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Final Report for the Western Regional Air Partnership (WRAP) Regional Modeling Center (RMC) for the Project Period March 1, 2004, through February 28, 2005

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Executive Summary

This report describes work completed for project year 2004 (March 1, 2004, through February 28, 2005) at the Regional Modeling Center (RMC), which comprises staff from the University of California, the University of North Carolina, and ENVIRON International Corporation. Funding for this work was provided by the Western Governors' Association's Western Regional Air Partnership (WRAP). This was the fourth year of a continuing project to analyze and model regional haze and visibility in the western United States. Listed below are the titles and purposes of the tasks that were included in the 2004 RMC work plan, which was developed in coordination with WRAP technical staff and the WRAP Modeling Forum.

- **Task 0.5, 2002 Ammonia Emissions Inventory for WRAP Region:** To review current ammonia emissions generation techniques and develop a GIS-based ammonia emissions model.
- **Task 1, Project Administration:** To manage the WRAP RMC activities, participate in WRAP conference calls, attend WRAP meetings, and prepare project status reports.
- **Task 2, Test, Improve, Quality Control, Obtain External Peer Review, and Finalize 36-km and 12-km MM5 Simulations for Eventual Use in CMAQ:** To perform MM5 modeling for 2002 on the 36-km Inter-RPO continental U.S. grid and a 12-km western U.S. WRAP grid.
- **Task 3, 2002 Base Year Emissions Modeling, Processing, and Analysis:** To revise the interim 2002 inventory by integrating missing emissions sources; to assimilate the results of applying the new analysis tools and QA plan for improving the emissions modeling process; and to integrate the final 2002 emissions inventories into a base 2002 emissions data set.
- **Task 4, Air Quality Model Evaluation for 2002 Annual Simulation:** To test the 2002 base year air quality modeling performed with CMAQ, including a preliminary simulation using the 2002 interim emissions inventory followed by several iterations with bug fixes or updates.
- **Task 5, Preparation and Reporting of Geographic Source Apportionment Results:** To implement, test, and apply Tagged Species Source Attribution PM algorithms in CMAQ.
- **Task 6, Further Analysis of Model Performance in Regard to the Contribution of Natural Emissions to Visibility Impairment:** To perform modeling without anthropogenic emissions to help elucidate natural background visibility levels.
- **Task 7, Evaluation and Comparison of Alternative Models:** To analyze alternative models to CMAQ for 2002 modeling.
- **Task 9, Testing and Further Improvements to the Windblown Dust Emissions Modeling Methodology:** To further refine and test the WRAP windblown dust model.
- **Task 10, Continued Improvement to Model Evaluation Software:** To continue developing model evaluation software for meteorology, emissions, and air quality modeling.
- **Task 11, Sensitivity Studies Designed to Evaluate Uncertainties in Fire Emissions:** To perform fire sensitivity simulations as requested by the Fire Emissions Joint Forum.

- **Task 12, Preliminary Meteorological, Emissions, and Air Quality Modeling Activities for Alaska:** To perform MM5 modeling of Alaska and preliminary dispersion modeling using a Lagrangian puff model.
- **Task 13, Training Courses for the WRAP States and Tribes:** To conduct training activities as needed to transfer datasets and technology to WRAP member tribes and states.

Section 1 of this report provides project background information. Sections 2 through 14 discuss the tasks in detail, and include lists of project deliverables as well as links to where they can be downloaded or viewed on the project web site, at <http://pah.cert.ucr.edu/aqm/308/>. Section 15 gives concise summaries of all the tasks.

The overall goal for 2004 was to develop, quality assure, test, and refine all model input data required to perform simulations of visibility for calendar year 2002. Visibility was modeled on both a continental 36-km domain and a higher-resolution 12-km domain for the WRAP region. A primary objective was to validate the modeling scenarios so that they can be used in subsequent analysis to support the development of State and Tribe Implementation Plans, which are due in December 2007. Most of these activities were performed under Tasks 1-4, 7, and 10.

Another major activity (Task 12) was the development of modeling scenarios to analyze visibility in Alaska. These data were developed independently of the conterminous WRAP region because Alaska is so far removed from the other WRAP states and because it has much lower emissions densities and longer transport distances. Alaska modeling required separate simulations that used a polar version of the meteorology model and that employed the CALPUFF model, which is more appropriate than grid-based models for studying visibility in Alaska.

The 2004 project year also included development of tools and model simulations to analyze the sources of haze. This activity was performed under Tasks 5 and 7. The CMAQ model was initially used to analyze source apportionment—that is, to identify particular emissions source categories and regions that are responsible for visibility impairment at individual receptor sites. Because of mass conservation errors in the modeling system, the source apportionment results in CMAQ were more qualitative than quantitative. We also evaluated the CAMx model's source apportionment tools, and plan to use CAMx in future source apportionment work.

Several model simulations were performed to assess CMAQ's sensitivity to changes in the fire emissions data (Task 11). Some key data needed for the fire sensitivity studies (e.g., detailed information on small fires) were not available, so the task definition was modified during 2004; the small fire sensitivity analysis and other plume rise analyses will now be completed in 2005.

In 2005-2006, the RMC will finish developing future visibility scenarios for 2018 to be used in additional modeling to support development of SIPs/TIPs. The ultimate goal is to transfer these data sets to the states and tribes so that they can carry out additional modeling analyses for their areas. During 2004 there were extensive discussions about what combination of training and technical support would be most beneficial for technology transfer. It was agreed that the most efficient approach would be to develop a standardized version of all data sets, computer software, and computer hardware, and that instructions for model setup and use would be provided on the project web site. Additionally, training classes will be offered on an “as needed” basis.

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Abbreviations

ACM	Asymmetric Convective Model
ADEC.....	Alaska Department of Environmental Conservation
AIM.....	Aerosol Inorganic Module
AML.....	ARC Macro Language
AoH.....	Attribution of Haze
AQS.....	Air Quality System
ARDB	Acid Rain Database
BART	Best Available Retrofit Technology
BC	boundary condition
BEIS.....	Biogenic Emissions Inventory System
BELD	Biogenic Emissions Landcover Database
BM	Betts-Miller
BRAVO.....	Big Bend Regional Aerosol and Visibility Observations Study
CAA	Clean Air Act
CAFO	confined animal feed operations
CALMET	California Meteorological Model
CALPUFF	California Puff Model
CAMx	Comprehensive Air quality Model with extensions
CAPE	convective available potential energy
CARB.....	California Air Resources Board
CASTNet.....	Clean Air Status and Trends Network
CB-IV.....	Carbon Bond IV (also referred to in the modeling community as CBIV, CB4)
CCM2.....	Community Climate Model 2
CCTM	CMAQ Chemical Transport Model
CEM	continuous emissions monitoring
CENRAP.....	Central Regional Air Planning Association
CEP	Carolina Environmental Program
CM	coarse mass (a term used in the context of the IMPROVE network; see also PMc)
CMAQ.....	Community Multiscale Air Quality
CMAS	Community Modeling and Analysis System
CMC.....	Chemical Mechanism Compiler
CMU	Carnegie Mellon University
CNG	compressed natural gas
CPC	Climate Prediction Center
CVS.....	Concurrent Versions System
CY02	calendar year 2002
DDM	decoupled direct method
DEAD	Dust Entrainment and Deposition

dV	deciview
EC	elemental carbon
EDAS	Eta Data Assimilation System
EEA	European Environment Agency
EGAS	Economic Growth Analysis System
EGU	electric generating utility
EPA	U.S. Environmental Protection Agency
ESSC	Earth System Science Center
FAQ	frequently asked question
FDDA	four-dimensional data assimilation
FEJF	Fire Emissions Joint Forum
FIPS	Federal Implementation Standards
GCVTC	Grand Canyon Visibility Transport Commission
GIS	geographic information system
GUI	graphical user interface
IC	initial condition
IDNR	Iowa Department of Natural Resources
IEH	Implicit-Explicit Hybrid
IMPROVE	Interagency Monitoring of Protected Visual Environments
IOA	index of agreement
IPR	Integrated Process Rates
IRR	Integrated Reaction Rates
KF	Kain-Fritsch
LADCO	Lake Michigan Air Directors Consortium
LAC	light-absorbing carbon
lat-lon	latitude-longitude
LPG	liquefied petroleum gas
LSM	land-surface model
LULC	land use/land cover
M4	Mechanism 4
MADM	Multicomponent Aerosol Dynamics Model
MADRID	Model of Aerosol Dynamics, Reaction, Ionization, and Dissolution
MANE-VU	Mid-Atlantic/Northeast Visibility Union
MM5	Fifth-Generation Penn State/NCAR Mesoscale Model
M-MRF	modified Medium-Range Forecast
MPE	model performance evaluation
MRF	Medium-Range Forecast
MRLC	Multi-Resolution Land Characterization
MRPO	Midwest Regional Planning Organization
NADP	National Atmospheric Deposition Program
NASS	National Agricultural Statistics Service
NCAR	National Center for Atmospheric Research
NCEP	National Centers for Environmental Prediction

NEI.....	National Emissions Inventory (NEI96 = 1996 version; NEI99 = 1999 version)
NLCD.....	National Land Cover Database
NNRP.....	NCAR/NCEP Reanalysis Project
NWS.....	National Weather Service
OC.....	organic carbon
ORD.....	Office of Research and Development
OSAT.....	Ozone Source Apportionment Technology
PAMS.....	Photochemical Assessment Monitoring Station
PAVE.....	Program for the Analysis and Visualization of Environmental data
PBL.....	planetary boundary layer
PDM.....	Plume Dynamics Model
PinG.....	plume-in-grid
PM.....	particulate matter
PM ₁₀	particulate matter $\leq 10\ \mu\text{m}$ in diameter
PM _{2.5}	particulate matter $\leq 2.5\ \mu\text{m}$ in diameter (referred to in this report as “fine particulate matter”)
PMc.....	coarse particulate matter: PM that ranges from 2.5 to $10\ \mu\text{m}$ in diameter (note that PMc is also referred to as CM in the context of the IMPROVE network)
PPM.....	Piecewise Parabolic Method
PSAT.....	PM Source Apportionment Technology
PX.....	Pleim-Xiu
QA.....	quality assurance
QAPP.....	quality assurance project plan
QC.....	quality control
QSSA.....	Quasi Steady State Approximation
RADM.....	Regional Acid Deposition Model
RAMS.....	Regional Atmospheric Modeling System
REMSAD.....	Regional Modeling System for Aerosols and Deposition
RHR.....	Regional Haze Rule
RMC.....	Regional Modeling Center
RMSE.....	root mean squared error
RPO.....	Regional Planning Organization
RRF.....	relative reduction factor
RRTM.....	Rapid Radiative Transfer Model
Rx.....	prescribed (used with “wildfires”)
SAPRC.....	Statewide Air Pollution Research Center
SCC.....	source classification code
SEARCH.....	Southeastern Aerosol Research and Characterization (monitoring network)
SEARCH_H.....	SEARCH monitoring network collecting hourly data (vs. daily [24-hour] data)
SIP.....	State Implementation Plans
SMOKE.....	Sparse Matrix Operator Kernel Emissions
SMVGEAR.....	Sparse-Matrix Vectorized Gear
SOA.....	secondary organic aerosols

SST.....	sea-surface temperature
STATSGO.....	State Soil Geographic
STN.....	Speciated Trends Network
TIP.....	Tribal Implementation Plan
TM.....	thematic mapper
TSD.....	Technical Support Document
TSSA.....	Tagged Species Source Apportionment
UAF.....	University of Alaska Fairbanks
UCR.....	University of California, Riverside
UNC.....	University of North Carolina
USDA.....	U.S. Department of Agriculture
USGS.....	U.S. Geological Survey
VISTAS.....	Visibility Improvement – State and Tribal Associations of the Southeast
VMT.....	vehicle miles traveled
VOC.....	volatile organic compound(s)
VRSM.....	Variable Size-Resolution Model
WEQ.....	Wind Erosion Equation
WRAP.....	Western Regional Air Partnership

1. Introduction

The Western Regional Air Partnership (WRAP) Regional Modeling Center (RMC) is responsible for performing air quality modeling simulations for the WRAP region's states and tribes in order to provide analytical results used in developing implementation plans under the U.S. Environmental Protection Agency (EPA) Regional Haze Rule. Responsibilities of the RMC include

- meteorological modeling;
- emissions processing and modeling;
- air quality and visibility modeling simulations;
- analysis, display, and reporting of modeling results; and
- storage and quality assurance of the modeling input and output files.

This document is a final report that discusses the activities the WRAP RMC performed from March 1, 2004, through February 28, 2005.

