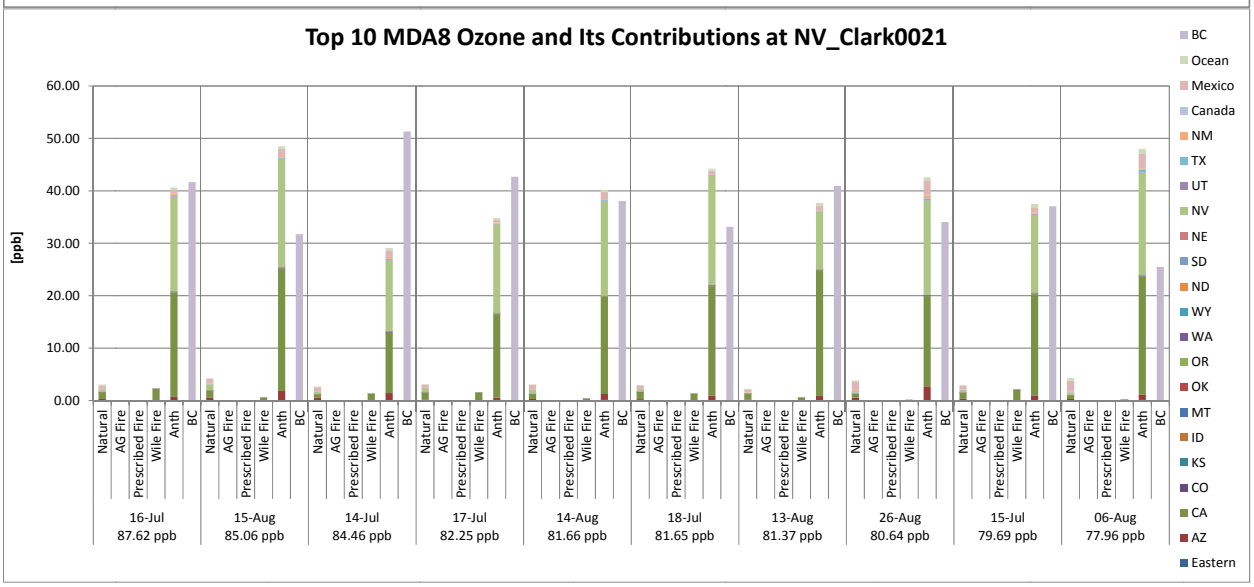
Cell B1 = Select State (Nevada in Example)

Cell B2 = Select County (Clark in Example)

Cell B3 = Select Monitoring Site (NV_Clark0021 in example)




Contributions to MDA8 Ozone [ppb]
Site: NV_Clark0021
Rank: 3 - 14 Jul, 2008
Total Ozone = 84.5 ppb
BC Ozone = 51.3 ppb (60.8%)
Wild Fire
Rx Fire
AG Fire
Mexico
Canada
Ocean
Natural
Eastern
NM
TX
UT
AZ
CA
NV
CO
KS
ID
MT
OK
OR
WA
WY
ND
SD
NE
AZ (1.43 ppb, 1.70%)
CA (11.46 ppb, 13.57%)
CO (0.14 ppb, 0.16%)
KS (0.01 ppb, 0.01%)
ID (0.05 ppb, 0.06%)
MT (0.00 ppb, 0.00%)
OK (0.00 ppb, 0.00%)
OR (0.11 ppb, 0.13%)
WA (0.06 ppb, 0.07%)
WY (0.05 ppb, 0.05%)
ND (0.00 ppb, 0.00%)
NE (0.01 ppb, 0.01%)
NV (13.42 ppb, 15.89%)
UT (0.23 ppb, 0.27%)
TX (0.11 ppb, 0.13%)
NM (0.36 ppb, 0.42%)
Eastern (0.00 ppb, 0.00%)
Canada (0.00 ppb, 0.00%)
Mexico (1.22 ppb, 1.45%)
Ocean (0.44 ppb, 0.52%)
Natural (2.65 ppb, 3.14%)
Wild Fire (1.38 ppb, 1
Rx Fire (0.00 ppb, 0.01%)
AG Fire (0.00 ppb, 0.00%)

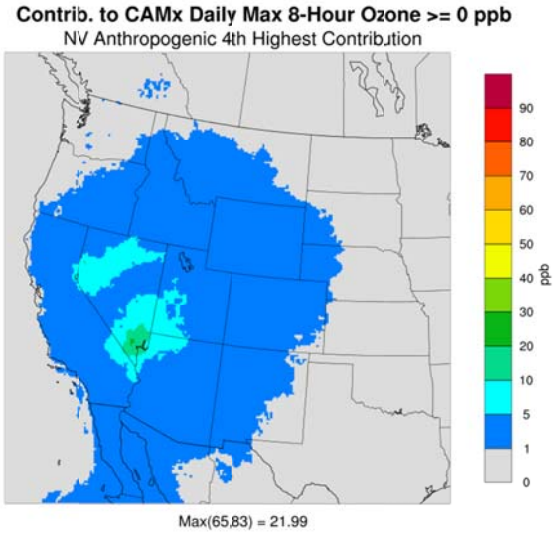

Top 10 MDA8 Ozone and Its Contributions at NV_Clark0021
[ppb]
60.00
50.00
40.00
30.00
20.00
10.00
0.00
Natural
AG Fire
Prescribed Fire
Wile Fire
Anth
BC
16-Jul
87.62 ppb
15-Aug
85.06 ppb
14-Jul
84.46 ppb
17-Jul
82.25 ppb
14-Aug
81.66 ppb
18-Jul
81.65 ppb
13-Aug
81.37 ppb
26-Aug
80.64 ppb
15-Jul
79.69 ppb
06-Aug
77.96 ppb
BC
Ocean
Mexico
Canada
NM
TX
UT
NV
NE
SD
ND
WY
WA
OR
OK
MT
ID
KS
CO
CA
AZ
Eastern

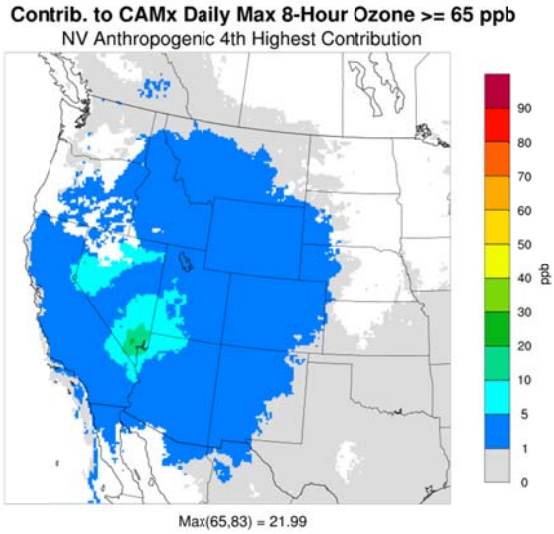
Appendix C

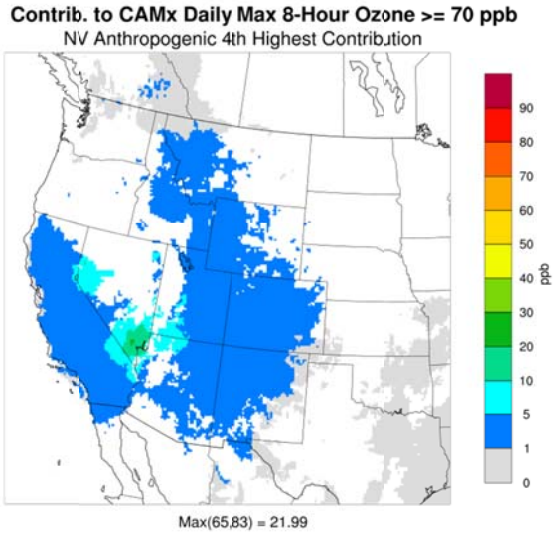
Spatial Maps of State-Specific Anthropogenic Emissions Contributions to Highest and Fourth Highest Modeled Daily Maximum 8-Hour Ozone Concentrations during 2008 Greater than 76 (current NAAQS), 70, 65, 60 (potential future NAAQS) and 0 (maximum contribution) ppb across the 12 km WESTUS and 36 km CONUS Domains

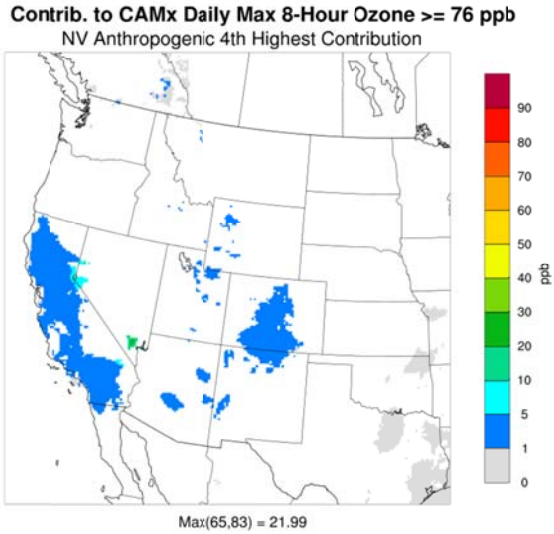
"Appendix_C_Spatial_O3_Anthro_State.zip" (38.2 Mb)

Examples follow for Nevada and Fourth Highest DMAX8 Ozone


Contrib. to CAMx Daily Max 8-Hour Ozone >= 0 ppb
NV Anthropogenic 4th Highest Contribution
90
80
70
60
50
40
30
20
10
5
1
0
ppb
Max(65,83) = 21.99


Contrib. to CAMx Daily Max 8-Hour Ozone >= 65 ppb
NV Anthropogenic 4th Highest Contribution
90
80
70
60
50
40
30
20
10
5
1
0
ppb
Max(65,83) = 21.99


Contrib. to CAMx Daily Max 8-Hour Ozone >= 70 ppb
NV Anthropogenic 4th Highest Contribution
90
80
70
60
50
40
30
20
10
5
1
0
ppb
Max(65,83) = 21.99


Contrib. to CAMx Daily Max 8-Hour Ozone >= 76 ppb
NV Anthropogenic 4th Highest Contribution
90
80
70
60
50
40
30
20
10
5
1
0
ppb
Max(65,83) = 21.99

Appendix D

CSAPR-Type Analysis for 2008 Upwind State Highest Contribution to Annual $PM_{2.5}$ Design Values in up to Five Downwind States using MATS

"Appendix_D_CSAPR_DVannPM_5_States.xlsx" (12.6 Mb)

<u>Plot1—Up to 5 Downwind States with Maximum Total Annual PM2.5 DV Greater than Threshold with "Significant" Contribution</u>

Cell B2 = Select Upwind State (Example for California)

Cell B3 = Select PM Species (Example for PM2.5)

Cell B4 = Select Annual $PM_{2.5}$ NAAQS Threshold for Analysis (12 µg/m^3 in Example)

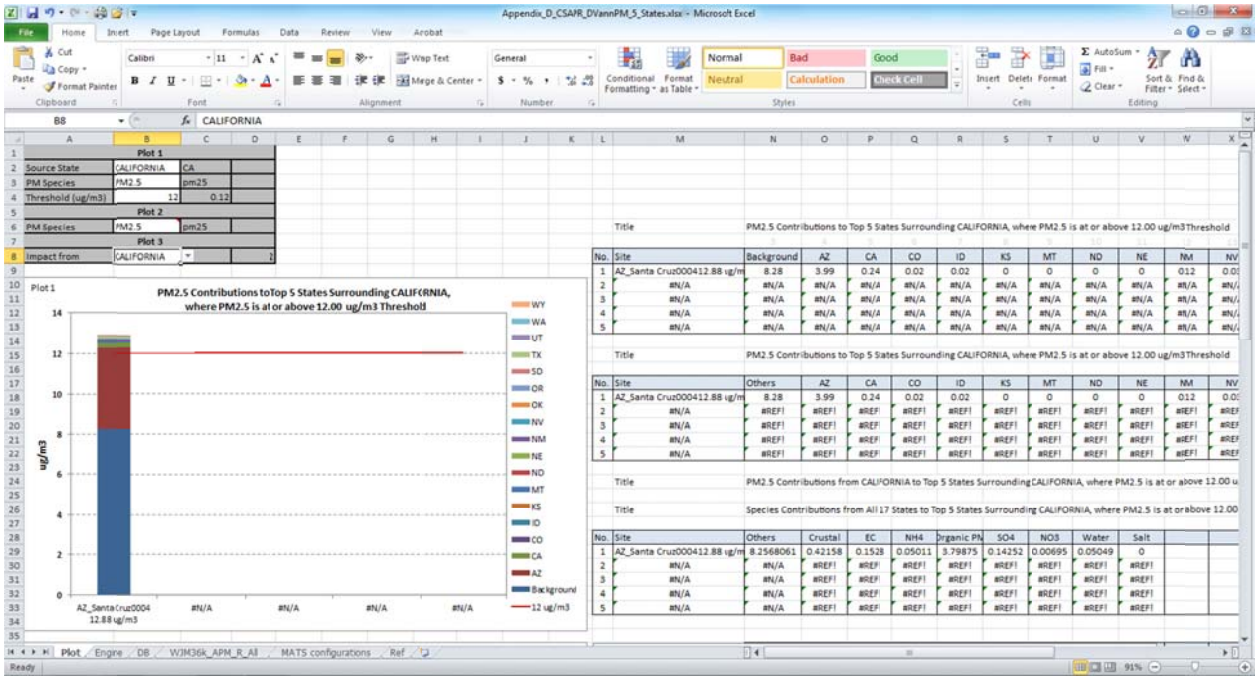
<u>Plot 2 – Total Concentration for Selected PM2.5 Species</u>

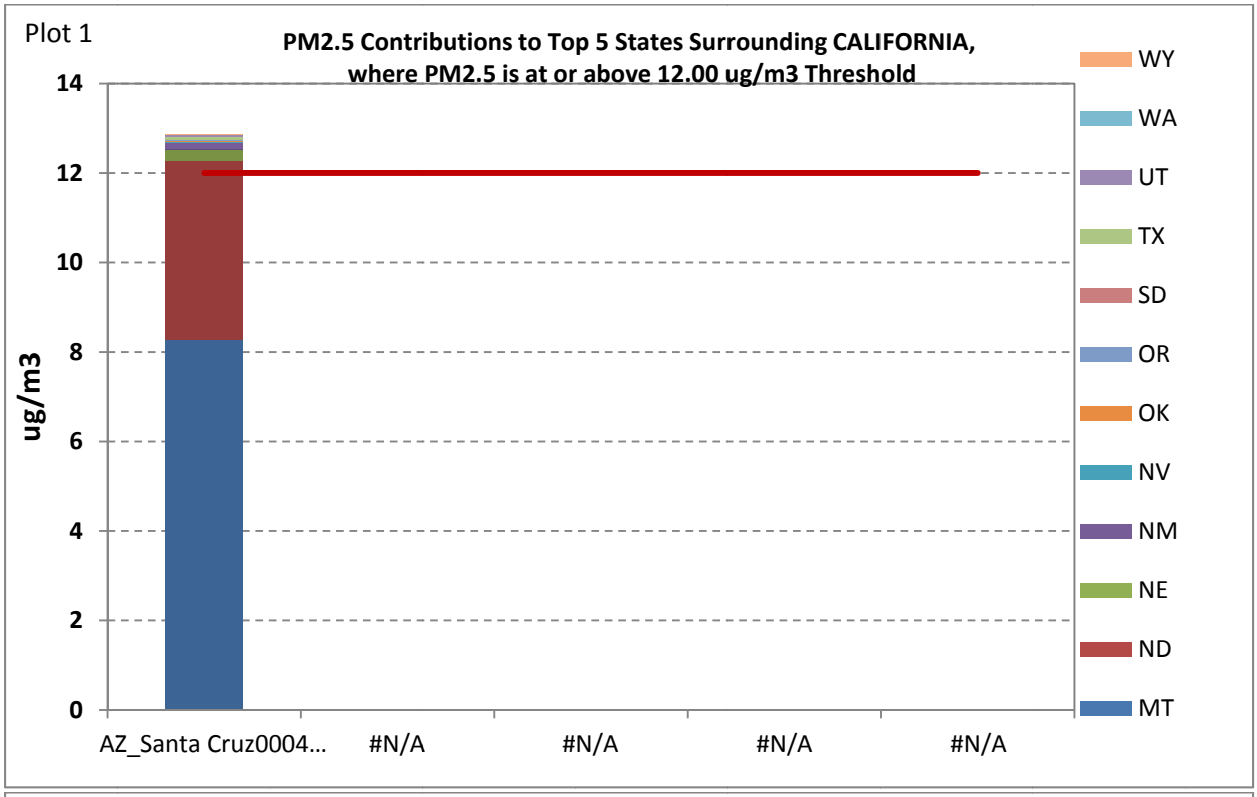
Cell B4 = PM2.5 Species (PM2.5 in Example so same as Plot1)