1.1 Background

1.1.1 Need for regional haze modeling

The Clean Air Act (CAA) establishes special goals for visibility in many national parks, wilderness areas, and international parks. Through the 1977 amendments to the Clean Air Act, Congress set a national goal for visibility as “the prevention of any future, and the remedying of any existing, impairment of visibility in mandatory Class I Federal areas which impairment results from manmade air pollution” (40 CFR 51.300). States are required to develop State Implementation Plans (SIPs) to attain visibility standards; also, tribes may opt to assume responsibility for visibility programs under 40 CFR Part 49 by developing Tribal Implementation Plans (TIPs). The goal of the Regional Haze Rule (RHR) is to achieve natural visibility conditions at 156 Federally mandated Class I areas by 2064. To achieve this goal, the RHR has set up milestone years of 2018, 2028, 2038, 2048, 2058, and 2064 to monitor progress toward natural visibility conditions. CAA Section 308 (§308) requires that the first visibility SIP/TIP be submitted to EPA by 2007-2008 to demonstrate progress toward natural visibility conditions in 2018 using the 2000-2004 five-year baseline.

Regional haze is linked to fine particulate matter (PM_{2.5}, which is particulate matter ≤ 2.5 μm in diameter), for which EPA has a new standard. PM_{2.5} SIPs/TIPs are to be submitted three years after designation of PM_{2.5} nonattainment areas. EPA performed the final designations of the PM_{2.5} nonattainment areas in December 2004, so the PM_{2.5} SIPs/TIPs are due by December 2007. As regional haze is intricately linked to PM_{2.5}, the PM_{2.5} and regional haze SIPs/TIPs are in the process of being aligned so that they would both be due by approximately December 2007 (January 2008). EPA designated 8-h ozone nonattainment areas in April 2004, which makes 8-h ozone SIPs/TIPs also due in 2007. States and tribes may use the integrated one-atmosphere

WRAP RMC base-year modeling as the regional component of the 8-h ozone attainment activities as well as for PM_{2.5} and regional haze. Those decisions will be based on schedule constraints, model performance, appropriateness of the episodes, feasibility, and need.

1.1.2 Role of the Western Regional Air Partnership

WRAP is one of five Regional Planning Organizations (RPOs) (Figure 1-1) that are responsible for coordinating development of SIPs and TIPs in selected areas of the United States to address the requirements of the RHR. The WRAP region is composed of states and tribal lands located within the boundaries of Alaska, Arizona, California, Colorado, Hawaii, Idaho, Montana, New Mexico, North Dakota, Oregon, South Dakota, Utah, Washington and Wyoming; it includes the Class I areas indicated in Figure 1-2. WRAP is a regional partnership of states, tribes, Federal agencies, stakeholders, and citizen groups that was established to initiate and coordinate activities associated with the management of regional haze and other air quality issues within the WRAP states; their role includes providing technical and policy tools to help states and tribes. The members of WRAP committees and forums (<http://wrapair.org/about/orgchart.htm>) consist of representatives from the affected stakeholder groups identified above. Committee and forum members are urged to communicate freely with their peers and professional associations so that they can adequately represent the views of that segment of the public. Each committee and forum is expected to translate technical materials into a form accessible to the public. More information about the WRAP organizational structure and activities is available at <http://wrapair.org/facts/forumdescribe.html>.



Figure 1-1. Regional Planning Organizations engaged in regional haze modeling.



Figure 1-2. Locations of Class I areas in the WRAP states.

1.1.3 WRAP strategic plan

On September 29, 2003, WRAP released their strategic plan for the years 2003-2008 (WGA, 2003): http://wrapair.org/WRAP/meetings/031014board/Tab_4_Strategic_Plan_Final.pdf. Prior to 2003, WRAP's activities focused on developing the Section 309 (§309) SIPs/TIPs that nine WRAP states may elect to opt into and thereby adopt the recommendations of the Grand Canyon Visibility Transport Commission (GCVTC). These §309 SIPs/TIPs address visibility at the 16 Class I areas on the Colorado Plateau (see Figure 1-2). In 2003, WRAP's efforts turned to performing the technical analyses needed to develop the §308 SIPs/TIPs that address all 116 Class I areas in the WRAP region. The WRAP 2003-2008 strategic plan is broken down into two phases (Table 1-1). It will be reviewed and revised in 2005.

Table 1-1. WRAP 2003 Strategic Plan (WGA, 2003).

	Phase I 2003-2005	Phase II 2005-2007
Purpose:	Dry run for Phase II. Hedge against earlier due dates.	Refine and apply Phase I approaches for SIP/TIP purposes.
Scale:	Regional.	Regional and subregional.
Apportionment:	1996 & 2002 source contributions. Areas each plan to address.	2002 source contributions. Reduction obligations.
Strategies:	Identify options, screen.	Perform cost/benefit, select, design.
Communications:	Public education.	Public acceptance.
Major state/tribe submittals:	2002 emissions inventories.	Modeling run specifications.

1.1.4 Organization of the Regional Modeling Center

The WRAP RMC is composed of researchers from the University of California, Riverside (UCR), ENVIRON International Corporation, and the University of North Carolina's Carolina Environmental Program (UNC-CEP). Dr. Gail Tonnesen of UCR is the Project Manager and Principal Investigator for the RMC. Mr. Ralph Morris and Mr. Zac Adelman lead the RMC efforts at ENVIRON and UNC-CEP, respectively. We are performing meteorological, emissions, and air quality modeling to support WRAP's efforts to comply with the requirements of the RHR. UCR hosts the RMC's computer center, which includes numerous Linux computer platforms and RAID disk storage systems. In the past, training of states, tribes, and others has been performed at UCR's facilities.

The primary modeling tools used by the RMC include the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Model (MM5) meteorological modeling system, the Sparse Matrix Operator Kernel Emissions (SMOKE) emissions modeling system, and the Models-3 Community Multiscale Air Quality (CMAQ) air quality modeling system. We have also performed some sensitivity tests using the Comprehensive Air Quality Model with extensions (CAMx) and Regional Modeling System for Aerosols and Deposition (REMSAD) air quality models. In addition, there are plans to apply MM5 and the California Meteorological Model/California Puff Model (CALMET/CALPUFF) modeling system to Alaska.

During 2002 and 2003, the RMC focused on performing the technical analysis needed to develop the §309 SIPs/TIPs for those states and tribes that elect to pursue the §309 process. We set up the SMOKE emissions and Models-3/CMAQ modeling system for 1996 for the western states using 36-km-resolution MM5 data, and performed the technical analysis needed for the §309 SIPs and TIPs. More details can be found in the Section 309 Technical Support Document (TSD) (WRAP, 2003) located at <http://wrapair.org/309/031215Final309TSD.pdf>.

In 2003, the RMC then turned its efforts to setting up the modeling tools needed to address the technical requirements of the §308 SIPs/TIPs. This included setting up the MM5, SMOKE, and

CMAQ modeling systems for calendar year 2002 (CY02) using a 36-km-resolution grid for the continental United States and a 12-km-resolution grid for the WRAP states. During 2004 and early 2005, we continued setting up the modeling infrastructure for CY02 to address the requirements of the WRAP strategic plan.

The RMC notes and understands the importance of the guidance contained in the WRAP Tribal Template (<http://wrapair.org/WRAP/reports/Gen-Tribe-Temp.pdf>). Work products from the RMC are reviewed by the WRAP Modeling Forum and any interested stakeholders.

1.2 Overview of RMC 2004 Activities

From March 2004 through February 2005, the RMC activities continued to focus on developing the modeling databases needed to address the technical requirements of the §308 SIPs/TIPs. This included not only setting up the emissions, meteorological, and air quality modeling for CY02, but also implementing a particulate matter (PM) source apportionment capability to obtain a preliminary assessment of source culpability to regional haze at Class I areas. Our work efforts also included separate meteorological and dispersion modeling for Alaska, a WRAP state with four Class I areas whose size and remoteness from the other states make it inefficient to include with the other states' modeling domain.

At the end of 2003, all 2003 RMC work was completed except for developing the new WRAP ammonia emissions model, for which the data collection efforts were not completed. This remaining work was rolled into the WRAP 2004 RMC work effort. The 2004 work plan (http://www.cert.ucr.edu/aqm/308/reports/RMC_2004_Workplan_Final_Version_03_01_04.pdf) was divided into 13 new tasks plus a task for the ammonia emissions work (Task 0.5). Note that Task 8 is not covered in this report because it did not receive funding for 2004.

- *Task 0.5—2002 Ammonia Emissions Inventory for WRAP Region:* This task was initiated in 2003 to develop a new GIS-based ammonia emissions model that uses high-resolution land cover data, new ammonia emission factors, and MM5 meteorological data to generate gridded, day-specific ammonia emissions.
- *Task 1—Project Administration:* Project management activities, including progress reports, interim and final reports, conference calls, and day-to-day management, were performed under this task. It also covered the purchase of computing hardware.
- *Task 2—Test, Improve, Quality Control, Obtain External Peer Review, and Finalize 36-km and 12-km MM5 Simulations for Eventual Use in CMAQ:* The MM5 meteorological modeling for CY02 for the continental U.S. at 36 km and the western U.S. at 12 km was performed under this task. This included sensitivity modeling to identify the optimal MM5 configuration, development of an MM5 modeling protocol, peer review of the MM5 approach, and the 2002 annual MM5 modeling.
- *Task 3—2002 Base Year Emissions Modeling, Processing, and Analysis:* This task covered setting up and performing the 2002 SMOKE emissions modeling at 36- and 12-km resolution.

- *Task 4—Air Quality Model Evaluation for 2002 Annual Simulation:* Under this task the RMC performed the CMAQ 2002 base case simulation and model performance evaluation.
- *Task 5—Preparation and Reporting of Geographic Source Apportionment Results:* Implementation of the Tagged Species Source Apportionment (TSSA) algorithms in CMAQ was performed under this task, along with the evaluation and application of the TSSA as part of the Attribution of Haze (AoH) study.
- *Task 6—Further Analysis of Model Performance in Regard to the Contribution of Natural Emissions to Visibility Impairment:* The use of models to aid in the definition of natural conditions was investigated under this task.
- *Task 7—Evaluation and Comparison of Alternative Models:* This task investigated and evaluated the benefits of applying alternative models to CMAQ.
- *Task 8—Improvement of WRAP Spatial, Chemical Speciation, and Temporal Allocation Profiles:* The purpose of this task was to improve several components of the emissions inventory. However, it was not funded during 2004.
- *Task 9—Testing and Further Improvements to the Windblown Dust Emissions Modeling Methodology:* This task refined the WRAP windblown dust model and applied it to 2002, and included a model performance evaluation.
- *Task 10—Continued Improvement to Model Evaluation Software:* Updates and enhancements to the UCR model evaluation software were performed under this task.
- *Task 11—Sensitivity Studies Designed to Evaluate Uncertainties in Fire Emissions:* The analysis of the sensitivity of PM and visibility to modeling assumptions made for wild-fires, prescribed burns, and agricultural burning was accomplished under this task.
- *Task 12—Preliminary Meteorological, Emissions, and Air Quality Modeling Activities for Alaska:* Meteorological and dispersion modeling for Alaska were evaluated under this task.
- *Task 13—Training Courses for the WRAP States and Tribes:* Any training requested was to be performed under this task.

2. Task 0.5: 2002 Ammonia Emissions Inventory for WRAP Region

2.1 Introduction

Ammonia (as ammonium nitrate and ammonium sulfate) plays an important role in the formation of particulate matter. Recent advances in understanding the health impacts of particulate pollution and the important role ammonia (NH_3) emissions play in the formation of secondary PM has spawned a great deal of new research into these emissions. Major sources of NH_3 emissions include livestock operations, fertilizer use, waste management, mobile sources, industrial point sources, and various biological sources such as human respiration, wild animals, and soil microbial processes. For each of these source categories there remain large uncertainties in the magnitude of emissions, the diurnal and seasonal variations, and the spatial distribution. Uncertainty in NH_3 emissions is a key source of uncertainty in modeling the formation of sulfate and nitrate aerosols. Thus, development of improved NH_3 emissions inventories is essential for modeling the formation of fine PM and regional haze, and for developing effective plans to mitigate visibility impairment at national parks, forests, and wilderness areas.