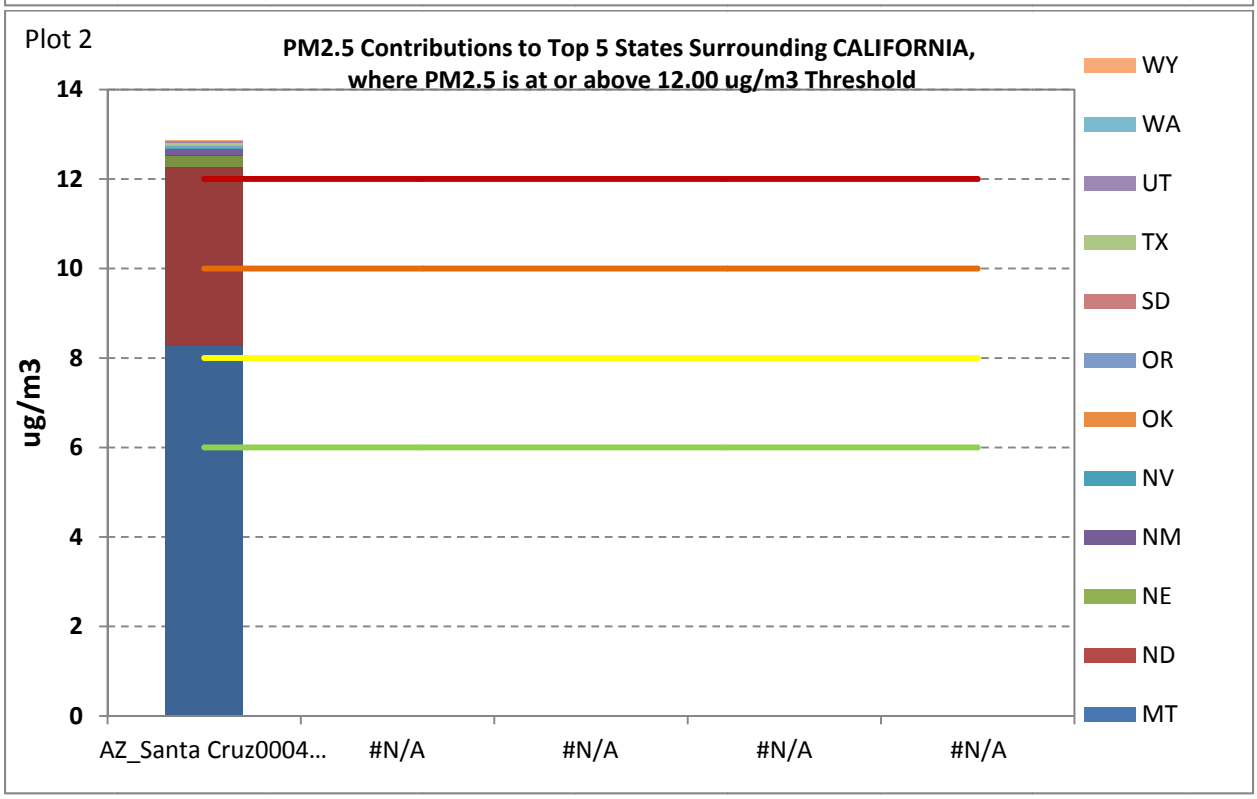
<u>Plot 3 – Upwind State PM2.5 Contribution to Downwind State Annual PM2.5 DV</u>

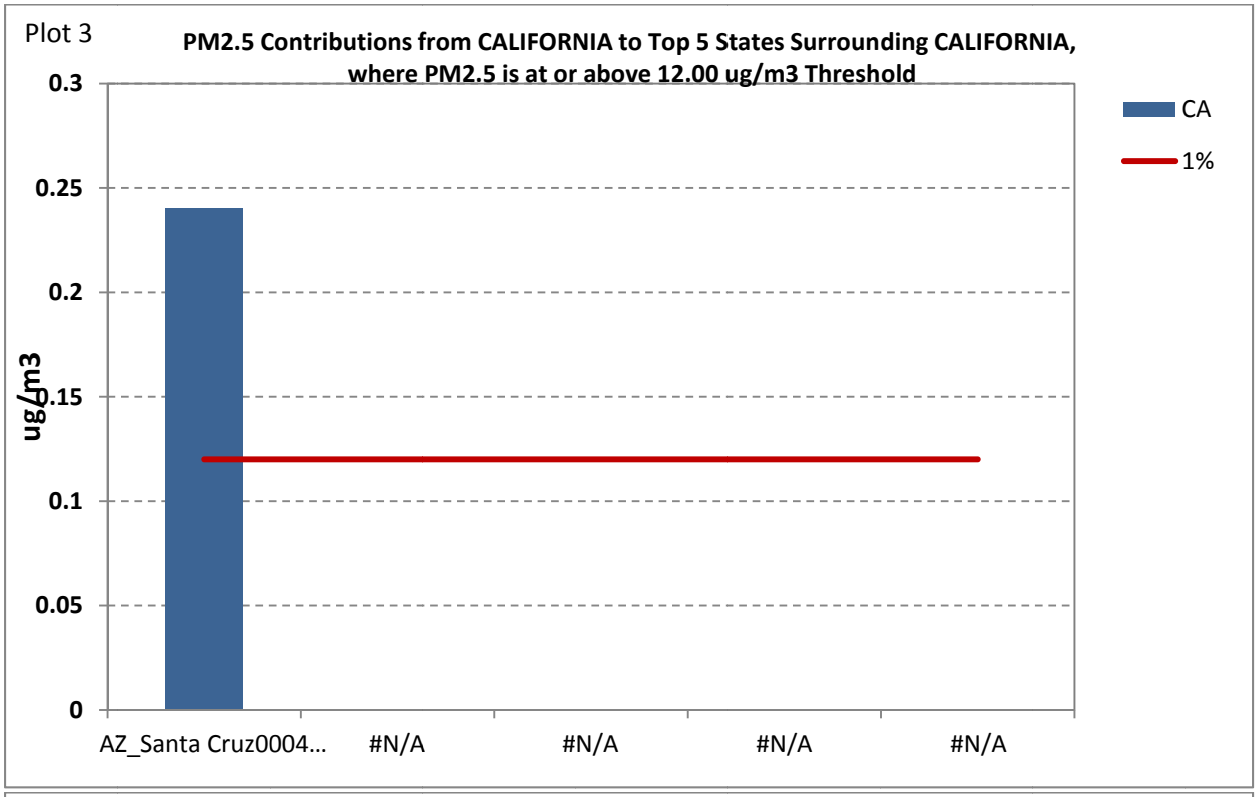
Cell B8 = Upwind State for Contribution (Example for California)

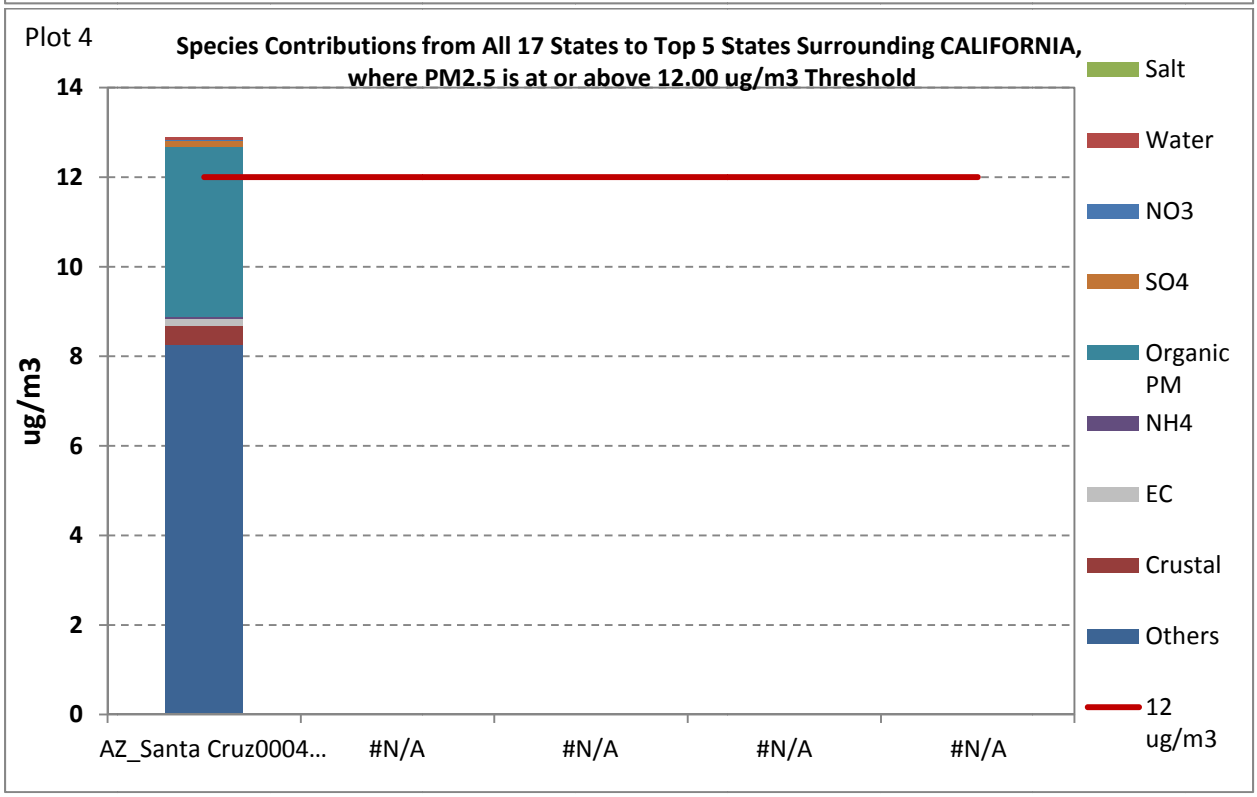
<u>Plot 4 – Species Contributions from 17 Western States + Remainder</u>




Plot 1
PM2.5 Contributions to Top 5 States Surrounding CALIFORNIA, where PM2.5 is at or above 12.00 ug/m3 Threshold
ug/m3
14
12
10
8
6
4
2
0
AZ_Santa Cruz0004...
#N/A
#N/A
#N/A
#N/A
WY
WA
UT
TX
SD
OR
OK
NV
NM
NE
ND
MT


Plot 2
PM2.5 Contributions to Top 5 States Surrounding CALIFORNIA, where PM2.5 is at or above 12.00 ug/m3 Threshold
ug/m3
14
12
10
8
6
4
2
0
AZ_Santa Cruz0004...
#N/A
#N/A
#N/A
#N/A
WY
WA
UT
TX
SD
OR
OK
NV
NM
NE
ND
MT


Plot 3
PM2.5 Contributions from CALIFORNIA to Top 5 States Surrounding CALIFORNIA, where PM2.5 is at or above 12.00 ug/m3 Threshold
ug/m3
0.3
0.25
0.2
0.15
0.1
0.05
0
AZ_Santa Cruz0004...
#N/A
#N/A
#N/A
#N/A
CA
1%

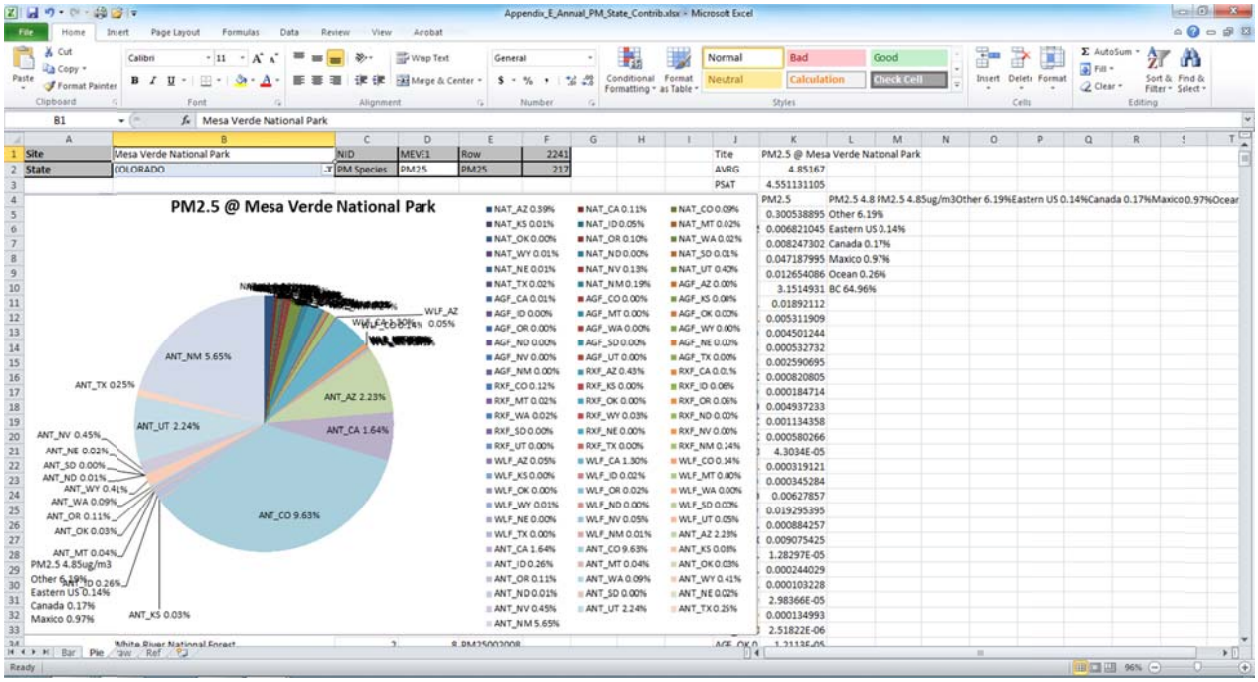

Plot 4
Species Contributions from All 17 States to Top 5 States Surrounding CALIFORNIA, where PM2.5 is at or above 12.00 ug/m3 Threshold
ug/m3
14
12
10
8
6
4
2
0
AZ_Santa Cruz0004...
#N/A
#N/A
#N/A
#N/A
Salt
Water
NO3
SO4
Organic PM
NH4
EC
Crustal
Others
12 ug/m3

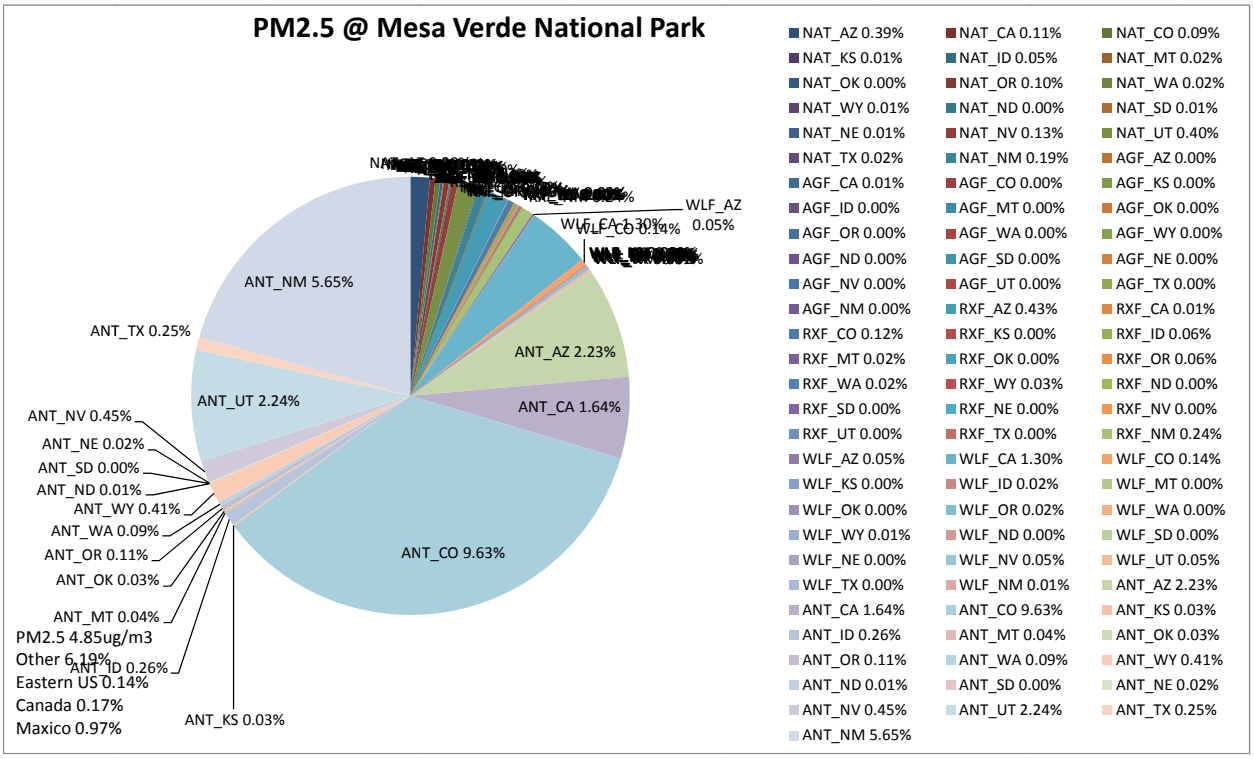
Appendix E

State Contributions to Modeled Annual $PM_{2.5}$ Concentrations in 2008 by Monitoring Site

"Appendix_E_Annual_PM_State_Contrib.xlsx" (23.8 Mb)

Cell B2 = State (Example for Colorado)
Cell B1 = Monitor in State (B2) (Example for Mesa Verde)




PM2.5 @ Mesa Verde National Park
WLF_AZ 0.05%
WLF_CA 1.30%
WLF_CO 0.14%
ANT_NM 5.65%
ANT_TX 0.25%
ANT_AZ 2.23%
ANT_CA 1.64%
ANT_UT 2.24%
ANT_NV 0.45%
ANT_NE 0.02%
ANT_SD 0.00%
ANT_ND 0.01%
ANT_WY 0.41%
ANT_WA 0.09%
ANT_OR 0.11%
ANT_OK 0.03%
ANT_MT 0.04%
PM2.5 4.85ug/m3
Other 6.19%
ANT_ID 0.26%
Eastern US 0.14%
Canada 0.17%
Maxico 0.97%
ANT_KS 0.03%
ANT_CO 9.63%
NAT_AZ 0.39%
NAT_CA 0.11%
NAT_CO 0.09%
NAT_KS 0.01%
NAT_ID 0.05%
NAT_MT 0.02%
NAT_OK 0.00%
NAT_OR 0.10%
NAT_WA 0.02%
NAT_WY 0.01%
NAT_ND 0.00%
NAT_SD 0.01%
NAT_NE 0.01%
NAT_NV 0.13%
NAT_UT 0.40%
NAT_TX 0.02%
NAT_NM 0.19%
AGF_AZ 0.00%
AGF_CA 0.01%
AGF_CO 0.00%
AGF_KS 0.00%
AGF_ID 0.00%
AGF_MT 0.00%
AGF_OK 0.00%
AGF_OR 0.00%
AGF_WA 0.00%
AGF_WY 0.00%
AGF_ND 0.00%
AGF_SD 0.00%
AGF_NE 0.00%
AGF_NV 0.00%
AGF_UT 0.00%
AGF_TX 0.00%
AGF_NM 0.00%
RXF_AZ 0.43%
RXF_CA 0.01%
RXF_CO 0.12%
RXF_KS 0.00%
RXF_ID 0.06%
RXF_MT 0.02%
RXF_OK 0.00%
RXF_OR 0.06%
RXF_WA 0.02%
RXF_WY 0.03%
RXF_ND 0.00%
RXF_SD 0.00%
RXF_NE 0.00%
RXF_NV 0.00%
RXF_UT 0.00%
RXF_TX 0.00%
RXF_NM 0.24%
WLF_AZ 0.05%
WLF_CA 1.30%
WLF_CO 0.14%
WLF_KS 0.00%
WLF_ID 0.02%
WLF_MT 0.00%
WLF_OK 0.00%
WLF_OR 0.02%
WLF_WA 0.00%
WLF_WY 0.01%
WLF_ND 0.00%
WLF_SD 0.00%
WLF_NE 0.00%
WLF_NV 0.05%
WLF_UT 0.05%
WLF_TX 0.00%
WLF_NM 0.01%
ANT_AZ 2.23%
ANT_CA 1.64%
ANT_CO 9.63%
ANT_KS 0.03%
ANT_ID 0.26%
ANT_MT 0.04%
ANT_OK 0.03%
ANT_OR 0.11%
ANT_WA 0.09%
ANT_WY 0.41%
ANT_ND 0.01%
ANT_SD 0.00%
ANT_NE 0.02%
ANT_NV 0.45%
ANT_UT 2.24%
ANT_TX 0.25%
ANT_NM 5.65%

Appendix F

CSAPR-Type Analysis for 2008 Upwind State Highest Contribution to 24-Hour $PM_{2.5}$ Design Values in up to Five Downwind States using MATS

"Appendix_F_CSAPR_DV24PM_5_States.xlsx" (12.8 Mb)

Plot1—Up to 5 Downwind States with Maximum Total 24-Hour $PM_{2.5}$ DV Greater than Threshold with "Significant" Contribution

Cell B2 = Select Upwind State (Example for California)

Cell B3 = Select PM Species (Example for PM2.5)

Cell B4 = Select 24-Hour $PM_{2.5}$ NAAQS Threshold for Analysis (35 µg/m^3 in Example)

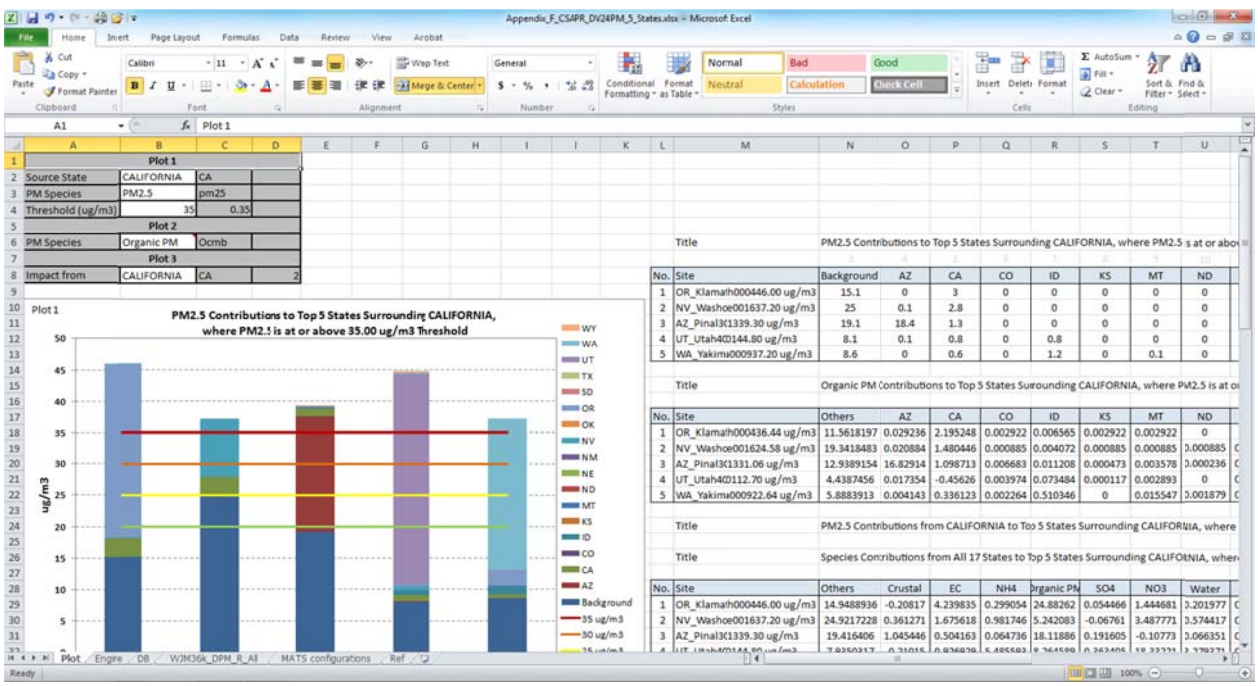
Plot 2 – Total Concentration for Selected $PM_{2.5}$ Species

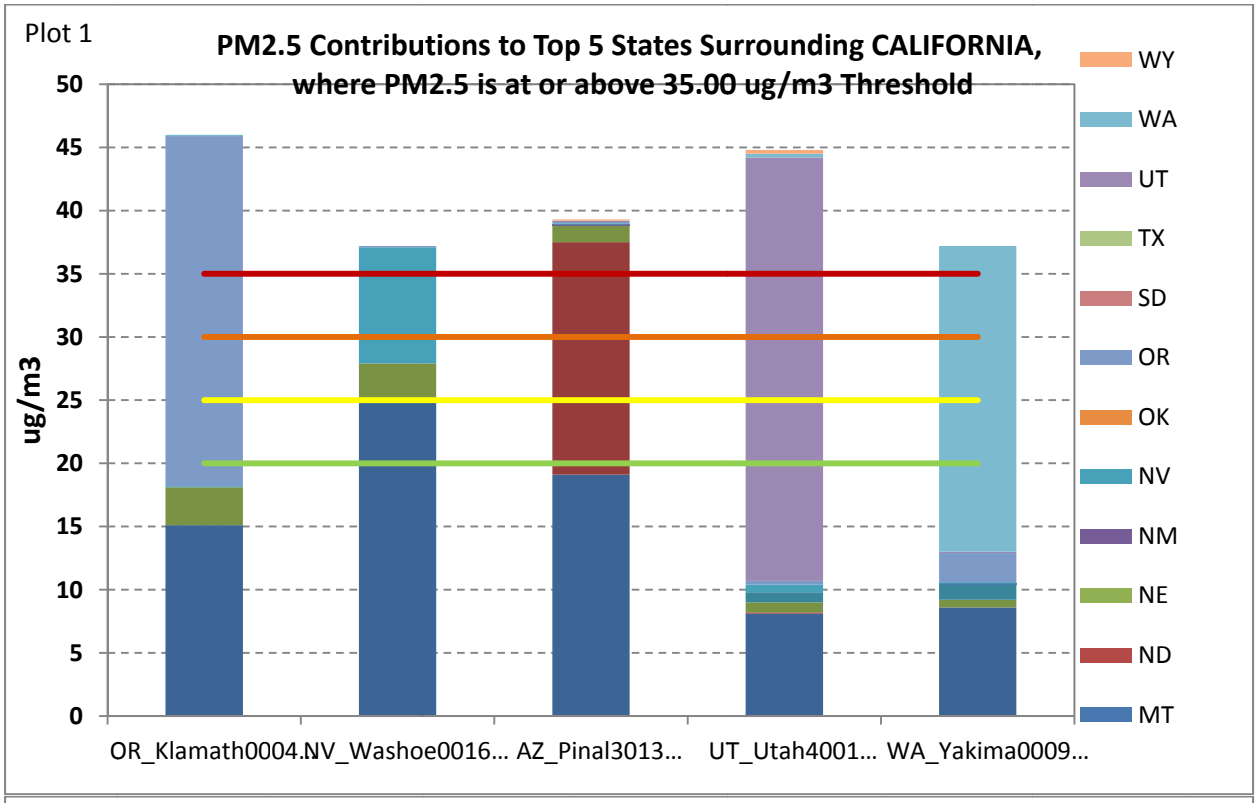
Cell B4 = Select PM2.5 Species (Organic Carbon in Example)

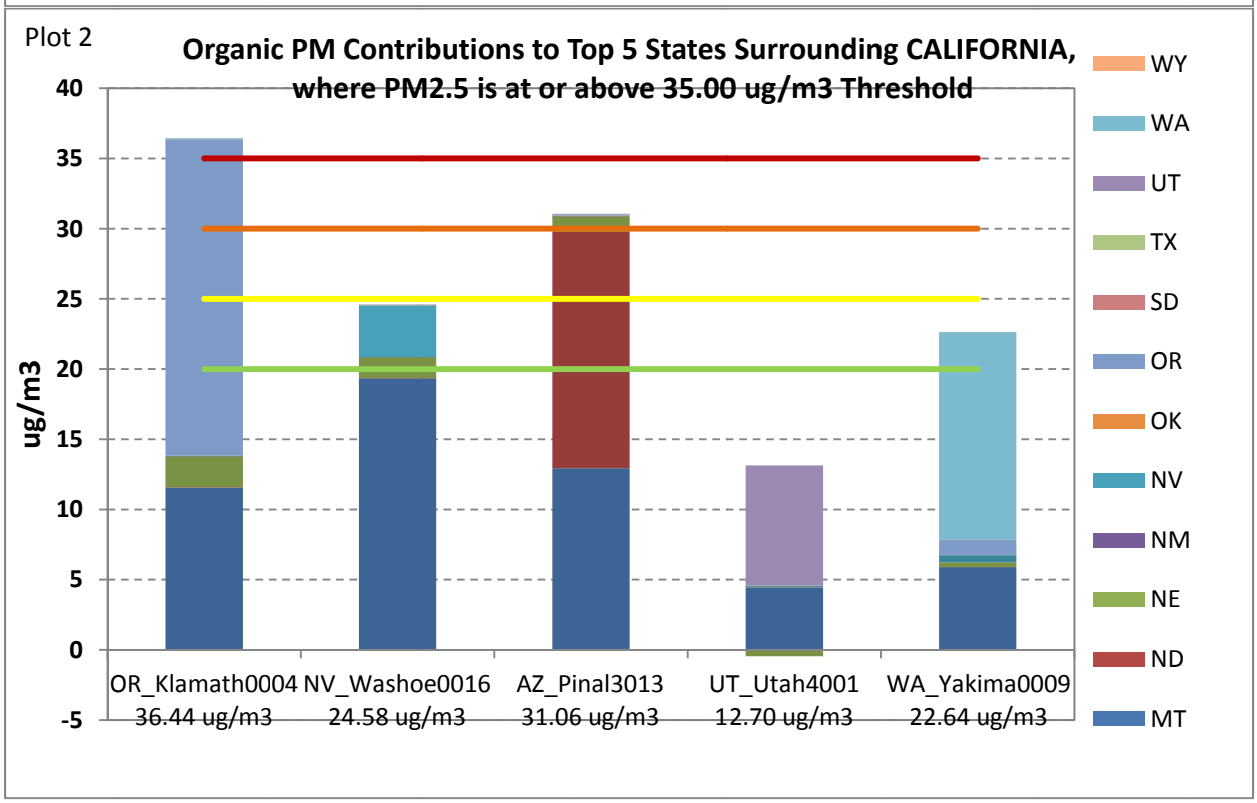
Plot 3 – Upwind State $PM_{2.5}$ Contribution to Downwind State 24-Hour $PM_{2.5}$ DV

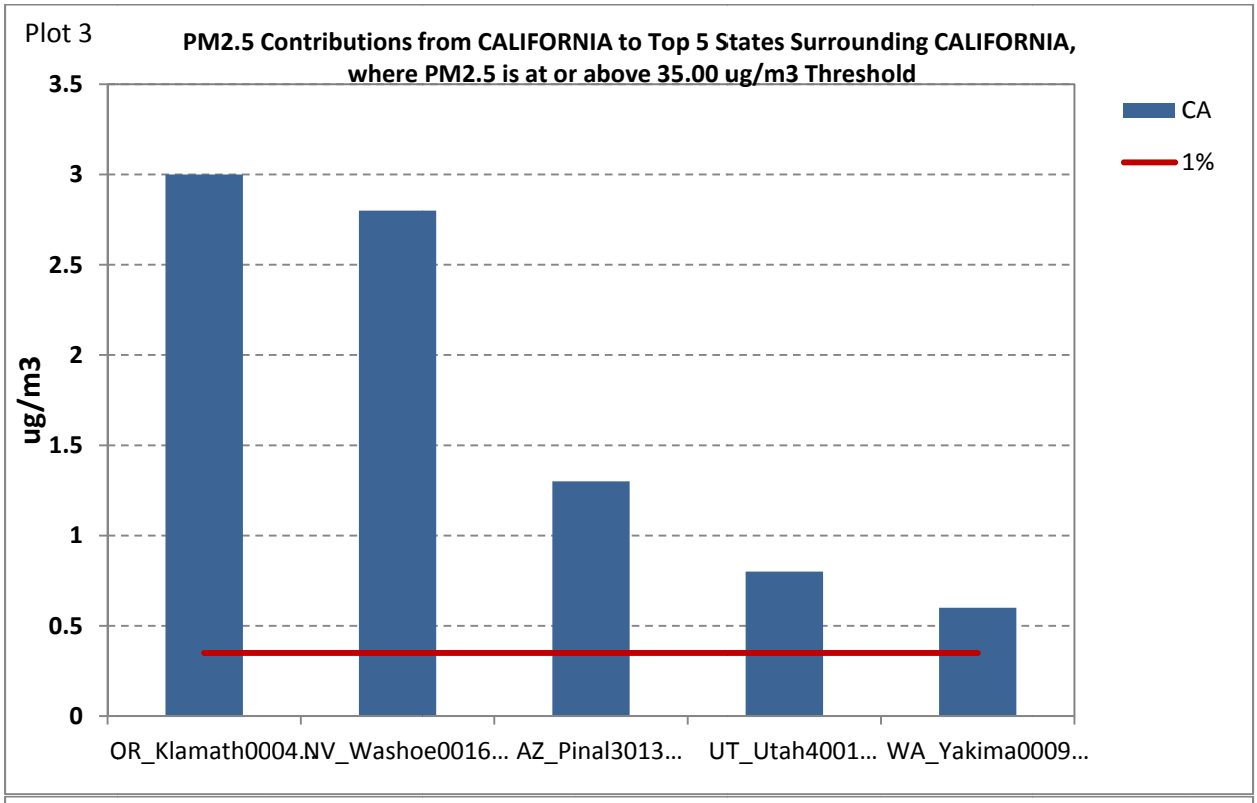
Cell B8 = Upwind State for Contribution (Example for California)