The understanding of ammonia emissions has significantly improved since the development of the 1996 National Emissions Inventory (NEI) that was used in the WRAP visibility modeling to meet CAA §309 requirements. WRAP funded the RMC to develop an improved NH_3 emissions inventory for the WRAP states and tribes to use in CAA §308 modeling. The development of this improved inventory involved a literature review of recent research in NH_3 emissions, the incorporation of environmental factors that influence the magnitude and temporal variation of ammonia emission, and the development of a geographic information system (GIS)-based modeling system for efficient generation of a gridded modeling inventory of ammonia emissions for CY02. We developed the inventory at a spatial resolution of 36 km on the RPO Unified Continental 36-km Modeling Grid domain (abbreviated in this report as “RPO Unified domain”), which is shown in Figure 2-1. This modeling grid is common to all five RPOs, with all emissions gridded to 36-km² cells for subsequent air quality modeling simulations. The source categories considered in the emissions inventory include the four major contributors of ammonia on a regional scale: livestock operations, fertilizer usage, domestic sources, and native soils. At the request of the WRAP Emissions Forum, we also included ammonia emissions from wild animals in the inventory.

As part of developing the improved inventory, we reviewed recent literature concerning ammonia emission factors for various source categories. Particular attention was given to identifying current research focusing on the temporal variation of ammonia emissions and the effects of environmental factors. The results of this literature review are documented in Chitjian and Mansell (2003a). The review identified a number of environmental factors affecting ammonia emission factors and temporal allocation of annual emission estimates; these factors include soil pH and meteorological data. Data on the effects were obtained from various sources, and the effects were incorporated into the modeling system used in creating the improved ammonia

emissions inventory. Chitjian and Mansell (2003b) present a detailed discussion of the environmental factors incorporated into the ammonia emissions modeling system, and their impacts on the resulting ammonia emissions are discussed in Mansell (2004a).

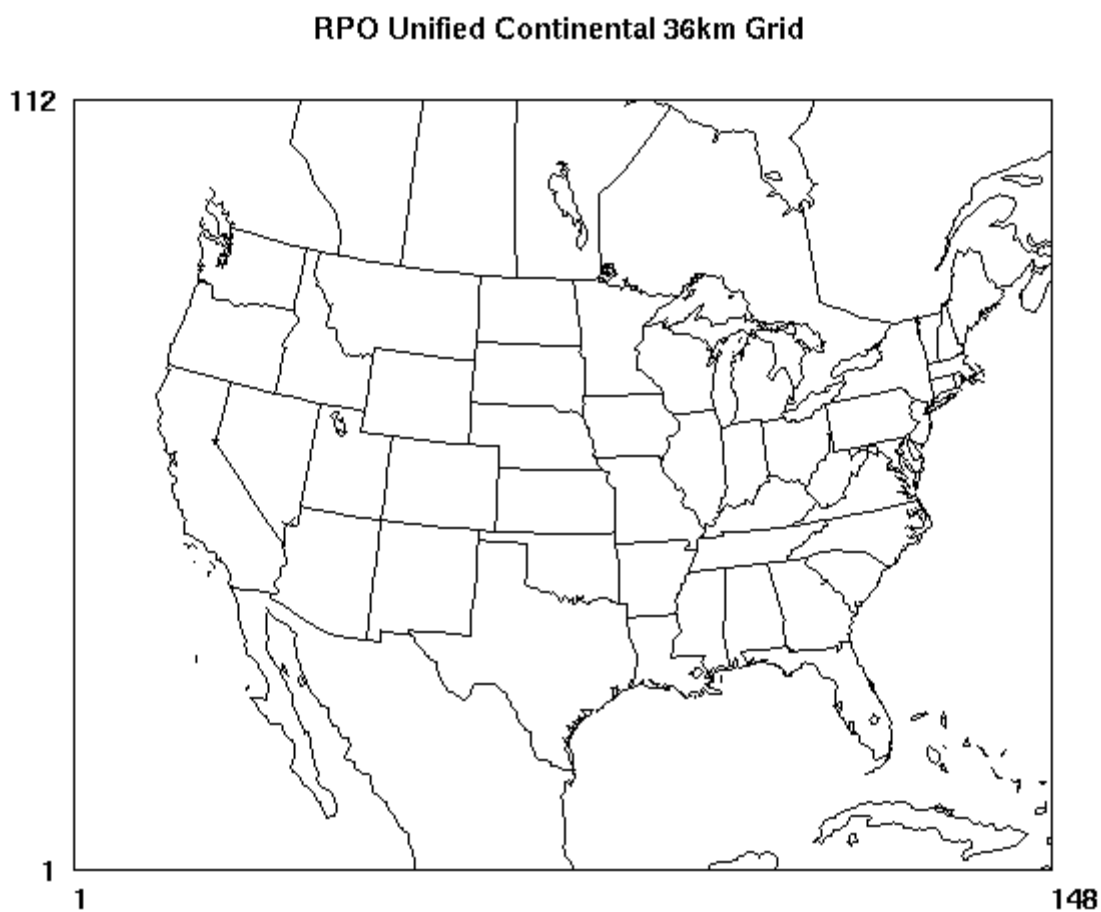


Figure 2-1. RPO Unified Continental 36-km Modeling Grid domain.

We developed a GIS-based modeling system using the latest version of ESRI's GIS, ArcGIS, and the ARC Macro Language (AML). The model incorporates the improved estimation algorithms just discussed, and includes a user-friendly graphical user interface (GUI) to facilitate implementation. It also allows easy modification of activity data, emission factors, and associations between the ammonia emission source categories' land use/land cover (LULC) characteristics. We populated the modeling system with all the data needed to produce an ammonia inventory for the U.S. portion of the RPO Unified domain for 2002 at a 36-km spatial resolution. The development of the GIS-based model is documented in Chitjian and Mansell (2003b).

2.2 Emissions Inventory Development

The development pathway of the 2002 ammonia emissions inventory is summarized below. (Chitjian and Mansell [2003a,b] and Mansell [2004a] provide greater detail.) Since WRAP forums other than the Air Quality Modeling Forum will be developing ammonia emissions inventories for mobile sources, industrial point sources, and fire sources, we considered only selected major and minor sources of ammonia emissions for our inventory: livestock operations, fertilizer usage, domestic sources, native soils, and wild animals. Table 2-1 shows the source categories and subcategories included in the inventory.

Table 2-1. Ammonia emission source categories included in the WRAP NH₃ inventory.

Major Source Category	Subcategories	Major Source Category	Subcategories
Livestock operations	Beef cattle	Domestic sources	Human respiration
	Dairy cattle		Human perspiration
	Swine		Infant cloth diapers
	Poultry		Infant disposable diapers
	Horses		Cats
	Sheep		Dogs
Fertilizer usage	Anhydrous ammonia	Native soils	Urban
	Aqueous ammonia		Barren/desert
	Nitrogen solutions		Deciduous forest
	Urea		Evergreen forest
	Ammonium nitrate		Mixed forest
	Ammonium sulfate		Shrubland
	Ammonium thiosulfate		Grassland
	Other straight nitrogen		Fallow
	Ammonium phosphates		Urban/recreational grasses
	N-P-K		Wetlands
	Calcium ammonium nitrate	Wild animals	Black bears
	Potassium nitrate		Grizzly bears
			Elk
			Deer

2.2.1 Emission factors

2.2.1.1 Livestock operations

Ammonia emissions from livestock were developed using county-level head counts and emission factors based on a literature review performed by Chinkin et al. (2003). Our inventory includes emissions for beef and dairy cattle, poultry, swine, sheep, and horses. The approach we used does not treat the individual processes leading to ammonia emissions from various management practices, which has been the subject of recent research in the emissions inventory development community. Rather, we used emission factors based on a “whole animal” approach. The factors used in developing the WRAP inventory are presented in Table 2-2.

Table 2-2. Livestock emission factors (kg/animal-yr).

Source Category	Emission Factor	Source Category	Emission Factor
Beef cattle	25.0	Swine	7.0
Dairy cattle	9.0	Horses	12.2
Poultry	0.1	Sheep	3.4

2.2.1.2 Fertilizer application

Ammonia emission estimates from fertilizer application were developed using emission factors from the European Environment Agency (EEA, 2002) as recommended in Chitjian and Mansell (2003b). Emission factors for fertilizer application are presented in Table 2-3. Fertilizer emission factors are adjusted as a function of soil pH. Based on research conducted by Potter et al. (2001), the emission factors are scaled by applying a scalar, a , to each factor, where a is calculated using the following relationship:

$$a = (0.3125 \cdot \text{pH}) - 1.01$$

Note that soil pH scalars were not applied to urea emission factors, as research has indicated that urea emissions are not affected by initial soil pH. Data for soil pH were derived from the State Soil Geographic (STATSGO) database from the U.S. Department of Agriculture (USDA, 1994). The soil pH data source and processing are discussed in more detail in Mansell (2004a).

Table 2-3. Fertilizer emission factors.

Fertilizer Type	%N	Fertilizer Type	%N
Anhydrous ammonia	4.0	Calcium ammonium nitrate	2.0
Aqueous ammonia	2.4	Ammonium thiosulfate	2.4
Nitrogen solutions	8.0	Other straight nitrogen	2.4

Fertilizer Type	%N	Fertilizer Type	%N
Urea	15.0	Ammonium phosphates	5.0
Ammonium nitrate	2.0	N-P-K	2.0
Ammonium sulfate	10.0	Potassium nitrate	2.4

2.2.1.3 Native soils

Natural soils can be both a source and a sink of ammonia emissions, depending on the ambient NH_3 concentrations, climatic conditions, and the conditions of the soils. While there are a number of researchers considering this issue, ammonia emissions from natural soils remain highly uncertain. For our inventory, ammonia emissions from natural soils were estimated based on emission factors developed or recommended by Battye et al. (2003) and Chinkin et al. (2003) (Table 2-4). Land use data used for the inventory were developed from the National Land Cover Database (<http://edcwww.cr.usgs.gov/pub/edcuser/vogel/states/>). A more complete description of the LULC data we used can be found in Section 2.2.5.1 and in Mansell (2004a). Emissions from agricultural lands are assumed to be included in the fertilizer application estimates.

Table 2-4. Emission factors for native soils.

Land Use Type	Emission Factor (kg/km ² -yr)	Land Use Type	Emission Factor (kg/km ² -yr)
Urban	10	Shrubland	400
Barren/desert land	10	Grassland	400
Deciduous forest	174	Fallow	205
Evergreen forest	54	Urban/recreational grasses	400
Mixed forest	114	Wetlands	400

Potter et al. (2001) estimated ammonia emissions from native soils based on several environmental variables, including monthly rainfall, surface air temperature, solar radiation, soil texture, land cover type, and vegetative type. The model first calculates the available mineral nitrogen substrate for ammonia emissions and then modifies this value by applying scalars for soil surface temperature (T , in K), pH, and soil moisture content (M , in g/g). The scalars are of the form

$$(1/\{1 + 10^{[0.09018 + 2729.92/(273.16+T) - (c \cdot \text{pH})]}\}) \cdot (1-M),$$

where c is a constant that determines the sensitivity to pH. The authors used $c=1.3$ (consistent with measurements they had made), and $c=10$ to produce results with minimal pH effects. Ammonia emissions were calculated for seven nonagricultural soil types. Emission factors derived from the model range from 6.5 kg/km²-yr for evergreen needle leaf forests, using a moderate pH effect, to 206 kg/km²-yr for mixed forests, using a minimal pH effect.

The emission factors presented in Table 2-4 have been modified for temperature and pH effects using the scalars described above. We used a value of $c=1.3$. Soil pH data were derived from the STATSGO database (USDA, 1994). Soil temperature and soil moisture content were taken from the meteorological data used in the development of the ammonia emissions inventory, as discussed in Section 2.2.5.3.

2.2.1.4 Domestic sources

Ammonia emissions from domestic source considered in the current inventory include human respiration and perspiration, disposable and cloth diapers, and domestic pets (cats and dogs). Table 2-5 presents the emission factors recommended by Chitjian and Mansell (2003b) and Chitjian et al. (2000).

Table 2-5. Emission factors for domestic ammonia sources.

Source	Emission Factor	Unit
Cats	0.348	lb N/cat/yr
Dogs	2.17	lb N/dog/yr
Human perspiration	0.55	lb NH ₃ /person/yr
Human respiration	0.0035	lb NH ₃ /person/yr
Cloth diapers	6.9	lb NH ₃ /infant/yr
Disposable diapers	0.36	lb NH ₃ /infant/yr

2.2.1.5 Wild animals

Ammonia emissions from wild animals considered in the current inventory include emissions from grizzly bears, black bears, elk, and deer. The emission factors presented in Table 2-6 were obtained from the Carnegie Mellon University (CMU) Ammonia Model (Strader et al., 2004).

Table 2-6. Emission factors for wild animal ammonia sources.