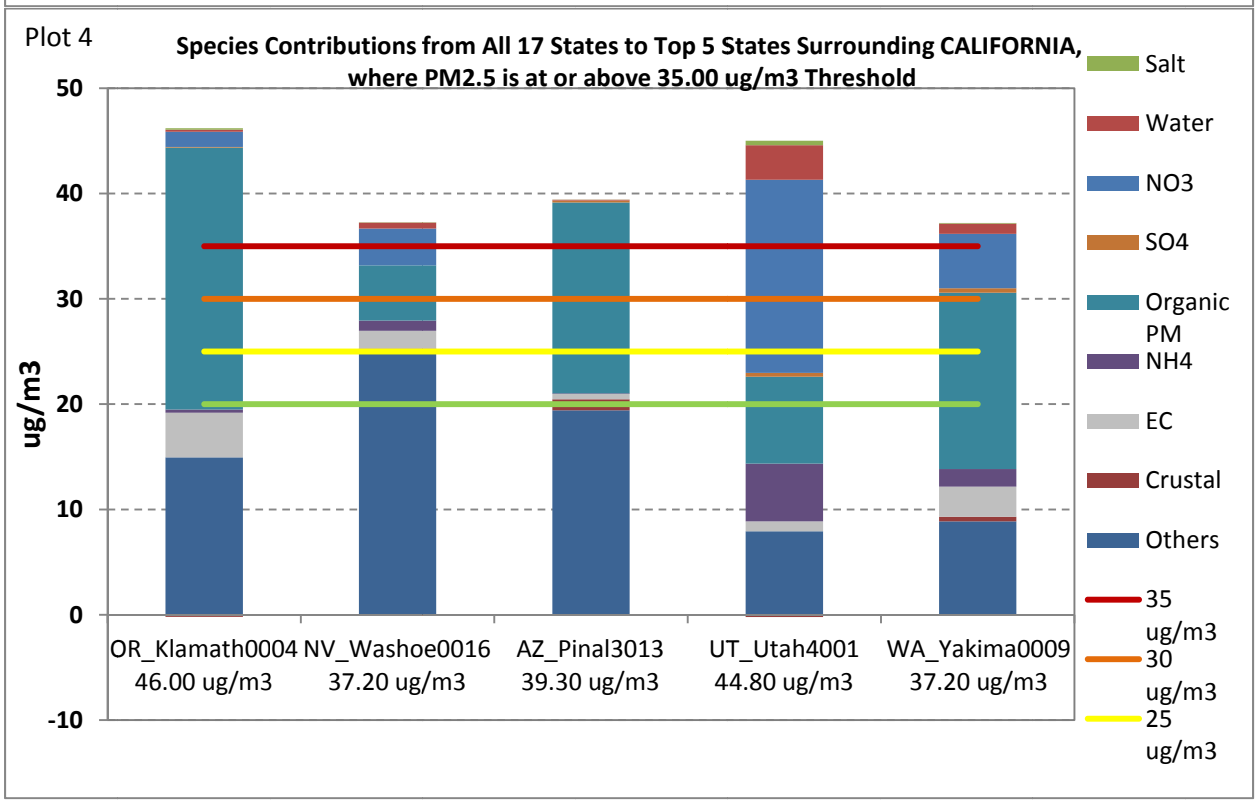
Plot 4 – Species Contributions from 17 Western States + Remainder




Plot 1
PM2.5 Contributions to Top 5 States Surrounding CALIFORNIA, where PM2.5 is at or above 35.00 ug/m3 Threshold
ug/m3
50
45
40
35
30
25
20
15
10
5
0
OR_Klamath0004.
NV_Washoe0016...
AZ_Pinal3013...
UT_Utah4001...
WA_Yakima0009...
WY
WA
UT
TX
SD
OR
OK
NV
NM
NE
ND
MT


Plot 2
Organic PM Contributions to Top 5 States Surrounding CALIFORNIA, where PM2.5 is at or above 35.00 ug/m3 Threshold
ug/m3
40
35
30
25
20
15
10
5
0
-5
OR_Klamath0004
36.44 ug/m3
NV_Washoe0016
24.58 ug/m3
AZ_Pinal3013
31.06 ug/m3
UT_Utah4001
12.70 ug/m3
WA_Yakima0009
22.64 ug/m3
WY
WA
UT
TX
SD
OR
OK
NV
NM
NE
ND
MT


Plot 3
PM2.5 Contributions from CALIFORNIA to Top 5 States Surrounding CALIFORNIA, where PM2.5 is at or above 35.00 ug/m3 Threshold
ug/m3
3.5
3
2.5
2
1.5
1
0.5
0
OR_Klamath0004...
NV_Washoe0016...
AZ_Pinal3013...
UT_Utah4001...
WA_Yakima0009...
CA
1%

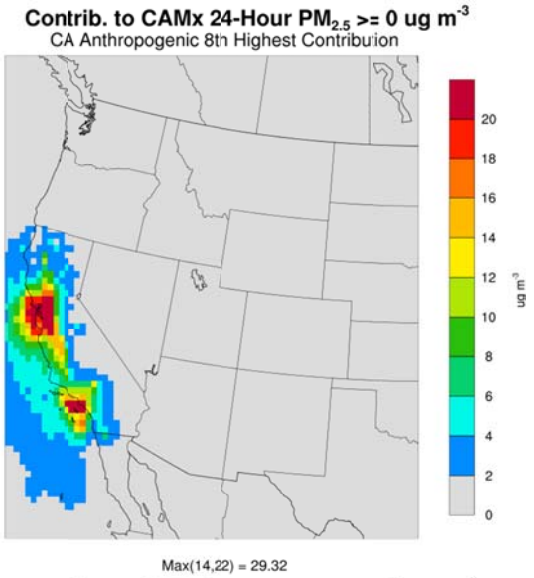

Plot 4
Species Contributions from All 17 States to Top 5 States Surrounding CALIFORNIA, where PM2.5 is at or above 35.00 ug/m3 Threshold
ug/m3
50
40
30
20
10
0
-10
OR_Klamath0004 46.00 ug/m3
NV_Washoe0016 37.20 ug/m3
AZ_Pinal3013 39.30 ug/m3
UT_Utah4001 44.80 ug/m3
WA_Yakima0009 37.20 ug/m3
Salt
Water
NO3
SO4
Organic PM
NH4
EC
Crustal
Others
35 ug/m3
30 ug/m3
25 ug/m3

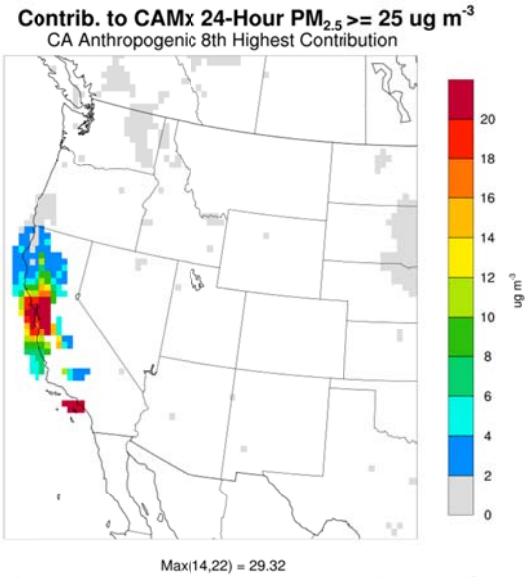
Appendix G

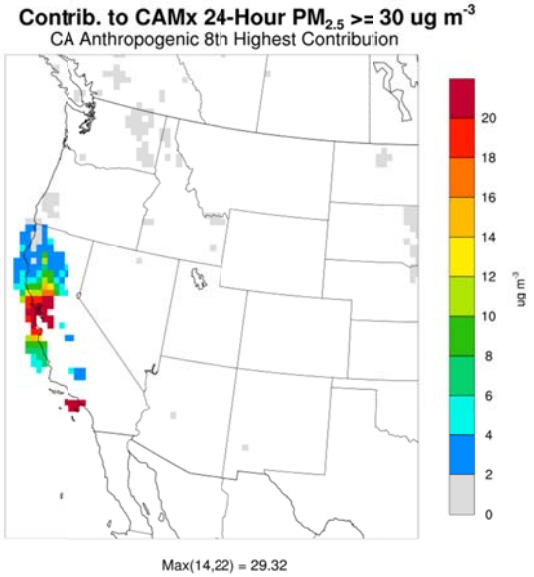
Spatial Maps of Modeled State-Specific Anthropogenic Emissions Contributions to Highest (1stmax) and Eighth (8thmax) Highest 24-Hour $PM_{2.5}$ Concentrations during 2008 greater than 35 (current NAAQS), 30, 25, 20 and 0 (maximum contribution) $\mu g/m^3$.

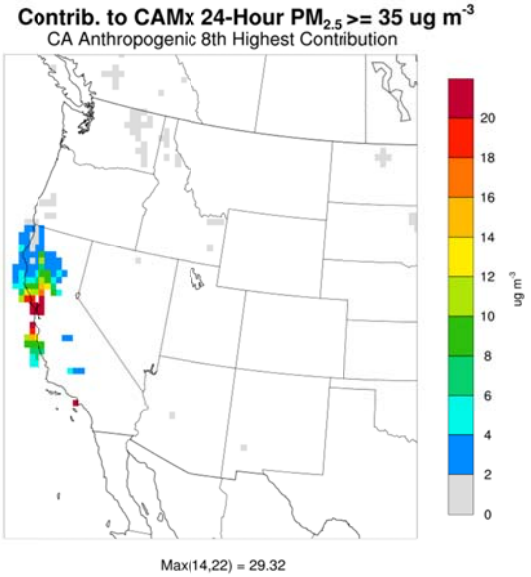
"Appendix_G_Spatial_24PM_Anthro_State.zip" (13.4 Mb)

Example follows for 8th High 24-Hour $PM_{2.5}$ and California


Contrib. to CAMx 24-Hour PM2.5 >= 0 ug m-3
CA Anthropogenic 8th Highest Contribution
20
18
16
14
12
10
8
6
4
2
0
ug m-3
Max(14,22) = 29.32


Contrib. to CAMx 24-Hour PM2.5 >= 25 ug m-3
CA Anthropogenic 8th Highest Contribution
20
18
16
14
12
10
8
6
4
2
0
ug m-3
Max(14,22) = 29.32


Contrib. to CAMx 24-Hour PM2.5 >= 30 ug m-3
CA Anthropogenic 8th Highest Contribution
20
18
16
14
12
10
8
6
4
2
0
ug m-3
Max(14,22) = 29.32


Contrib. to CAMx 24-Hour PM2.5 >= 35 ug m-3
CA Anthropogenic 8th Highest Contribution
20
18
16
14
12
10
8
6
4
2
0
ug m-3
Max(14,22) = 29.32

Appendix H

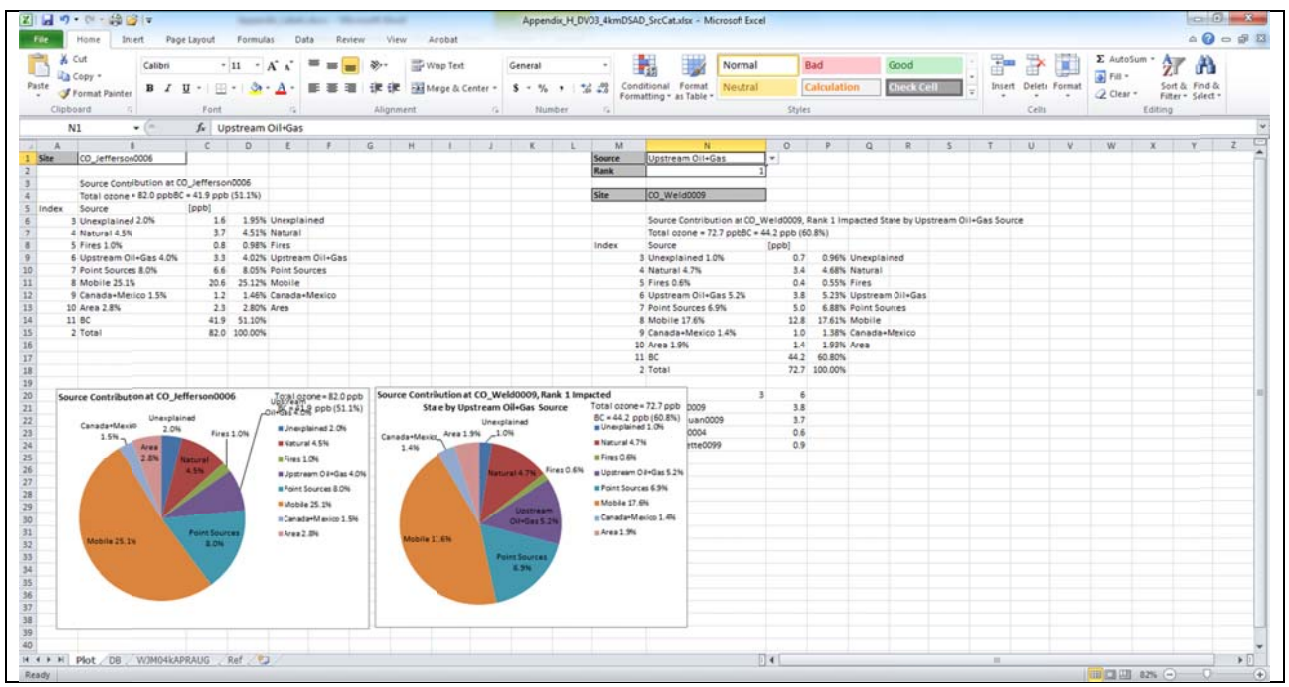
Source Category-Specific Contributions to 8-Hour Ozone Design Values at Monitoring Sites in the 4 km Detailed Source Apportionment Domain (DSAD) using MATS

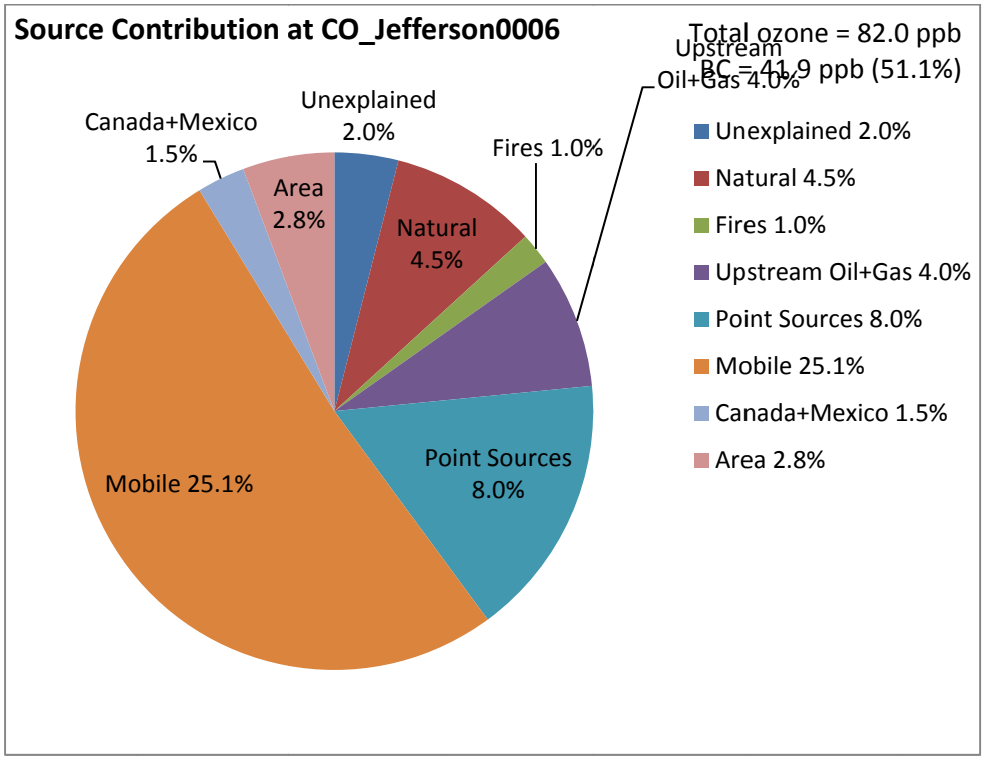
Cell B1 = Select Monitor in the DSAD Domain (CO_Jefferson0006 in example)

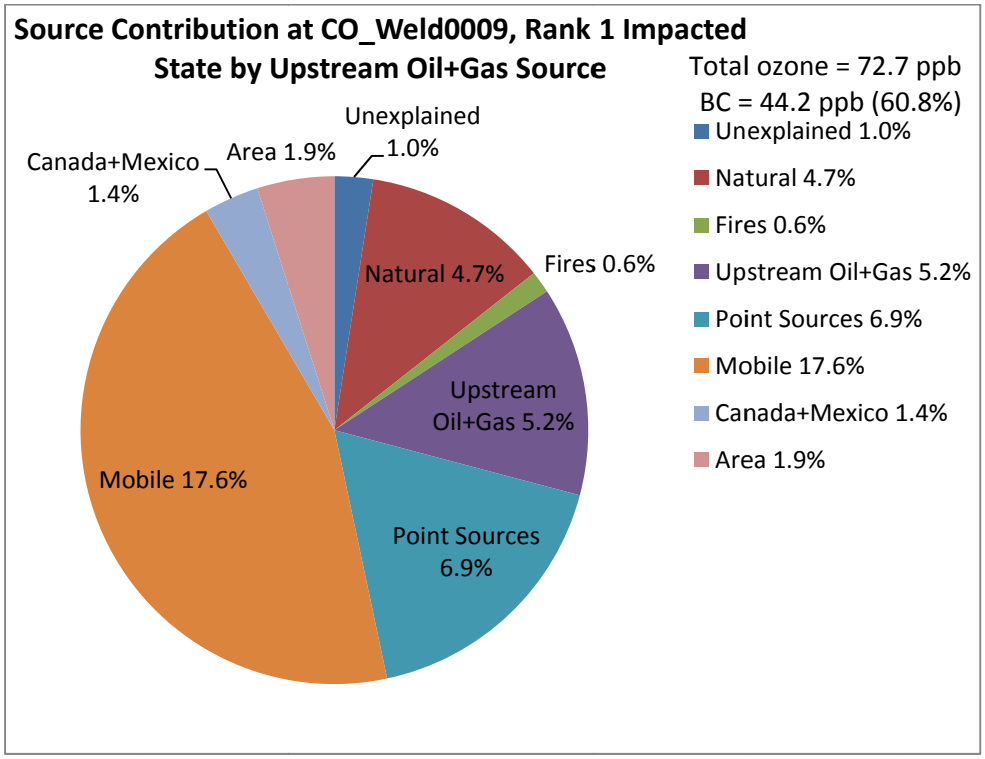
Maximum Contribution to 8-Hour Ozone Design Values in Each DSAD State (CO, NM, UT and WY) due to Major Source Categories using MATS