Source	Emission Factor	Unit
Black bears	0.378	kg NH ₃ /animal/yr
Grizzly bears	0.378	kg NH ₃ /animal/yr
Elk	1.707	kg NH ₃ /animal/yr
Deer	0.378	kg NH ₃ /animal/yr

2.2.2 Activity data

Complete listings of county-level activity data for all source categories considered in the ammonia inventory can be found in Mansell (2004b). Summaries are given below.

2.2.2.1 Livestock operations

Activity data for livestock ammonia emissions were based on total county-level animal head counts. We obtained animal head counts from the National Agricultural Statistics Service's (NASS) county livestock files (NASS, 2003).

2.2.2.2 Fertilizer application

Activity data for fertilizer ammonia emissions were based on county-level fertilizer usage data. Originally, we sought to obtain these data from a number of sources, including the Association of American Plant Food Control Officers (AAPFCO, 2003), the USDA agricultural census (2001), and the county crop files (NASS, 2003). However, these data did not provide the monthly or seasonal variation required for temporal allocation of the resulting emission estimates. As an alternative, fertilizer sales data obtained from the most recent version of the CMU Ammonia Model (Strader et al., 2004) were extracted and reformatted for use in our inventory. These data were available for calendar year 2002 on a monthly basis for each county in the conterminous U.S. The primary source of these data was the AAPFCO, with monthly variation based on crop planting times and fertilizer application times and rates as documented in Strader et al. (2004).

2.2.2.3 Native soils

The total area of each land use type from the LULC data used for this task provided the activity data for estimating soil emissions. These LULC data were developed from the National Land Cover Database (<http://edcwww.cr.usgs.gov/pub/edcuser/vogel/states/>).

2.2.2.4 Domestic sources

Activity data for domestic sources were based on the most recent U.S. Census (2000), and per capita pet ratios based on recommendations of Dickson et al. (1991).

2.2.2.5 Wild animals

As noted in Section 2.1, wild animal ammonia emissions were included in the inventory at the request of the WRAP Emissions Forum. Because this source category was added after the data collection efforts were completed, activity data for wild animals were obtained from the latest version of the CMU Ammonia Model (Strader et al., 2004). Note that these data were used “as is” (i.e., no additional quality assurance of the data was performed).

2.2.3 Temporal allocation

2.2.3.1 Livestock operations

A review of current literature revealed a lack in consistency of results quantifying temporal variations in ammonia emissions from livestock (Chitjian and Mansell, 2003a). However, most of the studies cited concluded that ammonia emissions from livestock display both a seasonal and a diurnal variation consistent, in general, with increased ammonia emissions associated with warmer temperatures.

Chinkin et al. (2003) recommend seasonal allocation factors derived from those proposed by Gilliland et al. (2002), which are based on inverse modeling results. The factors were adjusted to reflect the current recommended emission factors from EPA's Office of Research and Development (ORD) (U.S. EPA, 2002), which were not available at the time Gilliland and coworkers performed their modeling. The adjusted factors are shown in Table 2-7. Inspection of this table indicates a 3- to 4-fold increase in emissions during the warmest months. Also note that the minimum emissions occur during the late fall, as opposed to the coldest months; the minimum in fall is explained by the relatively dry conditions at that time of year.

Table 2-7. Monthly livestock allocation factors.

Month	Temporal Allocation Factor	Month	Temporal Allocation Factor
January	67	July	183
February	75	August	154
March	75	September	115
April	82	October	73
May	126	November	51
June	164	December	51

A discussion of the diurnal variation of livestock ammonia emissions is presented in Chitjian and Mansell (2003b). In general, the literature reports an increase in daytime emissions over nighttime emissions. Russell and Cass (1986) developed a theoretical equation to predict diurnal emission variations as a function of meteorological data. This equation relates hourly ammonia emission rates to temperature and wind speed, as follows:

$$E_i \propto [2.36^{(T_i-273)/10}] V_i A$$

where

E_i = ammonia emission rate at hour i from animal waste decomposition

A = daily total emission rate for ammonia from animal waste = $\sum E_i$

T_i = ambient temperature in Kelvin at hour i

V_i = wind speed in m/s at hour i (a minimum wind speed of 0.1 m/s was assumed)

For our inventory, the model of Russell and Cass was used to provide the diurnal variation of livestock ammonia emissions. This approach is consistent with first-principle assumptions.

Although the seasonal and diurnal variations presented here are both empirically based, they are consistent with theory and measurements showing increased ammonia volatilization rates with increased temperature and wind speed. The monthly allocation factors shown in Table 2-7 were used to allocate annual emission estimates to each month of the year.

2.2.3.2 Fertilizer application

Emissions from fertilizer application were temporally allocated monthly based on the monthly activity data (see Section 2.2.2.2). Diurnal variations in fertilizer emissions are expected, as temperature and wind speed affect ammonia production and volatilization. Our inventory used the equations developed by Russell and Cass (1986) to temporally allocate daily emissions to each hour of the day as a function of temperature and wind speed, as with livestock emissions. Chitjian and Mansell (2003b) provide a more detailed discussion of the temporal variation of fertilizer ammonia emissions.

2.2.3.3 Native soils

Temporal allocation of native soil ammonia emissions was calculated using the emission factor scalars described in Section 2.2.1.3, which are temporally resolved.

2.2.3.4 Domestic sources

The ammonia emissions from domestic sources were assumed to be temporally invariant. Thus, daily emissions can be estimated as the annual estimates divided by 365.

2.2.3.5 Wild animals

The ammonia emissions from wild animals were assumed to be temporally invariant. Thus, daily emissions can be estimated as the annual estimates divided by 365.

2.2.4 Spatial allocation

2.2.4.1 Livestock operations

Ideally, for spatial allocation of livestock ammonia emissions, the locations of large confined animal feed operations (CAFOs) should be used to geocode each CAFO within the modeling domain. In addition, grazing livestock must be spatially allocated from the county level to modeling grid cells using land use surrogates. For our inventory, geocoding of large CAFOs was not practical for the WRAP regional modeling domain, given the task schedule and budget constraints. Therefore, all livestock ammonia emissions were spatially allocated using surrogates based on the grassland and pasture land use categories (codes 71 and 81 in Table 2-8, which is discussed in Section 2.2.5.1).

2.2.4.2 Fertilizer application

Ammonia emissions from fertilizer application are spatially allocated as a function of land use types. We developed spatial allocation factors based on the agricultural land classes available in the LULC data used for this task.

2.2.4.3 Native soils

Native soil emissions are spatially allocated based on the land area for each land use category from the LULC data used for this task.

2.2.4.4 Domestic sources

Domestic animal ammonia emissions were spatially allocated by population density based on the 2000 U.S. Census.

2.2.4.5 Wild animals

Wild animal ammonia emissions were spatially allocated to forestland, shrubland, and grassland as determined by the LULC data used for this task.

2.2.5 Land use and environmental data

The land use and environmental data utilized in developing the WRAP ammonia emissions inventory are discussed below.

2.2.5.1 Land use/land cover

The default LULC data used in creating the inventory was based on the National Land Cover Database (NLCD). The NLCD was developed as part of a cooperative project between the U.S. Geological Survey (USGS) and EPA to produce a consistent land cover data layer for the entire conterminous U.S. based on 30-m Landsat thematic mapper (TM) data. The NLCD was developed from TM data acquired from the Multi-Resolution Land Characterization (MRLC) Consortium, a partnership of Federal agencies that produce or use land cover data. The partners include USGS (the National Mapping, Biological Resources, and Water Resources Divisions), EPA, the U.S. Forest Service, and the National Oceanic and Atmospheric Administration.

NLCD datasets are available as flat generic raster image files that are easily imported into a GIS (e.g., ARC/Info) and are provided in an Albers Conic Equal Area projection at a spatial resolution of 30 m. They can be found at <http://edcwww.cr.usgs.gov/pub/edcuser/vogel/states/>, along with a discussion on how they were developed. The land cover characteristics are defined in terms of the 21 separate categories given in Table 2-8. A sample display of the NLCD data is presented in Figure 2-2.

Table 2-8. NLCD land cover classification codes.

Code	Description	Code	Description
11	Open water	51	Shrubland
12	Perennial ice/snow	61	Orchards/vineyards/other
21	Low-intensity residential	71	Grassland/herbaceous
22	High-intensity residential	81	Pasture/hay
23	Commercial/industrial/transportation	82	Row crops
31	Bare rock/sand/clay	83	Small grains
32	Quarries/strip mines/gravel pits	84	Fallow
33	Transitional	85	Urban/recreational grasses
41	Deciduous forest	91	Woody wetlands
42	Evergreen forest	92	Emergent herbaceous wetlands
43	Mixed forest		

NLCD Landuse/Landcover

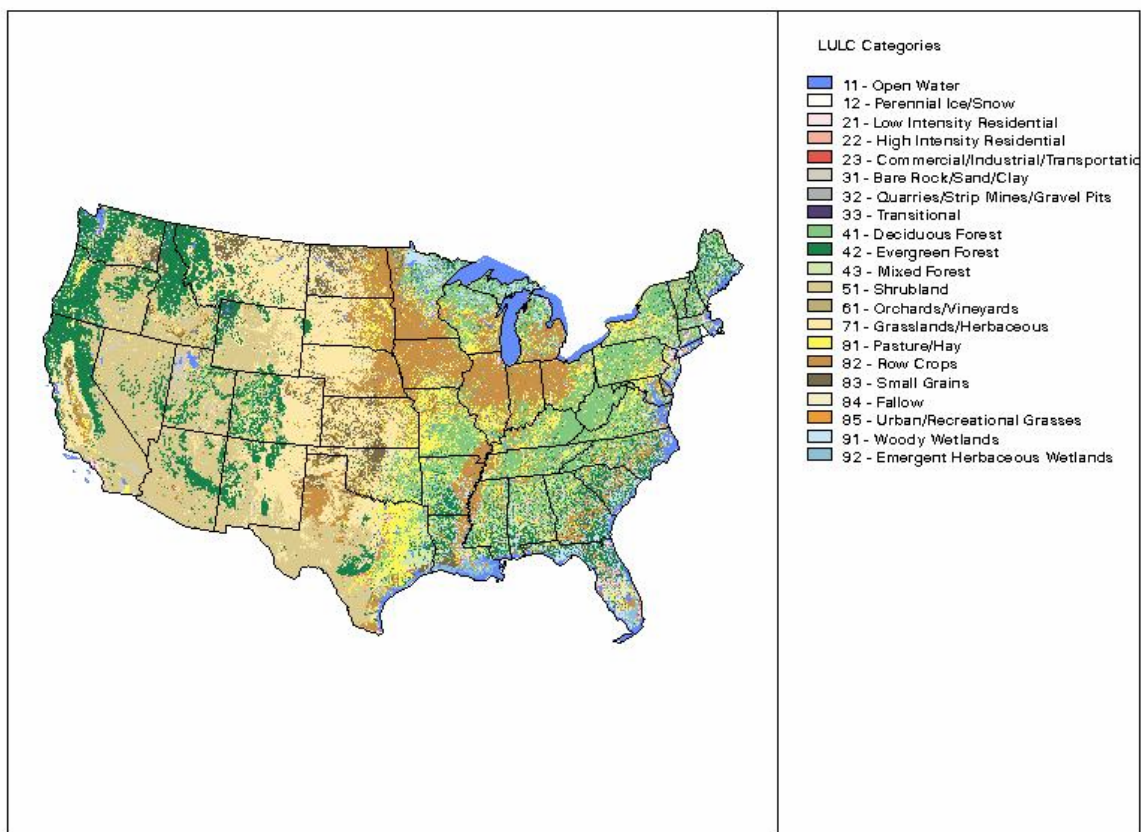


Figure 2-2. NLCD data for the conterminous United States.

2.2.5.2 Soil pH

The STATSGO database developed by USDA's Natural Resources Conservation Service was used to specify the soil pH necessary for developing our emissions inventory. These soils data are available as geospatial coverages and associated attribute tables for each state in the U.S., and require considerable effort to calculate and extract the relevant parameters. Detailed documentation of the database and data structures can be found in USDA (1994).

To reduce the resource-intensive data processing required with the complete STATSGO database, processed soils datasets were obtained from the Earth System Science Center (ESSC) at Pennsylvania State University via anonymous ftp at http://www.essc.psu.edu/soil_info/. The datasets archived by the ESSC include a single GIS coverage of soil pH for the conterminous U.S. (Figure 2-3).