Cell N1 = Source Category Selected (Upstream Oil and Gas in example)
Cell N2 = Rank 1 through 4 (Example selects state with highest O&G contribution)
Cell N4 = Identifies monitor with highest source category contribution (CO_Weld0009 in example)

"Appendix_H_DVO3_4kmDSAD_SrcCat.xlsx" (0.09 Mb)




Source Contribution at CO_Jefferson0006
Total ozone = 82.0 ppb
BC = 41.9 ppb (51.1%)
Unexplained 2.0%
Natural 4.5%
Fires 1.0%
Upstream Oil+Gas 4.0%
Point Sources 8.0%
Mobile 25.1%
Canada+Mexico 1.5%
Area 2.8%
Unexplained 2.0%
Natural 4.5%
Fires 1.0%
Upstream Oil+Gas 4.0%
Point Sources 8.0%
Mobile 25.1%
Canada+Mexico 1.5%
Area 2.8%

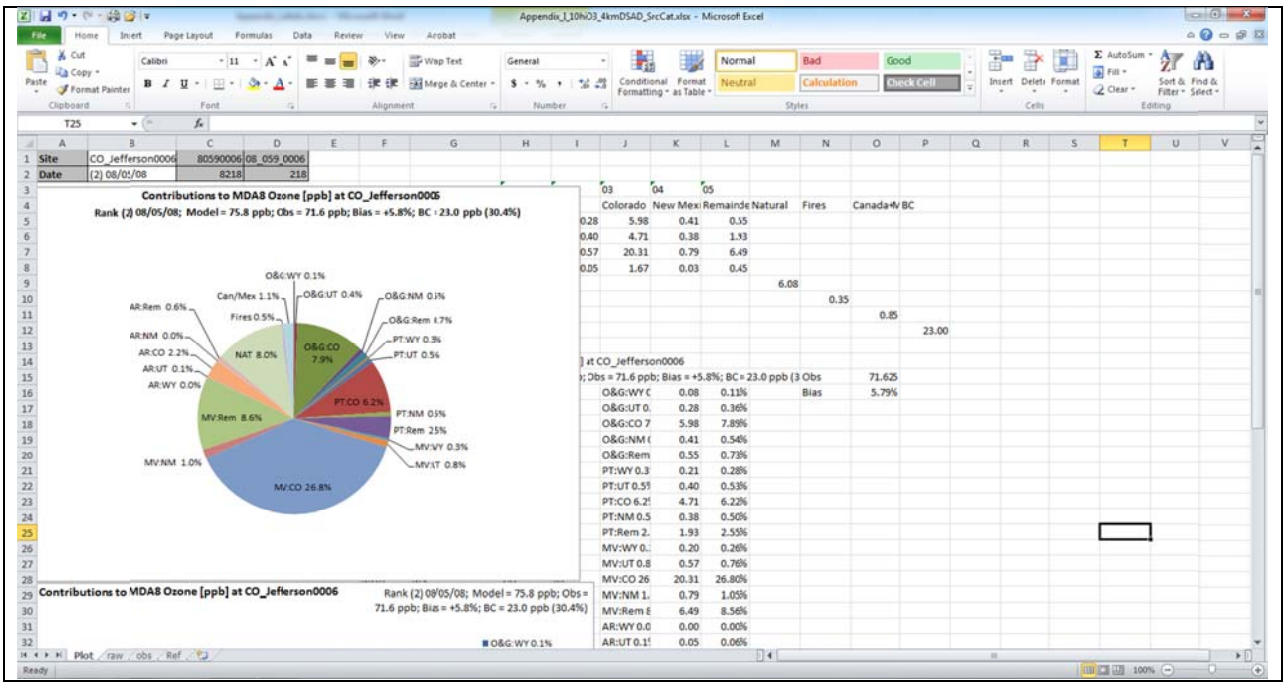

Source Contribution at CO_Weld0009, Rank 1 Impacted State by Upstream Oil+Gas Source
Total ozone = 72.7 ppb
BC = 44.2 ppb (60.8%)
Unexplained 1.0%
Natural 4.7%
Fires 0.6%
Upstream Oil+Gas 5.2%
Point Sources 6.9%
Mobile 17.6%
Canada+Mexico 1.4%
Area 1.9%
Unexplained 1.0%
Natural 4.7%
Fires 0.6%
Upstream Oil+Gas 5.2%
Point Sources 6.9%
Mobile 17.6%
Canada+Mexico 1.4%
Area 1.9%

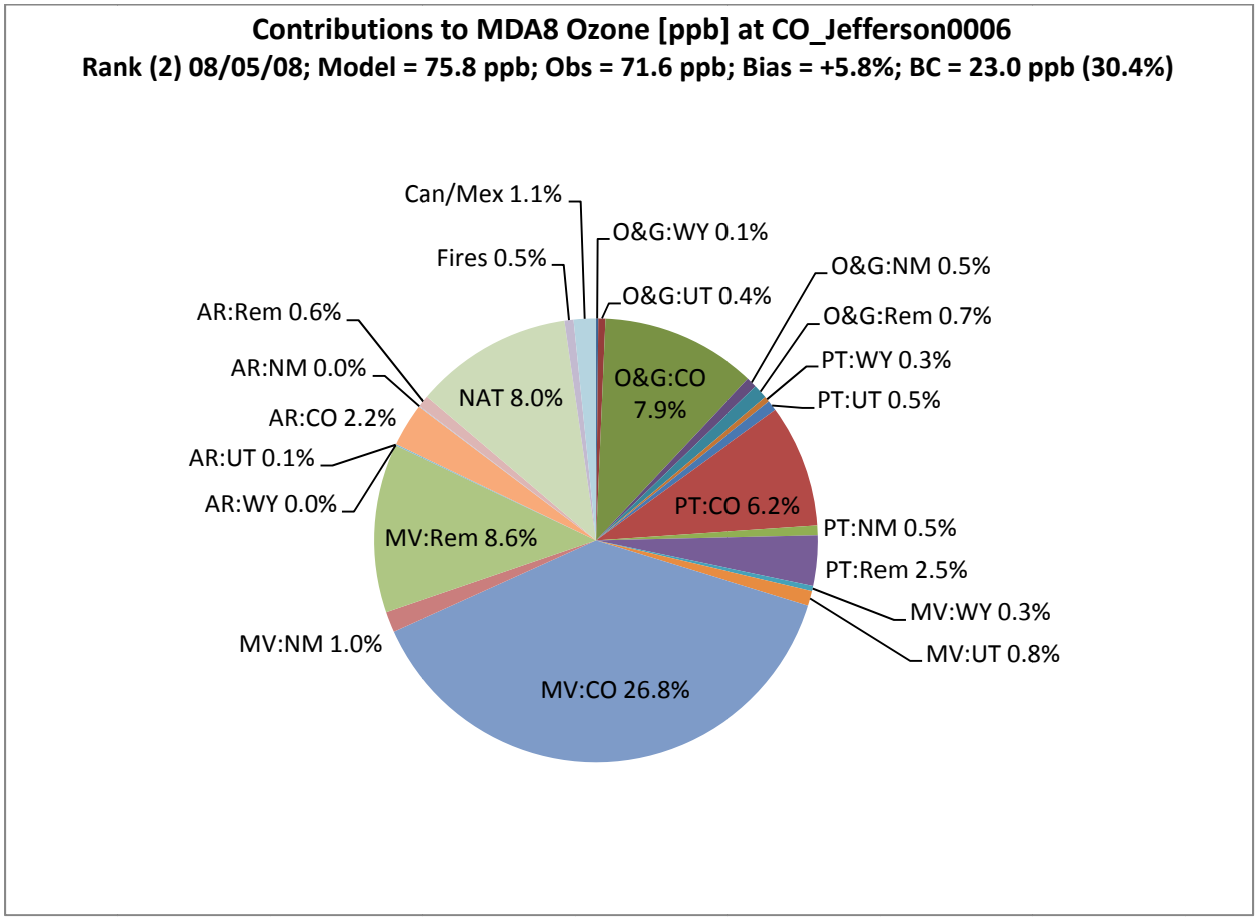
Appendix I

Source Category-Specific Contributions to Ten Highest Modeled Daily Maximum 8-Hour Ozone Concentrations at Monitoring Sites in the 4 km Detailed Source Apportionment Domain (DSAD)

"Appendix_I_10hiO3_4kmDSAD_SrcCat.xlsx" (2.3 Mb)

Cell B1 = Select Monitor in the DSAD Domain (CO_Jefferson0006 in example)
Cell B2 = Select Rank 1 through 10 (2 in example that gives 08/05/08 date)



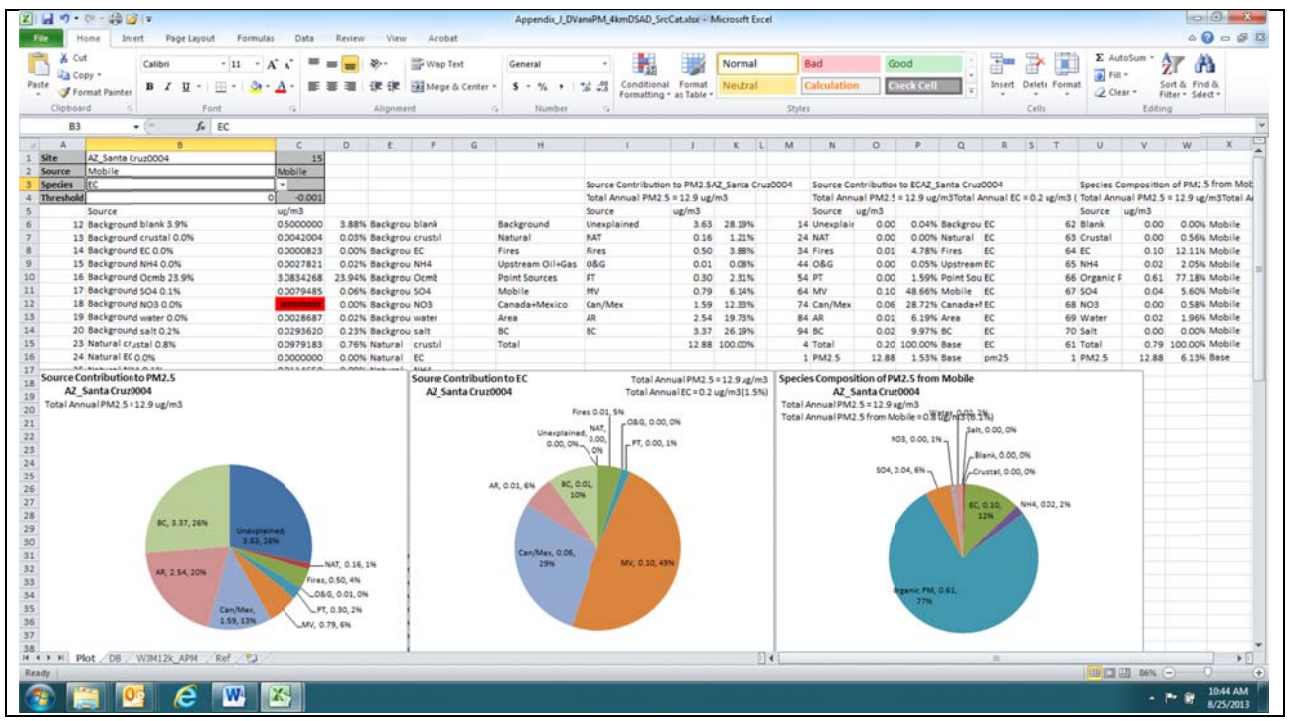

Contributions to MDA8 Ozone [ppb] at CO_Jefferson0006
Rank (2) 08/05/08; Model = 75.8 ppb; Obs = 71.6 ppb; Bias = +5.8%; BC = 23.0 ppb (30.4%)
Can/Mex 1.1%
O&G:WY 0.1%
Fires 0.5%
O&G:NM 0.5%
O&G:UT 0.4%
AR:Rem 0.6%
O&G:Rem 0.7%
AR:NM 0.0%
PT:WY 0.3%
NAT 8.0%
O&G:CO 7.9%
PT:UT 0.5%
AR:CO 2.2%
AR:UT 0.1%
AR:WY 0.0%
PT:CO 6.2%
PT:NM 0.5%
MV:Rem 8.6%
PT:Rem 2.5%
MV:WY 0.3%
MV:NM 1.0%
MV:UT 0.8%
MV:CO 26.8%

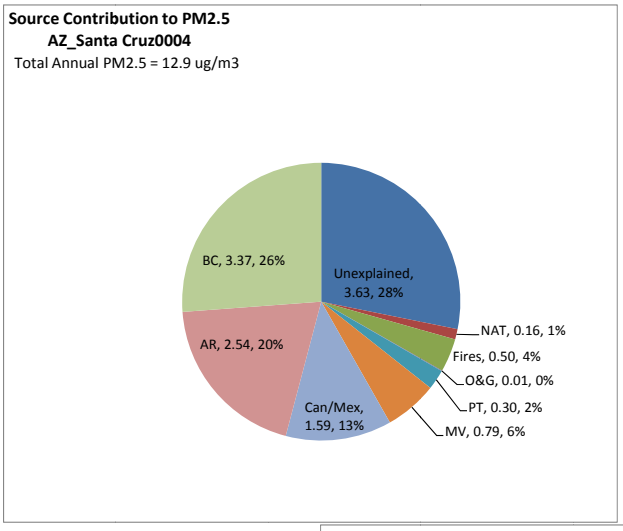
Appendix J

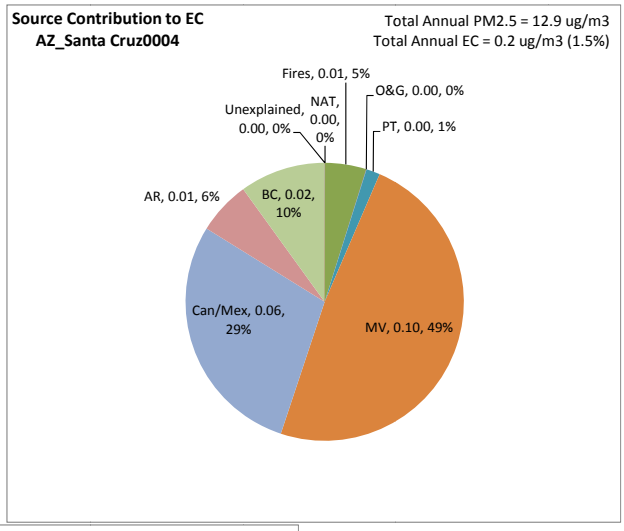
Source Category-Specific Contributions to Annual $PM_{2.5}$ Design Values at Monitoring Sites in the 12 km WESTUS Domain using MATS

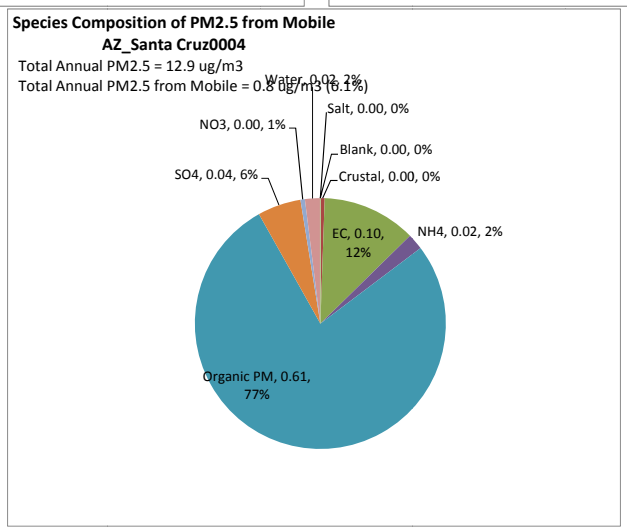
"Appendix_J_DVannPM_12kmWESTUS_SrcCat.xlsx" (1.8 Mb)

Cell B1 = Select Monitor in the 12 km WESTUS Domain for Contributions to Annual $PM_{2.5}$ Design Value (AZ_SantaCruz0004 in example)
Cell B2 = Select Source Category that will give second plot of contributions for that Source Category (Mobile in example)
Cell B3 = Select PM Species that will give third plot of contributions for that Species (EC in example)




Source Contribution to PM2.5
AZ_Santa Cruz0004
Total Annual PM2.5 = 12.9 ug/m3
Unexplained, 3.63, 28%
NAT, 0.16, 1%
Fires, 0.50, 4%
O&G, 0.01, 0%
PT, 0.30, 2%
MV, 0.79, 6%
Can/Mex, 1.59, 13%
AR, 2.54, 20%
BC, 3.37, 26%