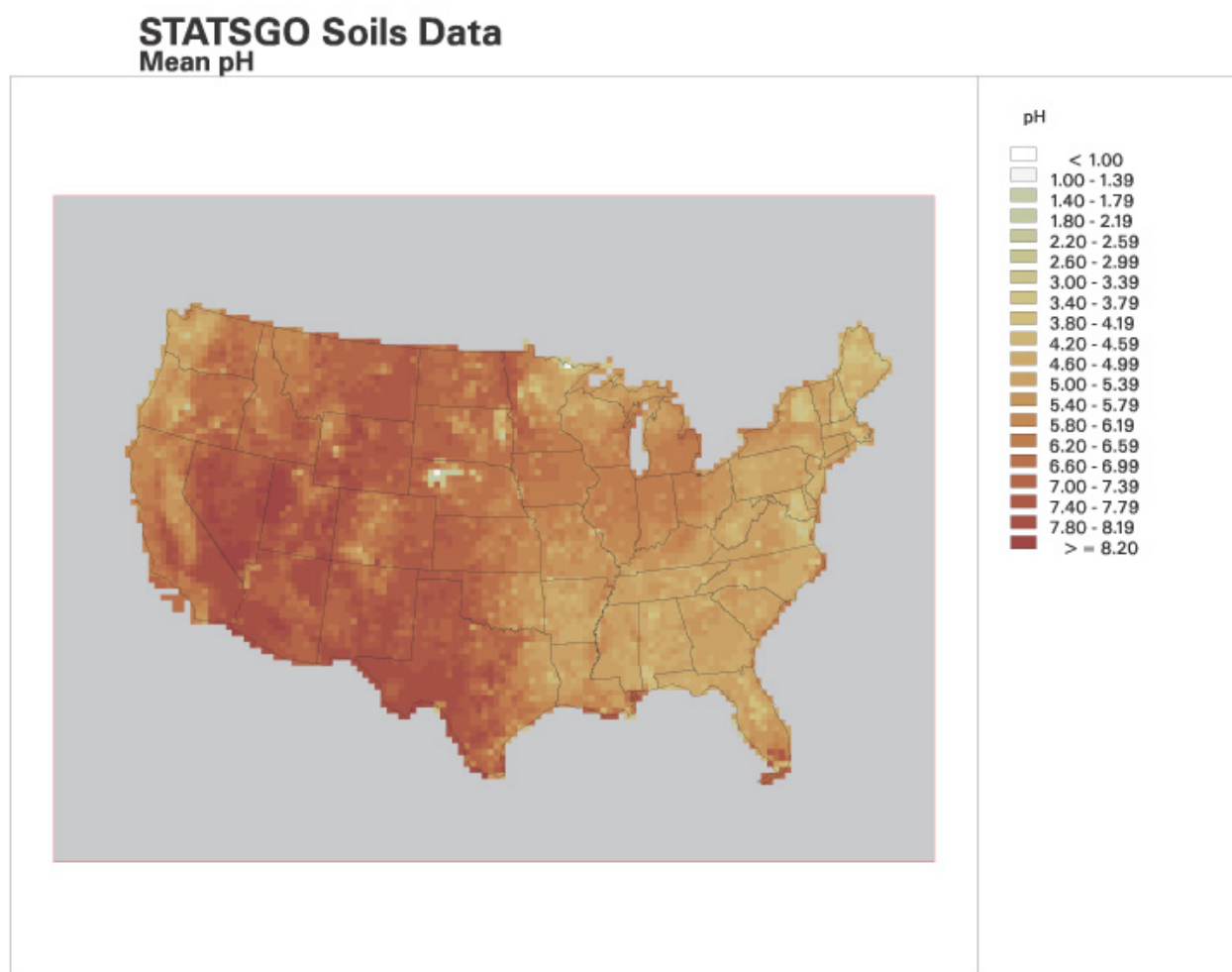


Figure 2-3. Mean soil pH for the conterminous United States.

2.2.5.3 Meteorological data

Meteorological data were derived from MM5 simulations for 2002 on the RPO Unified domain. Data required as input to the GIS-based ammonia emissions modeling system include wind speeds, ambient temperatures, soil temperatures, and soil moisture. These data were extracted from the MM5 output files and reformatted for use in the GIS-based modeling system.

2.2.6 GIS-based modeling

We developed a GIS-based modeling system to generate a gridded ammonia emissions inventory that includes the improvements identified for this project. The county-level activity data were used in conjunction with the appropriate emission factors and environmental factors described above to generate the gridded inventory on the RPO Unified domain. The inventory is temporally resolved hourly. A detailed discussion of the design and implementation of the modeling system is presented in Chitjian and Mansell (2003b).

As noted earlier, the GIS-based modeling system was developed using AML and the latest version of ArcGIS. The model incorporates our improved estimation algorithms, includes a user-friendly GUI, and allows easy modification of activity data, emission factors, and associations between ammonia emission source categories' LULC characteristics. The modeling system was populated with all the necessary data to produce an ammonia inventory for the U.S. portion of the RPO Unified domain for 2002 at a 36-km spatial resolution. See Chitjian and Mansell (2003b) for further information.

As discussed in Mansell (2004c), the modeling system applies gridding surrogates to the county-level emission estimates on an annual basis (or monthly for fertilizer application emissions). Effects of soil pH on the emission factors for fertilizer application are applied to the annual gridded ammonia emission estimates. Other environmental factors are incorporated in the temporal allocation modules, since these factors impact the diurnal variation of emissions through gridded, hourly temperatures and wind speeds. An exception applies for the emissions from native soils: for this source category, the effects of soil conditions (pH and moisture) and meteorological data are both incorporated in the emissions estimates during the temporal allocation process.

2.3 2002 Ammonia Emissions inventory

As stated earlier, the 2002 ammonia emissions inventory developed for this project includes the source categories of livestock operations, fertilizer usage, domestic sources, native soils, and wild animals; see Table 2-1 for the subcategories under each of these. Below we present the inventory in terms of the complete inventory and also by major source category. A comparison with the results of the CMU Ammonia Model is also presented. A more detailed discussion of the 2002 ammonia emissions inventory can be found in Mansell (2004a).

Table 2-9 shows the annual ammonia emissions estimates for calendar year 2002 by state for each of the five major source categories above. With the exception of the soil pH adjustments to fertilizer emission factors, the results presented here for fertilizer usage, livestock operations, and native soil emissions do not reflect the effects of environmental factors, as explained before. In

general, the ammonia inventory is dominated by livestock operations, fertilizer usage, and native soil emissions, as expected. This trend varies by state, with largely agricultural regions representing the majority of the emissions from these source categories. Although native soil ammonia emissions are highly uncertain, the variation in emissions from this category across states reflects the variation in land use types within each state. The magnitude of domestic-source emissions are reflective of the population in each state, based on the 2000 U.S. Census data used as activity data. Ammonia emissions from wild animals are based on activity data and emission factors extracted from the CMU Ammonia Model. The wild animal data were not scrutinized in detail, and clearly there are some omissions and/or inconsistencies in the datasets, as discussed in Section 2.3.5.

Figure 2-4 gives a graphical representation of the data in Table 2-9.

Table 2-9. Annual 2002 NH₃ emissions by state (tons).

State	Livestock Operations	Fertilizer Usage	Native Soils	Domestic Sources	Wild Animals	TOTAL
AL	34,306	5,562	15,793	2,259	7,500	65,419
AZ	10,331	12,109	102,837	2,553	1,798	129,628
AR	45,396	38,744	14,578	1,365	4,023	104,107
CA	97,721	78,052	102,447	16,704	302	295,225
CO	34,133	18,848	74,967	2,127	5,586	135,661
CT	1,802	796	1,937	1,668	375	6,577
DE	4,607	888	531	387	110	6,523
DC	0	0	9	272	0	281
FL	20,562	3,300	28,667	6,632	6	59,167
GA	38,408	6,468	18,229	4,132	5,203	72,440
ID	30,082	31,442	51,230	660	3,425	116,839
IL	48,391	120,817	6,361	6,137	3,699	185,405
IN	38,690	46,642	4,418	3,055	2,123	94,928
IA	159,638	120,694	6,729	1,472	1,500	290,032
KS	69,753	100,340	44,151	1,351	748	216,344
KY	34,476	26,858	12,066	2,049	2,184	77,633
LA	9,326	15,273	18,973	2,246	5,001	50,820
ME	2,321	924	10,449	645	1,299	15,638
MD	11,049	4,294	2,753	2,604	974	21,673
MA	1,487	405	3,059	3,079	304	8,334
MI	25,964	26,409	22,820	4,954	8,874	89,021
MN	86,787	114,864	26,827	2,460	4,587	235,525
MS	26,361	14,228	13,630	1,469	7,498	63,186
MO	62,834	61,084	16,543	2,798	3,820	147,079
MT	24,926	31,376	102,946	454	4,024	163,727
NE	80,050	91,584	48,356	859	1,255	222,105
NV	4,415	1,395	106,982	988	92	113,872

State	Livestock Operations	Fertilizer Usage	Native Soils	Domestic Sources	Wild Animals	TOTAL
NH	967	56	3,150	619	335	5,128
NJ	1,268	808	2,425	4,101	931	9,532
NM	21,397	5,599	112,468	913	1,414	141,791
NY	33,157	4,471	14,724	9,289	3,673	65,315
NC	101,463	6,771	17,005	4,071	5,517	134,827
ND	21,540	95,026	32,021	323	1,141	150,051
OH	34,443	55,453	7,192	5,632	2,049	104,769
OK	72,221	37,626	35,297	1,740	1,652	148,535
OR	17,325	22,988	55,624	1,691	3,361	100,989
PA	46,840	8,924	13,934	6,014	5,894	81,605
RI	112	56	450	507	52	1,176
SC	10,754	3,864	10,081	2,025	4,249	30,973
SD	50,786	66,051	43,705	386	1,316	162,244
TN	29,369	14,680	12,330	2,861	3,704	62,944
TX	146,410	83,349	175,959	10,502	18,012	434,233
UT	17,458	2,091	62,973	1,150	1,623	85,295
VT	6,529	624	3,087	309	635	11,183
VA	26,787	8,352	12,851	3,501	4,021	55,512
WA	18,349	17,300	28,024	2,911	2,186	68,771
WV	6,449	1,331	9,465	911	3,790	21,947
WI	73,031	28,807	16,352	2,674	6,932	127,795
WY	15,159	11,037	93,013	246	2,944	122,400
TOTAL	1,755,633	1,448,659	1,620,414	137,752	151,744	5,114,202

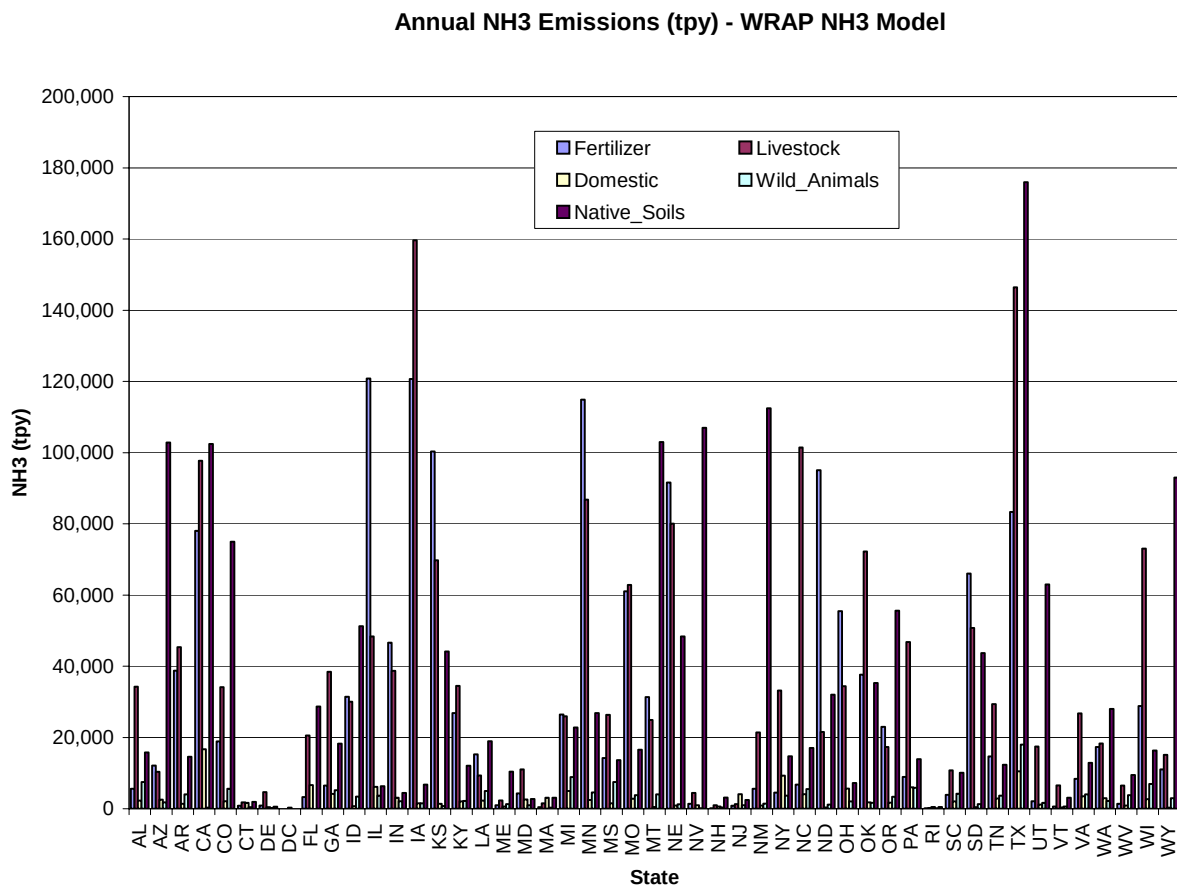


Figure 2-4. 2002 annual NH₃ emissions by source category and state in tons per year (tpy).

2.3.1 Livestock operations

Figure 2-5 presents the 2002 annual livestock emissions by animal type for each the WRAP states. Beef cattle, dairy cattle, and swine contribute approximately 87% of the total livestock emissions across all 13 states. The majority of dairy cattle emissions are found in California. Beef cattle emissions are more evenly distributed across the WRAP region, with the exception of Arizona and Nevada; South Dakota shows the highest amount of ammonia emissions from beef cattle. The remaining source categories (swine, poultry, horses, and sheep) are minor contributors of livestock ammonia emissions across the WRAP region.

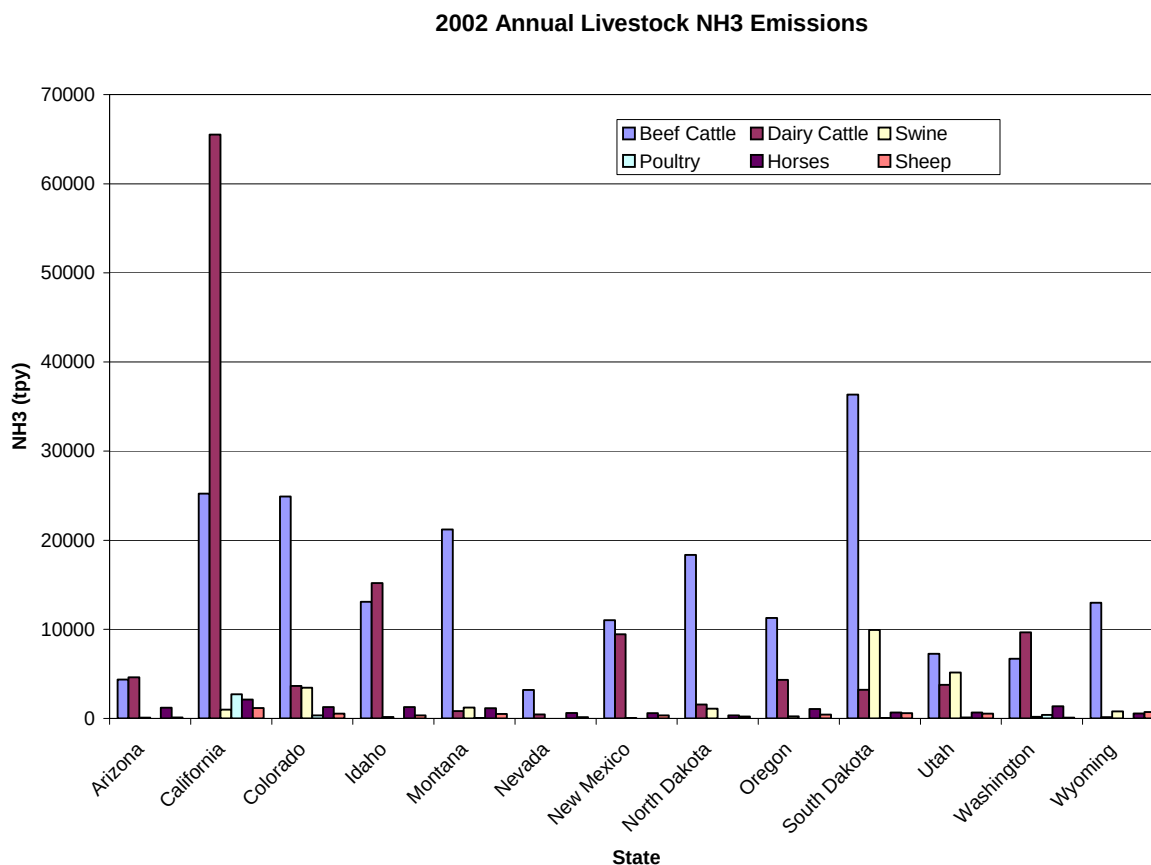


Figure 2-5. Annual livestock NH₃ emissions by animal type for WRAP states.

Tabulated livestock ammonia emissions by state and animal type are presented in Mansell (2004a), as is the spatial distribution of total annual livestock ammonia emissions. Both the county-level emissions and the gridded emission estimates generated using the display modules of the GIS-based modeling system are given in the draft report for this task (Mansell, 2004a).

2.3.2 Fertilizer application

Figure 2-6 shows the 2002 annual fertilizer application emissions by fertilizer type for the WRAP states. The majority of fertilizer ammonia emissions are found in California and the Dakotas. The distribution among the various fertilizer types can also be seen. Note that these emission summaries include the dependence of emission factors on soil pH. As expected, states with large agricultural regions dominate the fertilizer-usage ammonia emissions.

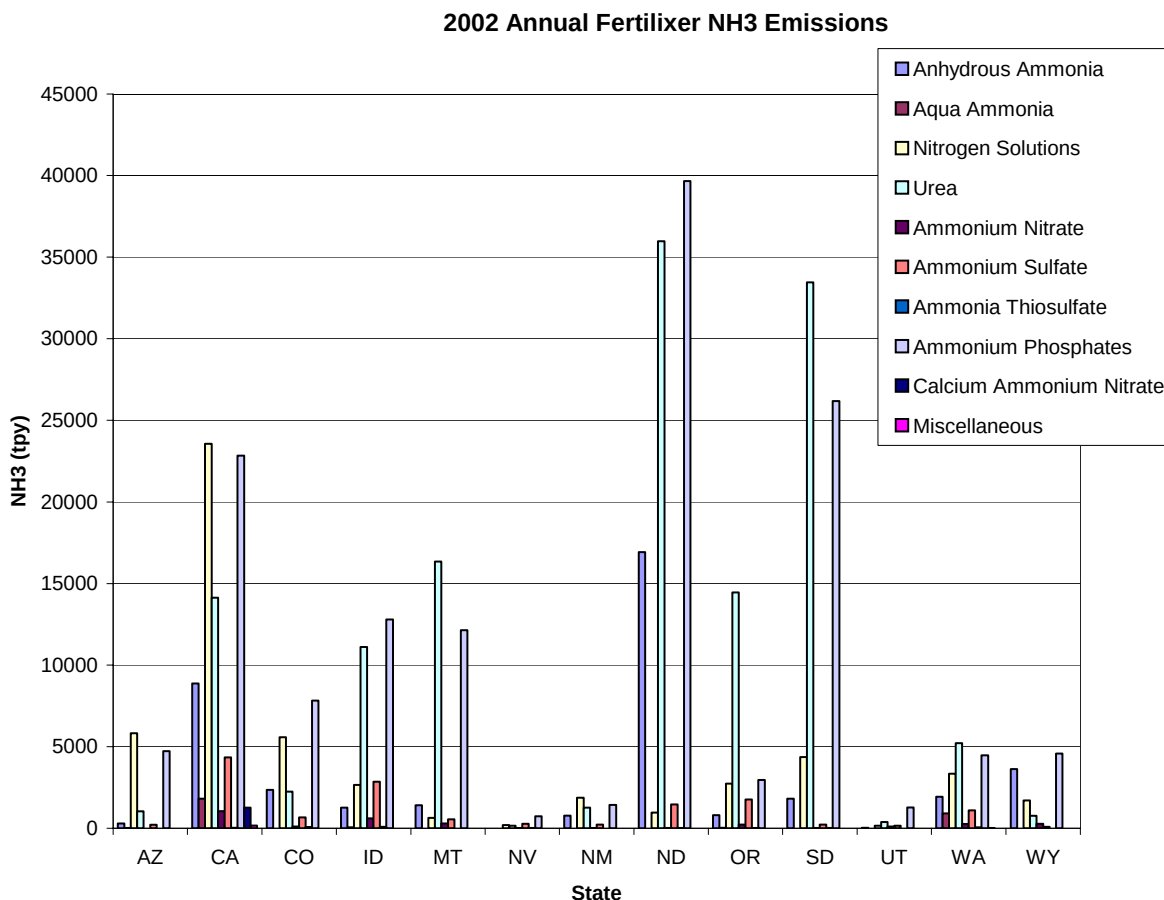


Figure 2-6. Annual fertilizer NH₃ emissions by fertilizer type for WRAP states.

Tabulated fertilizer-usage ammonia emissions by state and fertilizer type can be found in Mansell (2004a), as can the spatial distribution of total monthly fertilizer-usage ammonia emissions.

To assess the impact of the adjustments made to account for soil pH, we estimated the emissions for this source category based on unadjusted emission factors. Figure 2-7 displays the annual fertilizer ammonia emissions both with emission factor adjustments (dataset a0) and without them (dataset a1). The difference between these two cases is relatively minor at the state level. The differences are both positive and negative, as the soil pH varies regionally.

Comparison of Annual Fertilizer NH₃ Emissions - Datasets a1 vs a0

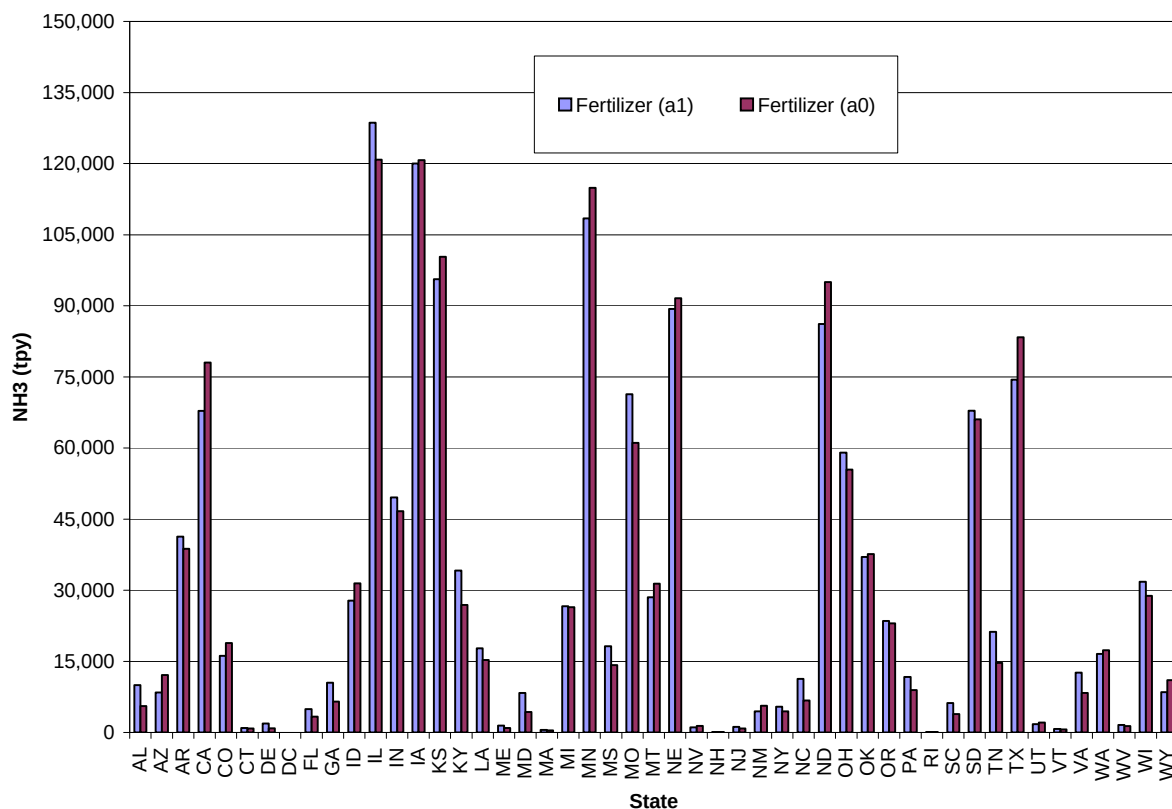


Figure 2-7. Annual fertilizer NH₃ emissions: dataset a0 is with pH effects, dataset a1 is without them.