Source Contribution to EC
AZ_Santa Cruz0004
Total Annual PM2.5 = 12.9 ug/m3
Total Annual EC = 0.2 ug/m3 (1.5%)
Fires, 0.01, 5%
O&G, 0.00, 0%
NAT, 0.00, 0%
Unexplained, 0.00, 0%
PT, 0.00, 1%
AR, 0.01, 6%
BC, 0.02, 10%
Can/Mex, 0.06, 29%
MV, 0.10, 49%

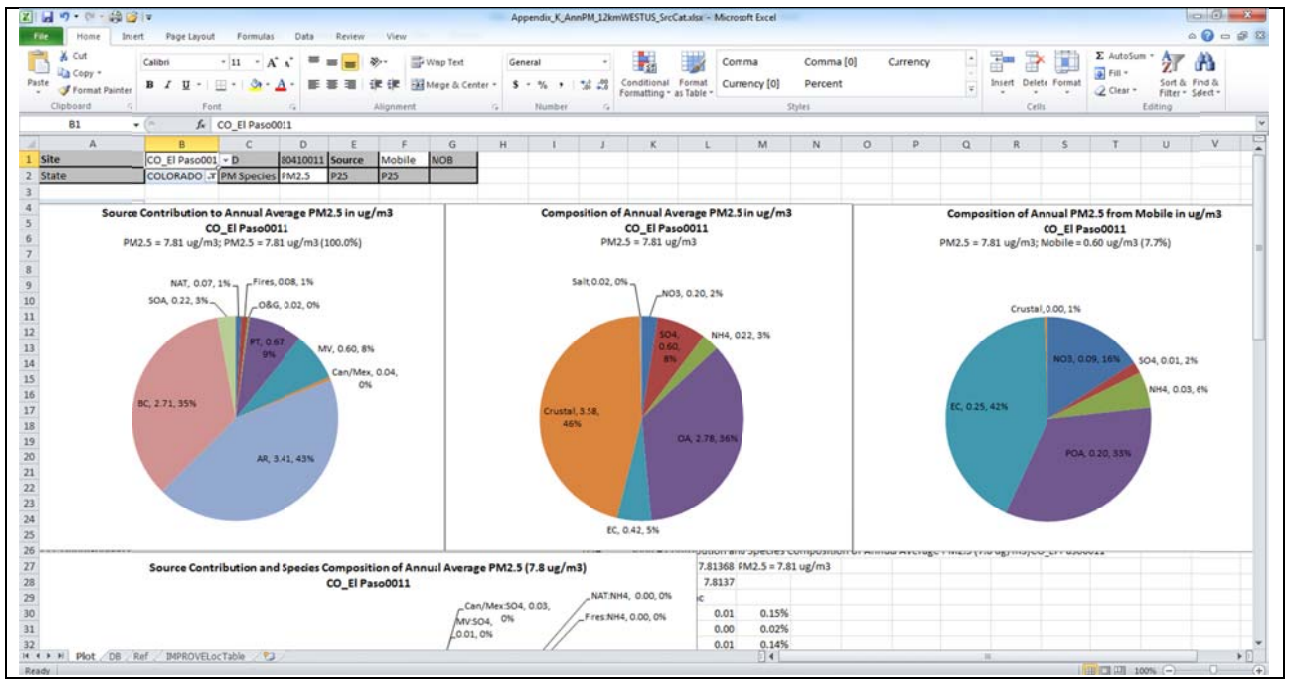

Species Composition of PM2.5 from Mobile
AZ_Santa Cruz0004
Total Annual PM2.5 = 12.9 ug/m3
Total Annual PM2.5 from Mobile = 0.8 ug/m3 (6.1%)
Water, 0.02, 2%
Salt, 0.00, 0%
NO3, 0.00, 1%
Blank, 0.00, 0%
SO4, 0.04, 6%
Crustal, 0.00, 0%
EC, 0.10, 12%
NH4, 0.02, 2%
Organic PM, 0.61, 77%

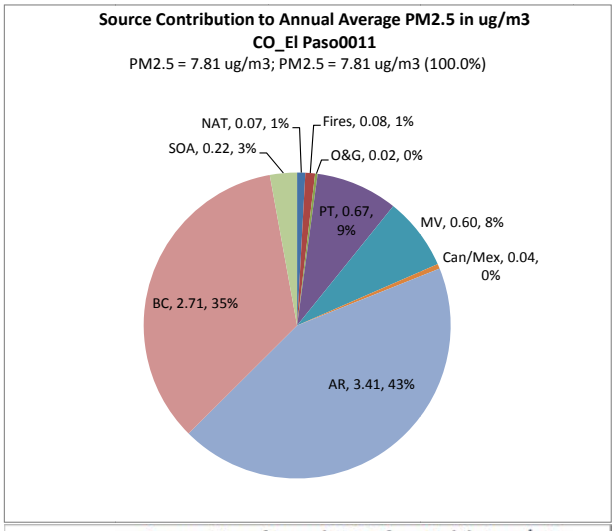
Appendix K

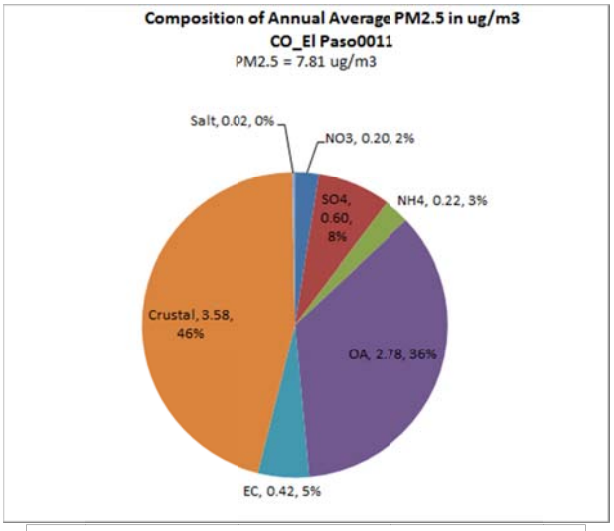
Source Category-Specific Contributions to Modeled Annual $PM_{2.5}$ Concentrations ($\mu g/m^3$) at Monitoring Sites in the 12 km WESTUS Domain

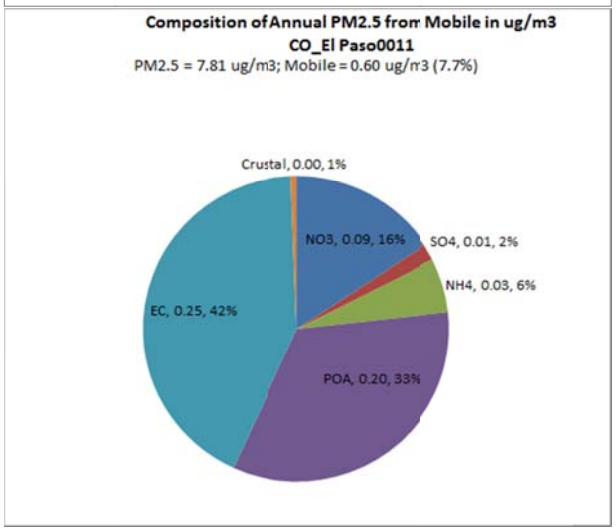
"Appendix_K_AnnPM_12kmWESTUS_SrcCat.xlsx" (4.0 Mb)

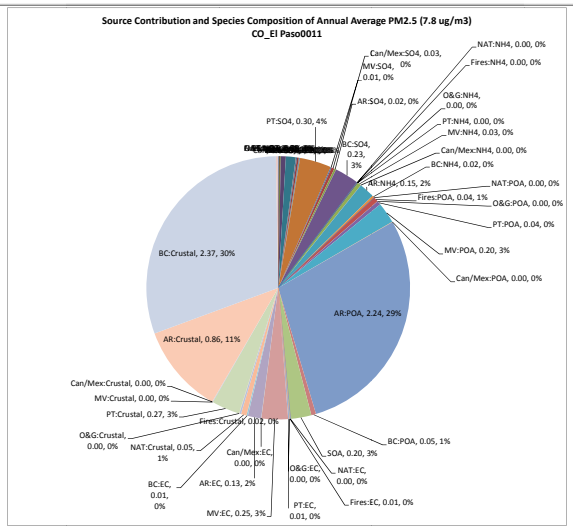
Cell B2 = Select State for Monitoring Site (Colorado in example)
Cell B1 = Select Monitoring Site (CO_ElPaso0011)
Cell D2 = Select PM Species for Source Apportionment Pie Chart (PM2.5 in example)
Cell F1 = Select Source Category for Additional Pie Chart (Mobile in example)




Source Contribution to Annual Average PM2.5 in ug/m3
CO_El Paso0011
PM2.5 = 7.81 ug/m3; PM2.5 = 7.81 ug/m3 (100.0%)
NAT, 0.07, 1%
Fires, 0.08, 1%
SOA, 0.22, 3%
O&G, 0.02, 0%
PT, 0.67, 9%
MV, 0.60, 8%
Can/Mex, 0.04, 0%
BC, 2.71, 35%
AR, 3.41, 43%


Composition of Annual Average PM2.5 in ug/m3
CO_El Paso0011
PM2.5 = 7.81 ug/m3
Salt, 0.02, 0%
NO3, 0.20, 2%
SO4, 0.60, 8%
NH4, 0.22, 3%
Crustal, 3.58, 46%
OA, 2.78, 36%
EC, 0.42, 5%


Composition of Annual PM2.5 from Mobile in ug/m3
CO_El Paso0011
PM2.5 = 7.81 ug/m3; Mobile = 0.60 ug/m3 (7.7%)
Crustal, 0.00, 1%
NO3, 0.09, 16%
SO4, 0.01, 2%
NH4, 0.03, 6%
EC, 0.25, 42%
POA, 0.20, 33%

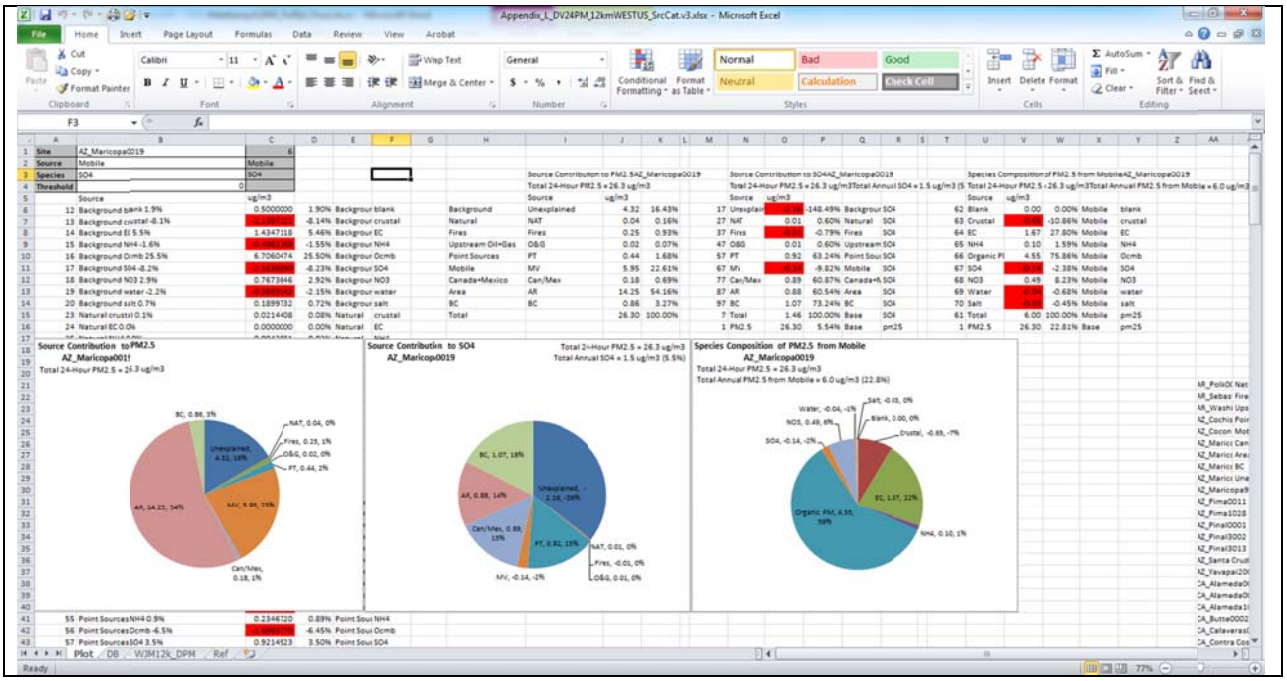

Source Contribution and Species Composition of Annual Average PM2.5 (7.8 ug/m3)
CO_El Paso0011
Can/Mex:SO4, 0.03, 0%
MV:SO4, 0.01, 0%
AR:SO4, 0.02, 0%
PT:SO4, 0.30, 4%
BC:SO4, 0.23, 3%
NAT:NH4, 0.00, 0%
Fires:NH4, 0.00, 0%
O&G:NH4, 0.00, 0%
PT:NH4, 0.00, 0%
MV:NH4, 0.03, 0%
Can/Mex:NH4, 0.00, 0%
BC:NH4, 0.02, 0%
AR:NH4, 0.15, 2%
NAT:POA, 0.00, 0%
Fires:POA, 0.04, 1%
O&G:POA, 0.00, 0%
PT:POA, 0.04, 0%
MV:POA, 0.20, 3%
Can/Mex:POA, 0.00, 0%
BC:Crustal, 2.37, 30%
AR:POA, 2.24, 29%
AR:Crustal, 0.86, 11%
Can/Mex:Crustal, 0.00, 0%
MV:Crustal, 0.00, 0%
PT:Crustal, 0.27, 3%
Fires:Crustal, 0.02, 0%
O&G:Crustal, 0.00, 0%
NAT:Crustal, 0.05, 1%
Can/Mex:EC, 0.00, 0%
BC:POA, 0.05, 1%
SOA, 0.20, 3%
NAT:EC, 0.00, 0%
O&G:EC, 0.00, 0%
BC:EC, 0.01, 0%
AR:EC, 0.13, 2%
MV:EC, 0.25, 3%
PT:EC, 0.01, 0%
Fires:EC, 0.01, 0%

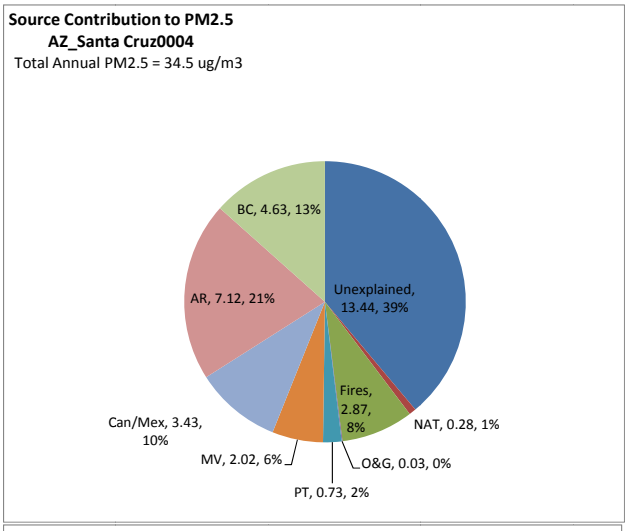
Appendix L

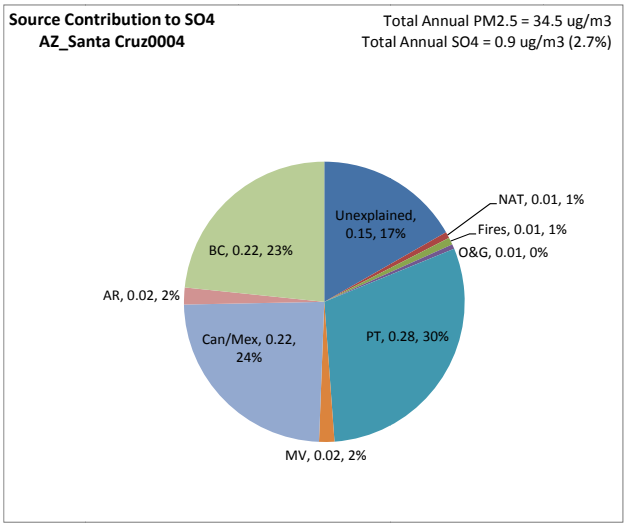
Source Category-Specific Contributions to 24-Hour $PM_{2.5}$ Design Values at Monitoring Sites in the 12 km WESTUS Domain using MATS

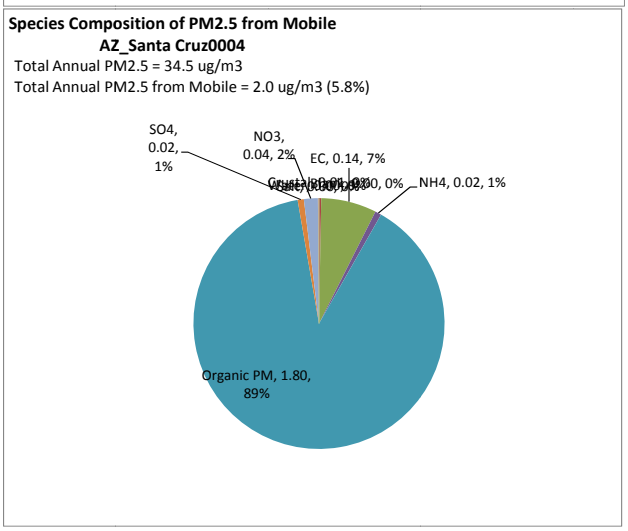
"Appendix_L_DV24PM_12kmWESTUS_SrcCat.xlsx" (2.0 Mb)

Cell B1 = Select Monitor in the 12 km WESTUS Domain for Contributions to 24-Hour $PM_{2.5}$ Design Value (AZ_SantaCruz0004 in example)
Cell B2 = Select Source Category that will give second plot of contributions for that Source Category (Mobile in example)
Cell B3 = Select PM Species that will give third plot of contributions for that Species (SO4 in example)




Source Contribution to PM2.5
AZ_Santa Cruz0004
Total Annual PM2.5 = 34.5 ug/m3
BC, 4.63, 13%
AR, 7.12, 21%
Unexplained, 13.44, 39%
Fires, 2.87, 8%
NAT, 0.28, 1%
Can/Mex, 3.43, 10%
MV, 2.02, 6%
O&G, 0.03, 0%
PT, 0.73, 2%


Source Contribution to SO4
AZ_Santa Cruz0004
Total Annual PM2.5 = 34.5 ug/m3
Total Annual SO4 = 0.9 ug/m3 (2.7%)
Unexplained, 0.15, 17%
NAT, 0.01, 1%
Fires, 0.01, 1%
O&G, 0.01, 0%
BC, 0.22, 23%
AR, 0.02, 2%
Can/Mex, 0.22, 24%
PT, 0.28, 30%
MV, 0.02, 2%

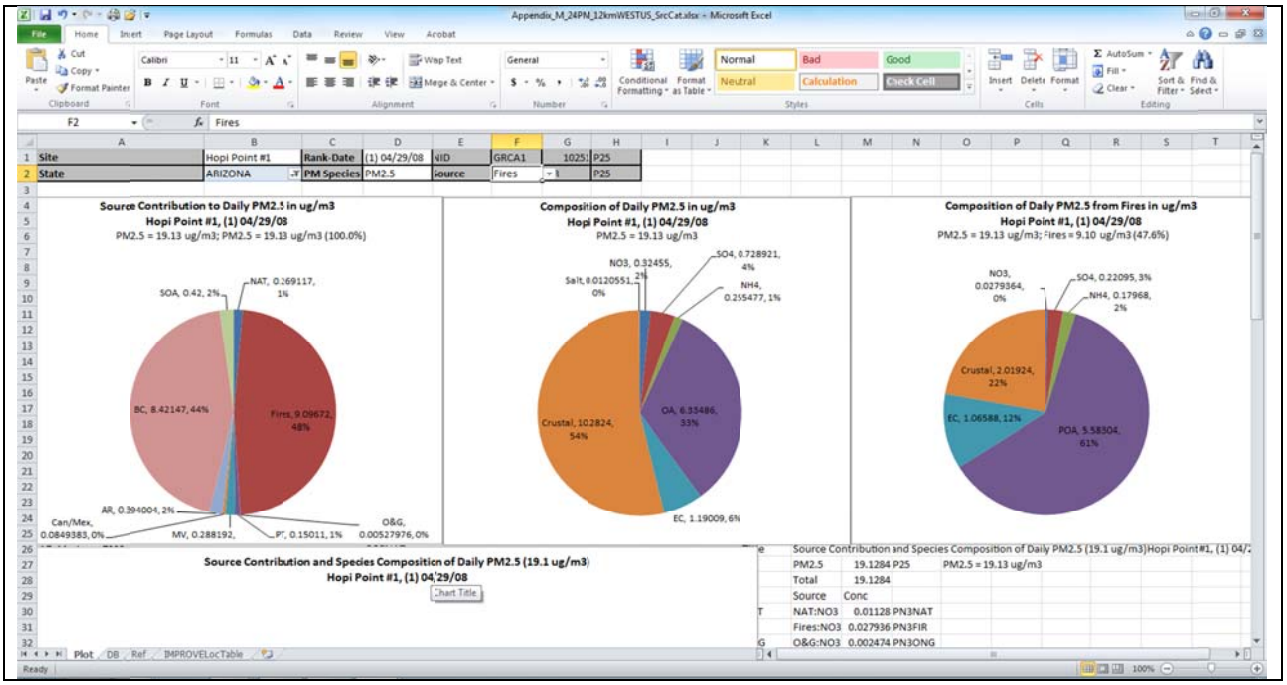

Species Composition of PM2.5 from Mobile
AZ_Santa Cruz0004
Total Annual PM2.5 = 34.5 ug/m3
Total Annual PM2.5 from Mobile = 2.0 ug/m3 (5.8%)
SO4, 0.02, 1%
NO3, 0.04, 2%
EC, 0.14, 7%
NH4, 0.02, 1%
Organic PM, 1.80, 89%

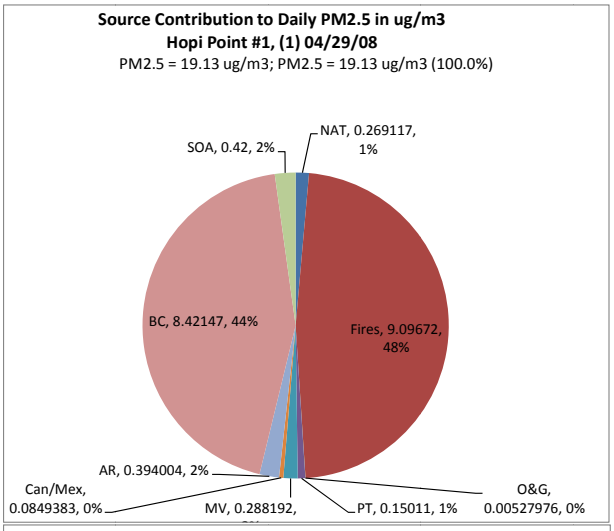
Appendix M

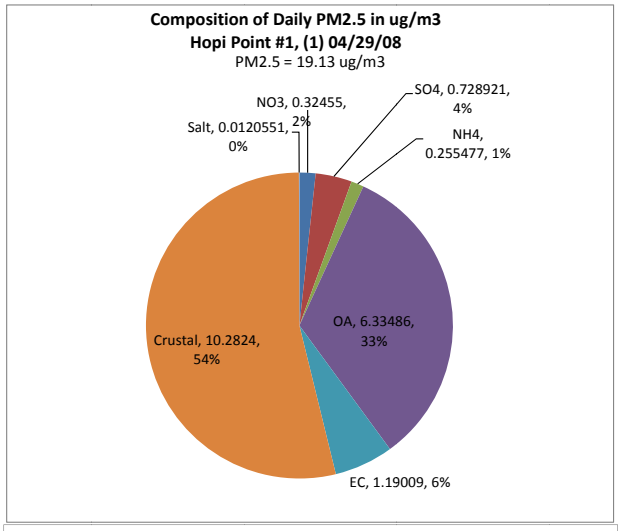
Source Category-Specific Contributions to Ten Highest Modeled 24-Hour $PM_{2.5}$ Concentrations ($\mu g/m^3$) at Monitoring Sites in the 12 km WESTUS Domain

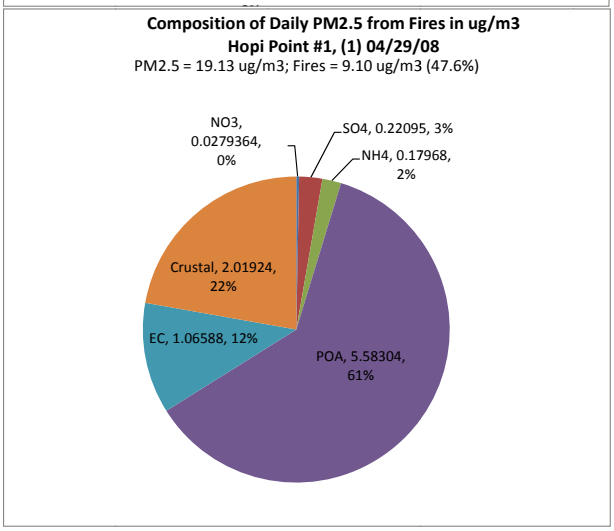
"Appendix_M_24PM_12kmWESTUS_SrcCat.xlsx" (4.0 Mb)

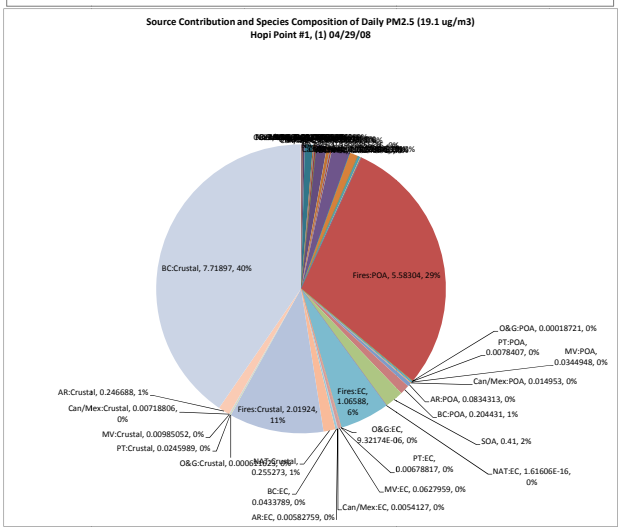
Cell B2 = Select State for Monitoring Site (Arizona in example)
Cell B1 = Select Monitoring Site (Hopi Point #1 in example)
Cell D1 = Selection One of 10 Highest Dates (Rank #1 on 04/29/08 in example)
Cell D2 = Select PM Species for Separate Source Category Apportionment Pie Chart (PM2.5 in example)
Cell F2 = Select Source Category for Additional Pie Chart (Fires in example)




Source Contribution to Daily PM2.5 in ug/m3
Hopi Point #1, (1) 04/29/08
PM2.5 = 19.13 ug/m3; PM2.5 = 19.13 ug/m3 (100.0%)
NAT, 0.269117, 1%
SOA, 0.42, 2%
BC, 8.42147, 44%
Fires, 9.09672, 48%
AR, 0.394004, 2%
Can/Mex, 0.0849383, 0%
MV, 0.288192,
PT, 0.15011, 1%
O&G, 0.00527976, 0%


Composition of Daily PM2.5 in ug/m3
Hopi Point #1, (1) 04/29/08
PM2.5 = 19.13 ug/m3
NO3, 0.32455, 2%
SO4, 0.728921, 4%
Salt, 0.0120551, 0%
NH4, 0.255477, 1%
OA, 6.33486, 33%
Crustal, 10.2824, 54%
EC, 1.19009, 6%


Composition of Daily PM2.5 from Fires in ug/m3
Hopi Point #1, (1) 04/29/08
PM2.5 = 19.13 ug/m3; Fires = 9.10 ug/m3 (47.6%)
NO3, 0.0279364, 0%
SO4, 0.22095, 3%
NH4, 0.17968, 2%
Crustal, 2.01924, 22%
EC, 1.06588, 12%
POA, 5.58304, 61%


Source Contribution and Species Composition of Daily PM2.5 (19.1 ug/m3)
Hopi Point #1, (1) 04/29/08
BC:Crustal, 7.71897, 40%
Fires:POA, 5.58304, 29%
O&G:POA, 0.00018721, 0%
PT:POA, 0.0078407, 0%
MV:POA, 0.0344948, 0%
Can/Mex:POA, 0.014953, 0%
AR:POA, 0.0834313, 0%
BC:POA, 0.204431, 1%
SOA, 0.41, 2%
NAT:EC, 1.61606E-16, 0%
Fires:EC, 1.06588, 6%
O&G:EC, 9.32174E-06, 0%
PT:EC, 0.00678817, 0%
MV:EC, 0.0627959, 0%
Can/Mex:EC, 0.0054127, 0%
AR:EC, 0.00582759, 0%
BC:EC, 0.0433789, 0%
NAT:Crustal, 0.255273, 1%
O&G:Crustal, 0.00051025, 0%
PT:Crustal, 0.0245989, 0%
MV:Crustal, 0.00985052, 0%
Can/Mex:Crustal, 0.00718806, 0%
AR:Crustal, 0.246688, 1%
Fires:Crustal, 2.01924, 11%

Appendix N

Annual Sulfur and Nitrogen Wet and Dry Deposition at IMPROVE Monitors by Species

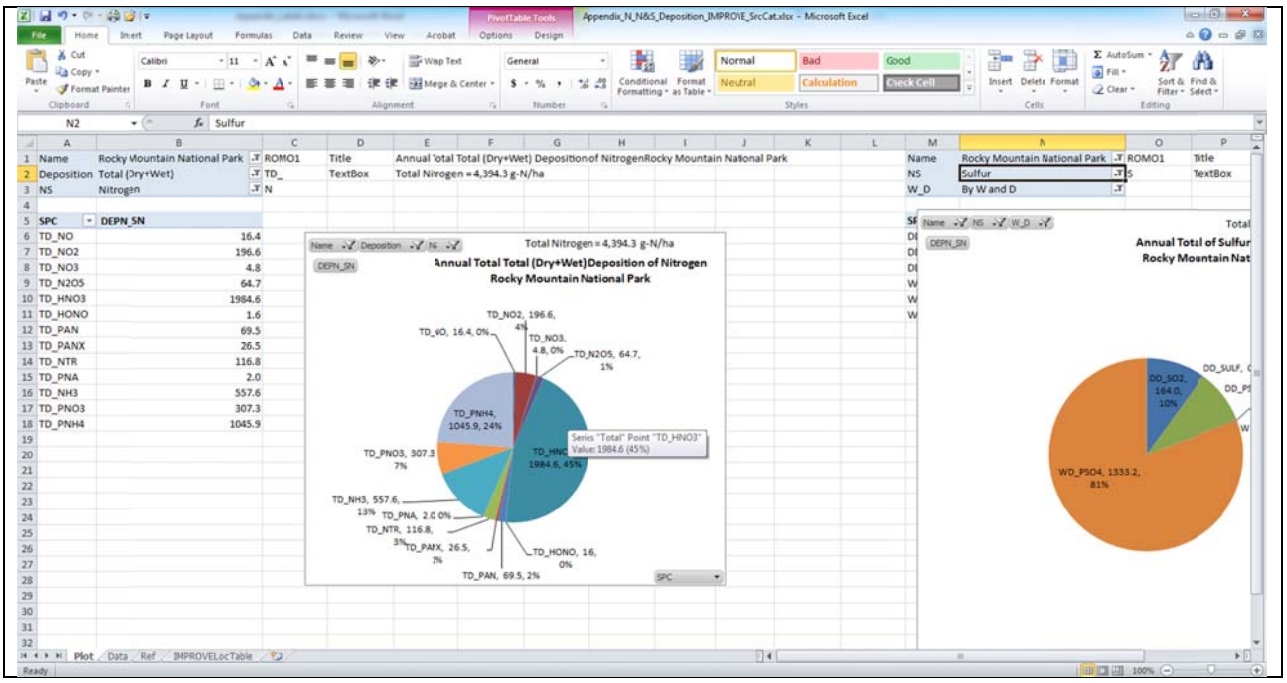
"Appendix_N_N&S_Deposition_IMPROVE_SrcCat.xlsx" (1.3 Mb)