2.3.3 Native soils

Figure 2-8 presents the 2002 annual native soil ammonia emissions by land use type for the WRAP states. Note that these emission summaries do not reflect the dependence of soil emissions on environmental factors; as discussed in Mansell (2004a), these factors are incorporated during the temporal allocation procedures in the modeling system. The variation seen in soil emissions across the WRAP region reflects the land use characteristics of each state. These emissions are dominated by shrubland and grassland, which reflects the characteristics of the land use/cover types in the western U.S. and their relatively high emission factors. The spatial distribution of total annual native soil ammonia emissions is presented in the draft report for this task (Mansell, 2004a).

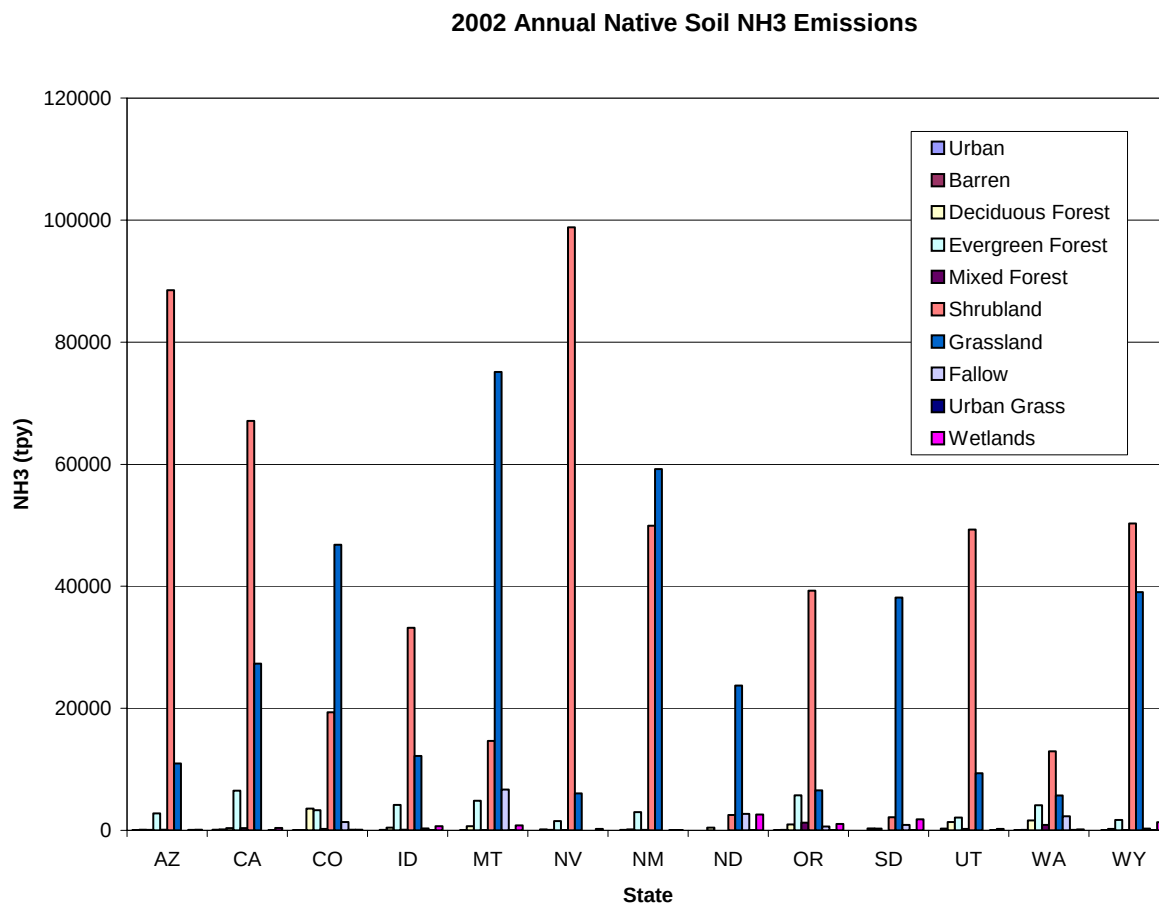


Figure 2-8. Annual native soil NH₃ emissions by land use type for WRAP states.

2.3.4 Domestic sources

Figure 2-9 gives the 2002 annual ammonia emissions from domestic sources for the 13-state WRAP region. The magnitude of domestic-source emissions reflects the population in each state, based on the 2000 U.S. Census data used as activity data. Emissions from California dominate the contribution to the inventory from this source category, reflecting the state's higher population. Displays of the spatial distribution of total annual domestic-source ammonia emissions are presented in Mansell (2004a).

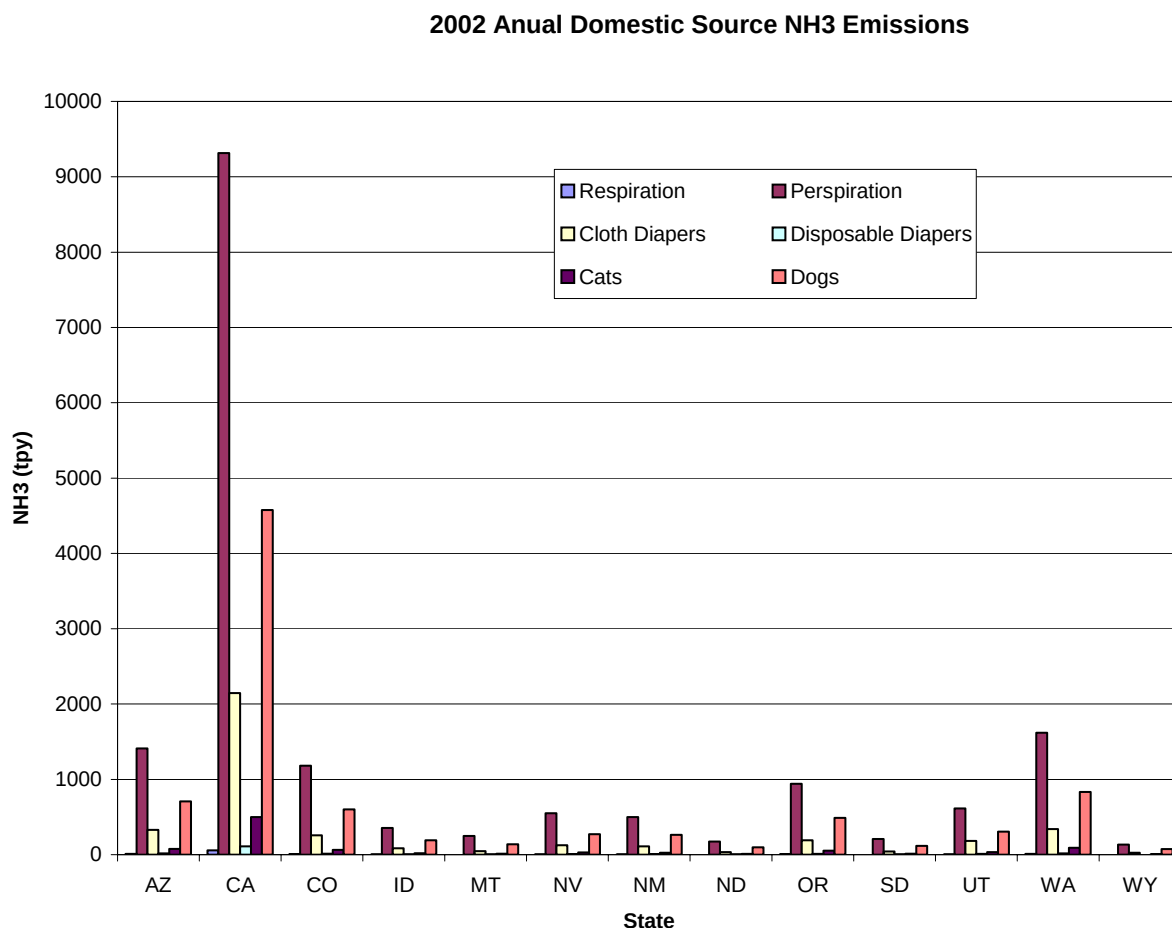


Figure 2-9. Annual domestic-source NH₃ emissions by source type for WRAP states.

2.3.5 Wild animals

Figure 2-10 presents the 2002 annual ammonia emissions from wild animals for the WRAP states. Domainwide, results are dominated by the deer emissions estimates, consistent with the large deer populations in the activity data. While elk populations are considerably smaller than those of other animals in most states (based on the CMU data), the emission factor for elk is much higher, resulting in a significant contribution by elk to the wild animal source category emissions. However, as noted previously, the activity data and emission factors were taken from the CMU Ammonia Model “as is.” The emission results highlight some of the deficiencies in those datasets. For example, although the figure shows that elk dominate the emissions, in reality a significant contribution from deer should be seen in several of the states. This is not reflected in the CMU activity datasets; for California, for instance, the data show no deer populations. The spatial distribution of total annual wild animal ammonia emissions is presented in the draft task report (Mansell, 2004a). A review of the displays in that report also highlights dataset problems for Florida and Nevada. As this source category is a relatively minor contributor to the overall ammonia emissions inventory, no corrective action was taken to rectify these problems.

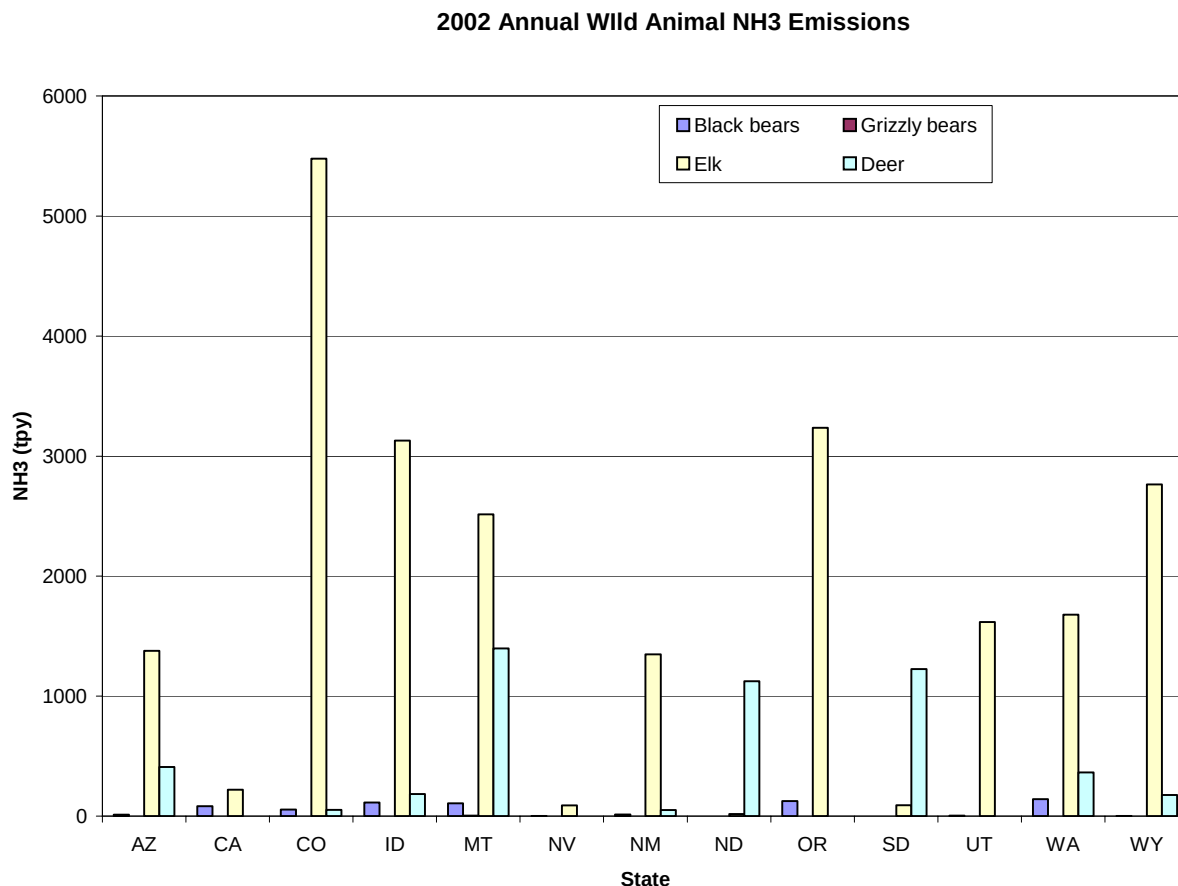


Figure 2-10. Annual wild animal NH₃ emissions by animal type for WRAP states.