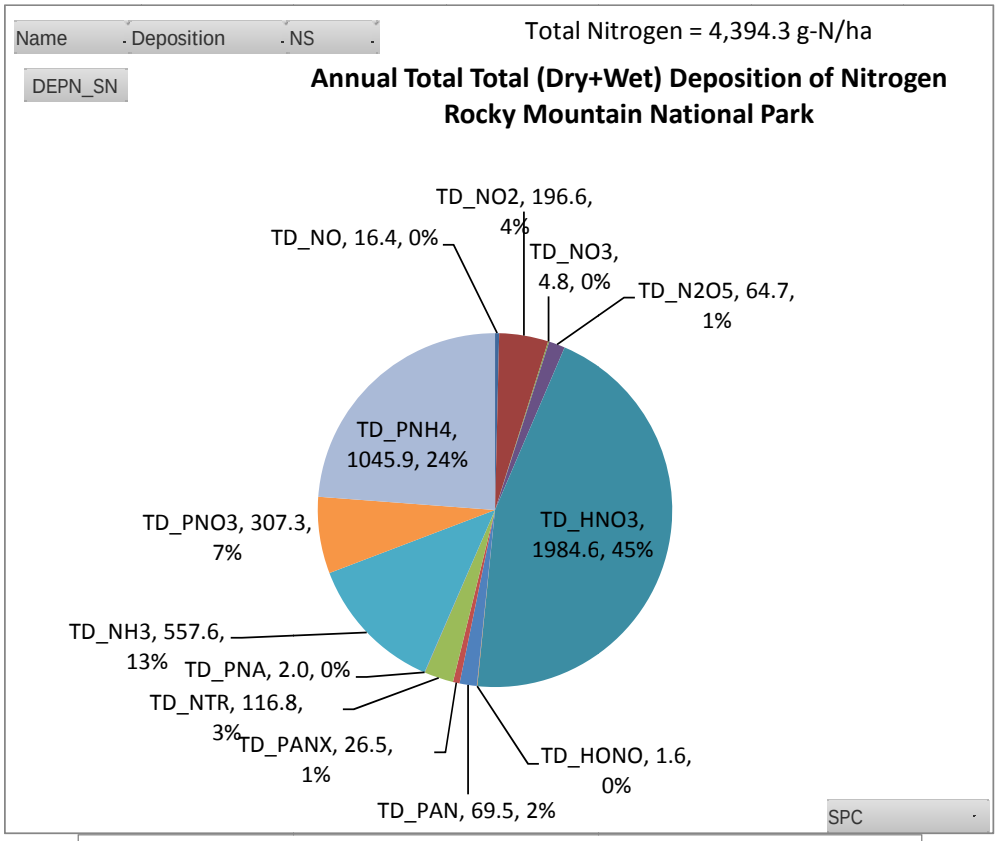
<u>First Pie Chart</u>

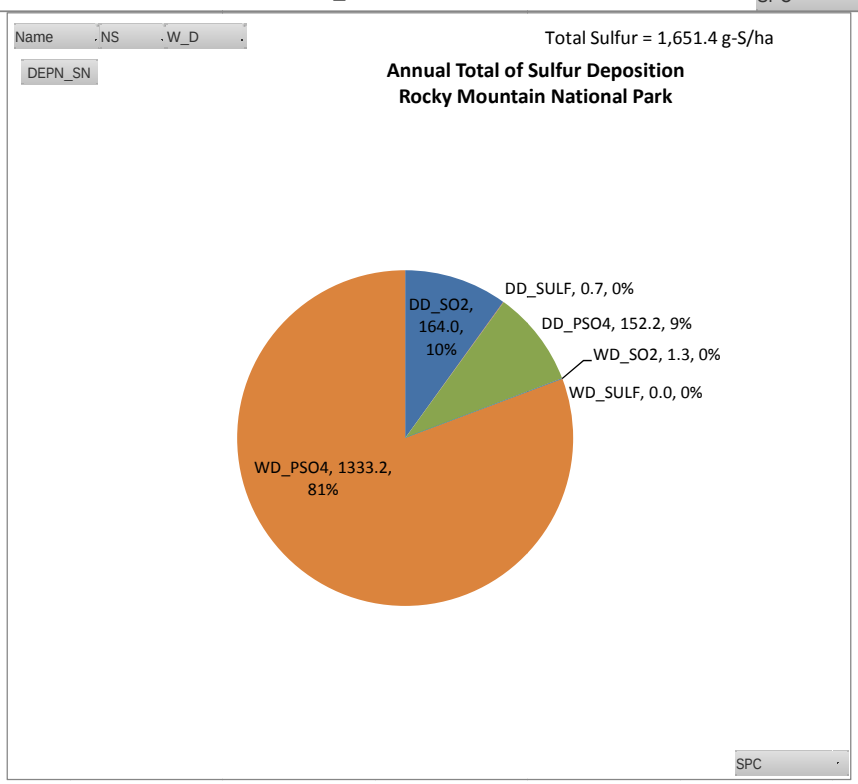
Cell B1 = Select IMPROVE Monitoring Site (ROMO1 in example)
Cell B2: Select whether want Wet, Dry or Total Deposition (Total in example)

<u>Second Pie Chart</u>

Cell N1 = Select IMPROVE Monitoring Site (ROMO1 in example)
Cell N2 = Select whether want Sulfur or Nitrogen (Sulfur in example)
Cell N3 = Select whether want by Wet and Dry or by Total Deposition




Name
Deposition
NS
DEPN_SN
Total Nitrogen = 4,394.3 g-N/ha
Annual Total Total (Dry+Wet) Deposition of Nitrogen
Rocky Mountain National Park
TD_NO2, 196.6, 4%
TD_NO, 16.4, 0%
TD_NO3, 4.8, 0%
TD_N2O5, 64.7, 1%
TD_PNH4, 1045.9, 24%
TD_PNO3, 307.3, 7%
TD_HNO3, 1984.6, 45%
TD_NH3, 557.6, 13%
TD_PNA, 2.0, 0%
TD_NTR, 116.8, 3%
TD_PANX, 26.5, 1%
TD_HONO, 1.6, 0%
TD_PAN, 69.5, 2%
SPC

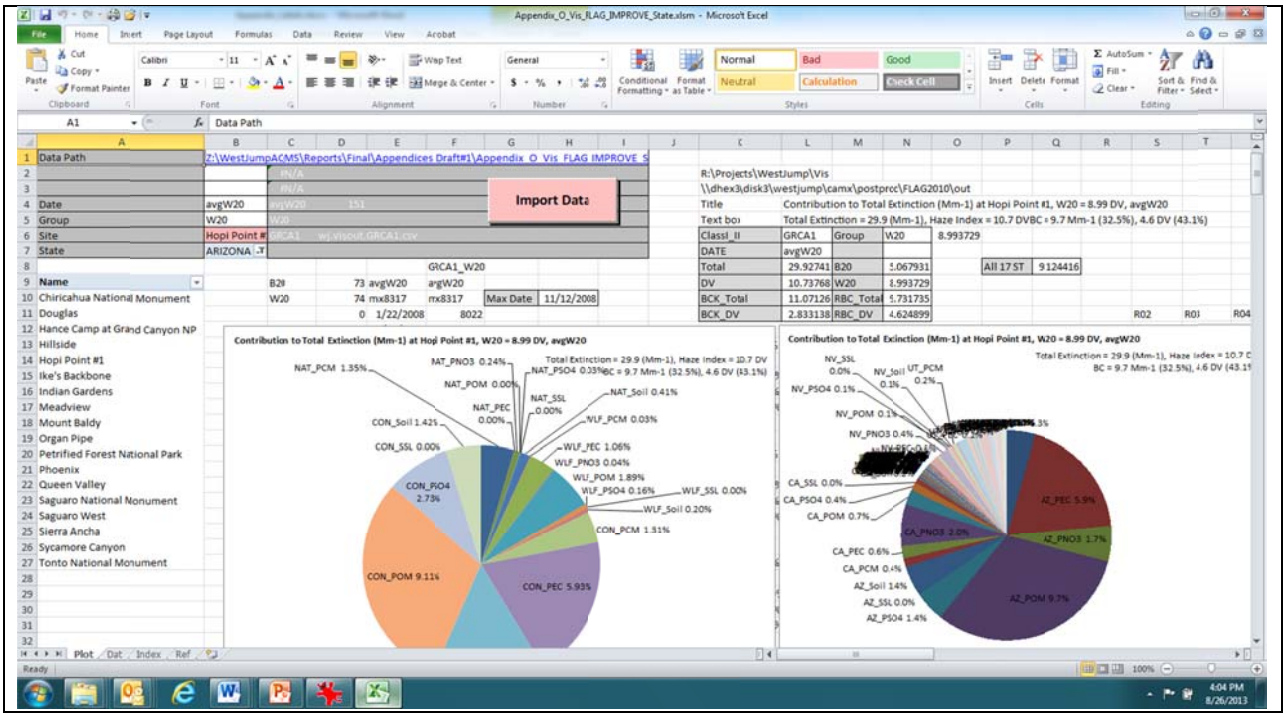

Name
NS
W_D
DEPN_SN
Total Sulfur = 1,651.4 g-S/ha
Annual Total of Sulfur Deposition
Rocky Mountain National Park
DD_SULF, 0.7, 0%
DD_SO2, 164.0, 10%
DD_PSO4, 152.2, 9%
WD_SO2, 1.3, 0%
WD_SULF, 0.0, 0%
WD_PSO4, 1333.2, 81%
SPC

Appendix O

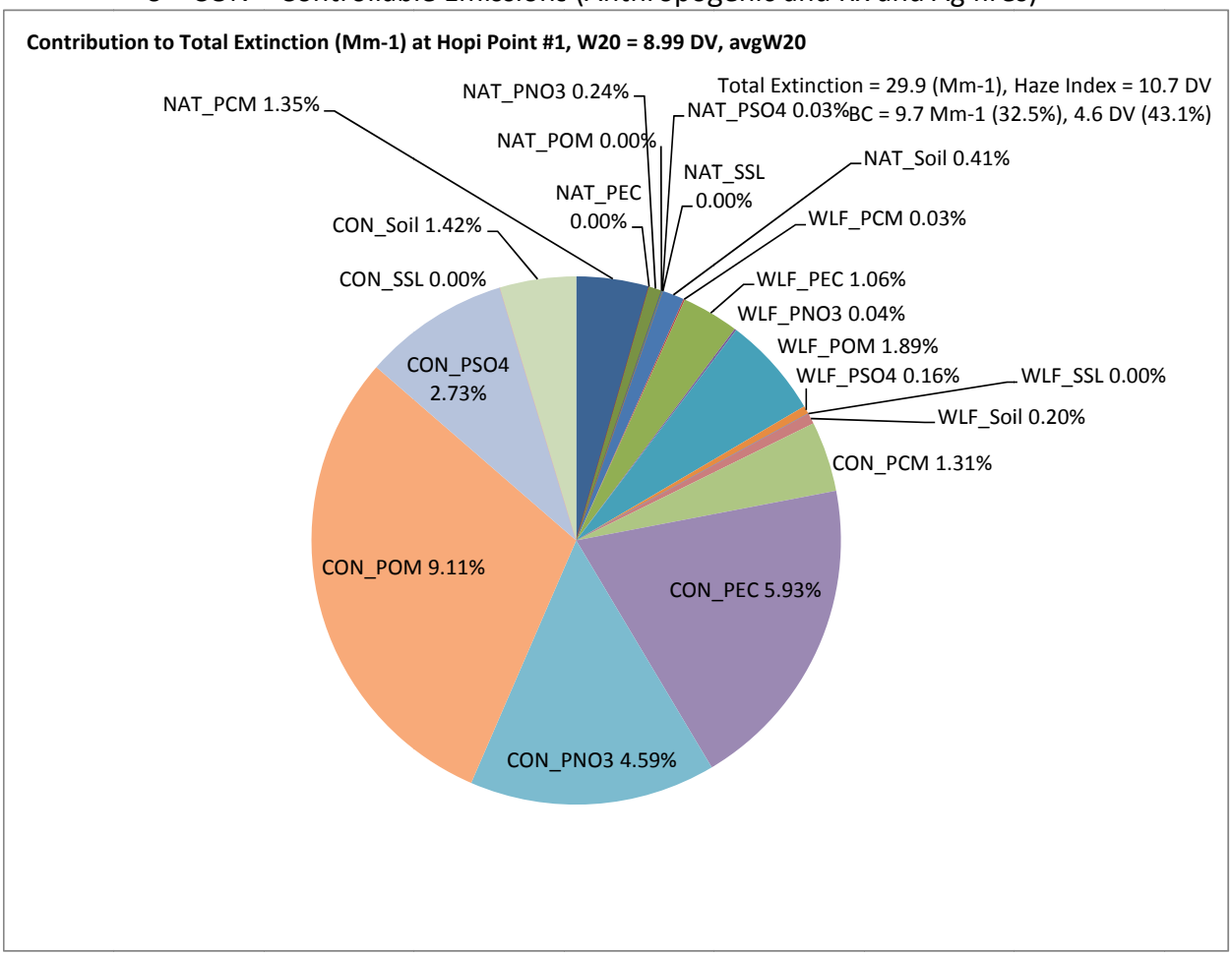
Western State-Specific Modeled Contributions to Visibility Impairment at IMPROVE Monitoring Sites for Modeled Worst (W20) and Best (B20) 20% Days during 2008

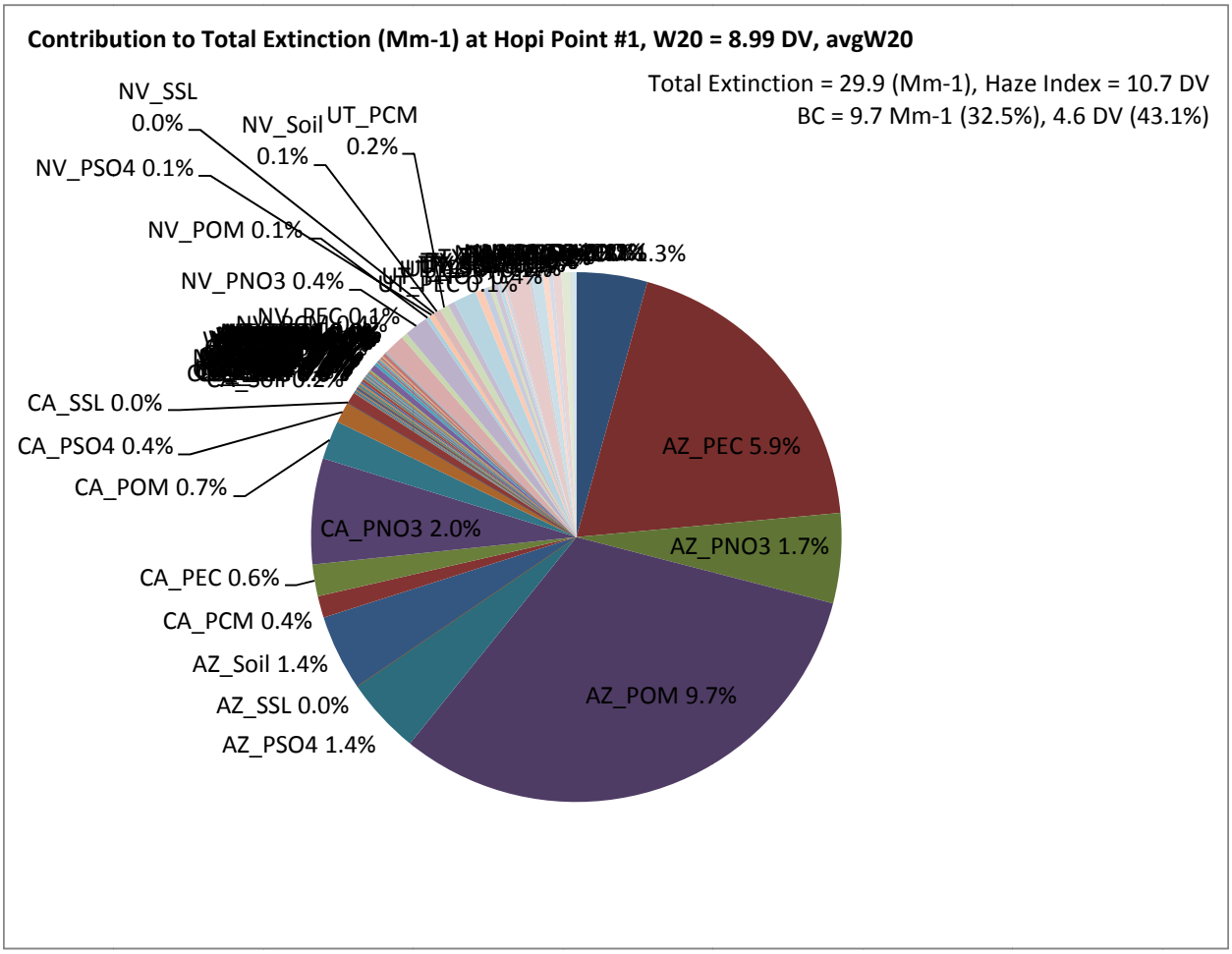
"Appendix_O_Vis_FLAG_IMPROVE_State-xlsm" (3.0 Mb)
(Note: May have to enable macros etc. depending on security settings in your Excel setup)

Cell B1 = Path where site-specific .crv files are stored
Cell B7 = State for monitor desired (Arizona in example)
Cell B6 = Monitoring Site in State (Hopi Point in example, GRCA)
Once a new monitoring site is selected data needs to be imported through the pink "Import Data" button
Cell B5 = Select whether want W20 or B20 days (W20 in example)
Cell B4 = Select individual day or average for display (avgW20 in example)



- Pie Chart displays are just for the 17 western states
- Total extinction without Rayleigh is in cell L8 (29.9 Mm^{-1} in example)
- Background Sources (i.e., EUSA, Mexico, Canada, Off-Shore and SOA) extinction is in cell L10 (11.1 Mm^{-1})
- Boundary Condition (BC) contribution is in plots (9.7 Mm^{-1} in example)
- Pie Chart breaks down 17 state contributions to extinction either by Source Category and Species (left plot) or by State and Species (right plot). Three Source Categories are used:
    - NAT = Natural Emissions (Biogenic, Lightning, Sea Salt and WBD)
    - WLF = Wild Fires
    - CON = Controllable Emissions (Anthropogenic and Rx and Ag fires)




Contribution to Total Extinction (Mm-1) at Hopi Point #1, W20 = 8.99 DV, avgW20
Total Extinction = 29.9 (Mm-1), Haze Index = 10.7 DV
BC = 9.7 Mm-1 (32.5%), 4.6 DV (43.1%)
NV_SSL 0.0%
NV_Soil 0.1%
UT_PCM 0.2%
NV_PSO4 0.1%
NV_POM 0.1%
NV_PNO3 0.4%
CA_SSL 0.0%
CA_PSO4 0.4%
CA_POM 0.7%
CA_PNO3 2.0%
CA_PEC 0.6%
CA_PCM 0.4%
AZ_Soil 1.4%
AZ_SSL 0.0%
AZ_PSO4 1.4%
AZ_POM 9.7%
AZ_PNO3 1.7%
AZ_PEC 5.9%