2.3.6 Comparison with CMU emission estimates

We compared the ammonia emissions inventory we developed against results obtained from the CMU Ammonia Model for the source categories considered. This comparison served as a check on the reasonableness and consistency of our inventory, as well as an assessment of the various environmental factors incorporated in the modeling system. The CMU model was applied for all states in the conterminous U.S. to obtain monthly and annual ammonia emission estimates for the five major source categories estimated for the WRAP.

Figure 2-11 compares the total 2002 annual ammonia emissions, by state, between the CMU model and the WRAP inventory. In general, the overall state-level emission totals were comparable for most states. For some states, the CMU emission estimates were higher than those from the WRAP model, while for others the WRAP model estimates were the higher ones. Certainly, differences in the estimation methodologies, activity data, and emission factors contributed to these differences in ammonia emissions. For example, the CMU model treats livestock emissions using a processed-based approach, while our system considers this source category using a “whole animal” approach. Other differences and similarities between the two inventories are

described in Mansell (2004a) for each major source category. Considering the emissions uncertainties associated with some source categories (e.g., native soils), overall the two inventories compared quite favorably. A more complete comparison between the WRAP and CMU ammonia emissions inventories is presented and discussed in Mansell (2004a).

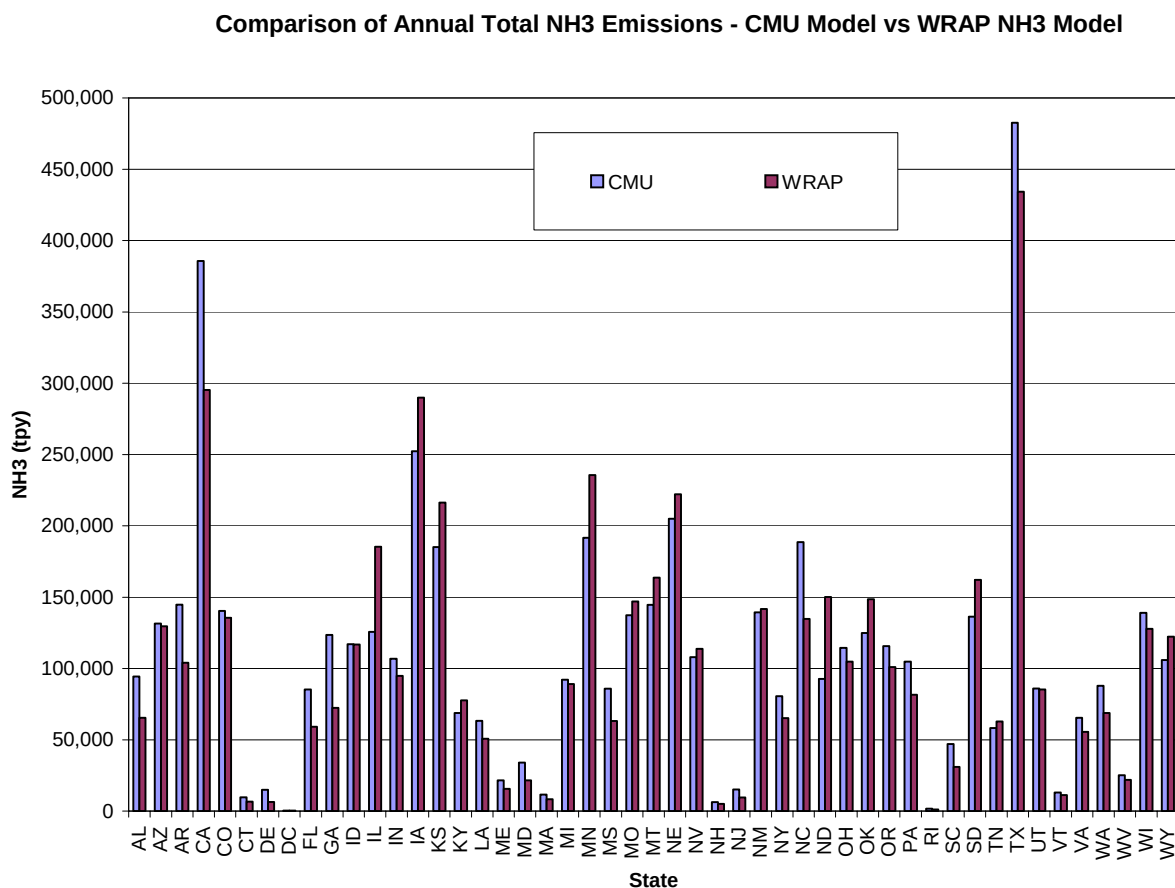


Figure 2-11. Comparison of total 2002 annual ammonia emissions between the CMU and WRAP models.

2.4 Summary and Recommendations

The results of the WRAP ammonia emissions inventory improvement task are summarized below. Also included here are recommendations regarding improvements in data quality and enhancements to the ammonia inventory and emissions modeling system.

2.4.1 Summary

We created a gridded modeling ammonia emissions inventory for the following major source categories: livestock operations, fertilizer application, native soils, domestic sources, and wild animals (see Table 2-1 for a breakdown). We developed the inventory using the improvements and estimation methodologies described above and documented in detail in Chitjian and Mansell (2003a,b). The improvements, based on a literature survey of recent research in ammonia emissions inventory development, were associated with the effects of environmental parameters on the emission factors, and temporal and spatial allocation of ammonia emissions for several source categories. A GIS-based ammonia emissions modeling system was developed and applied for calendar year 2002 to generate a gridded, hourly emissions inventory for the WRAP modeling domain at a spatial resolution of 36 km. The data sources and environmental factors used in the inventory improvements are presented in more detail in the draft task report (Mansell, 2004a).

The 2002 ammonia emissions inventory for the WRAP domain is dominated, on a regional scale, by fertilizer application and livestock operation emissions. This result is entirely consistent with the current understanding of ammonia emissions within the air quality and emissions modeling community. Ammonia emission from native soils, while a major component of the overall inventory, remains highly uncertain. The uncertainty arises mainly from unresolved issues in the research community regarding whether soils act as a source or a sink of ammonia. Ammonia emissions from domestic sources, while only a small contributor to the total regional ammonia inventory, can be a major source of emissions on smaller, urban scales. The wild animal ammonia emissions, although only a small portion of the inventory, were included at the request of the WRAP Emissions Forum.

A comparison of the WRAP ammonia inventory with similar results obtained from the CMU Ammonia Model was summarized above and is discussed in greater detail in Mansell (2004a). Based on state-level comparisons, the results of this task are seen to be consistent with existing ammonia emissions inventories. Evaluation of the differences and similarities, and further investigation of the two emissions inventories for detailed source categories at the county level, may provide useful insights into potential enhancements to the inventory and the emissions modeling system.

2.4.2 Recommendations

We make the following recommendations with respect to improving data quality and refining the ammonia inventory and emissions modeling system:

- The quality and detail of activity data collected for the study should be improved. In particular, livestock head counts for large CAFOs should be obtained and reconciled with the county-level activity data. This would allow improved spatial allocation of these large CAFO sources as point emissions sources.
- The current inventory could be improved further by obtaining detailed information on the specific types of livestock. For example, the current inventory considered beef cattle and dairy cattle in aggregate (i.e., independent of the specific processes occurring at the farm

level and using a single “whole animal” emission factor.) Given the recent trend toward a process-based emission estimation methodology, emission factors for the different stages of an animal’s lifetime are available and can be used, given the appropriate activity data. Similarly, the WRAP model treated poultry as a composite, rather than separately for broilers, layers, pullets, etc., for which emission factors are available.

- The temporal allocation of the inventory would benefit from the collection of activity data on a monthly basis for livestock operations, as is done for fertilizer usage data.
- Ammonia emissions from native soils should be evaluated to see whether implementing some of the modeling techniques currently undergoing research and development with respect to ammonia emission and deposition would improve their estimation.
- The existing inventory was generated at a spatial resolution of 36 km, for two reasons: the air quality modeling will be conducted at this resolution, and the meteorological data necessary for applying the various environmental factors used for this task were available only at 36-km resolution at the time the inventory was developed. Higher spatial resolution of meteorological data would allow development of emissions data at a higher resolution, thus improving the overall spatial allocation of various emission source categories. The GIS-based modeling system is already capable of handling modeling domains of arbitrary spatial resolution. Results from running the ammonia model using the latest 12-km MM5 modeling results will be documented in the final report for this task.
- While domestic-source ammonia seems to be a relatively small component of the inventory, refinement of these emissions estimates using 2002 population estimates would provide additional improvements in the overall emissions inventory.
- The activity data used in developing the wild animal emissions should be reviewed and updated to address the various problems and omissions we identified.
- Some additional ammonia emission sources could be added to the current inventory. The ammonia emissions modeling system we developed is designed to treat essentially any source category, provided the activity and emission factor data are available.
- With respect to source classification of anthropogenic versus natural, all source categories estimated by the ammonia model except native soils and wild animal emissions should be considered anthropogenic sources of ammonia emissions.

2.5 Status of Task 0.5 Deliverables

Table 2-10 gives the status of each Task 0.5 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 2-10. Status of the Task 0.5 deliverables.

Deliverable	Status
Draft final task report	Delivered August 26, 2004
Final task report	Expected completion: March 18, 2005
User's guide and modeling system	Expected completion: March 18, 2005

3. Task 1: Project Administration

3.1 Project Administration

Project administration activities included communicating with WRAP members and other WRAP contractors; participating in monthly conference calls with the RMC project management team and with the WRAP Air Quality Modeling Forum; attending or participating by teleconference in meetings with several of the other WRAP forums; preparing project reports and a quality assurance project plan (QAPP); and maintaining and updating the project web page and project mailing lists.

During 2004, the RMC team participated in the following meetings:

- Air Quality Modeling Forum Meeting, January, Phoenix, AZ
- RPO Modeling Discussion Group Meeting, May, Denver, CO
- Attribution of Haze Meeting, July, Denver, CO
- Emissions Forum Conference Call, August 27
- Fire Emissions Joint Forum Meeting (by phone), September 9, Worley, ID
- Attribution of Haze Meeting, September, Salt Lake City, UT
- Attribution of Haze Meeting, November, Las Vegas, NV
- Fire Emissions Joint Forum Meeting, December, Las Vegas, NV

Because the RMC contract in 2004 included projects under the direction of the WRAP's Air Quality Modeling Forum, Fire Emissions Joint Forum, Dust Emissions Joint Forum, and Emissions Forum, there were frequent conference calls to coordinate and report progress on the various subtasks within the work plan.

3.2 Computer Systems Administration

Computer systems administration included maintenance, updates, expansion, and optimization of the computing systems. All emissions, meteorology, and air quality modeling was performed on RMC computer equipment located at UCR; staff from UNC-CEP and ENVIRON have accounts on these computer systems. Much of the computer hardware used for the WRAP modeling was purchased in 2001 or early 2002, and is no longer under warranty. As a result, considerable effort was required to maintain and repair the computing systems.

We also experimented with new CPUs, network equipment, and system configurations to optimize the computer system performance during 2004. UCR had previously ported CMAQ to Linux, implemented a parallel version of CMAQ in Linux, and ported CMAQ to the 64-bit Opteron CPUs. During 2004 we attempted to port CMAQ to the Apple G5/PowerPC CPU (a

new 64-bit CPU that was priced competitively with Athlon and Intel CPUs). We were motivated to complete the port because we felt that the Apple/G5 systems would have better performance and be more reliable than PC systems. After considerable effort invested in porting the code, however, we were unable to achieve good performance of CMAQ on the G5/PowerPC platform. We still believe it would be worthwhile to consider operating CMAQ on the G5 in the long term, but the effort needed to optimize CMAQ for the G5/PowerPC platform will require greater resources than were available to the RMC in 2004 for this activity. The CMAS Center at UNC-CEP is currently working on this project. Given that the RMC is already heavily invested in PC/Linux systems, we plan to complete the project with PC/Linux hardware; however, we recommend that states and tribes who are purchasing new hardware consider the G5 systems if the CMAS Center is able to optimize CMAQ and SMOKE for that platform.

Within the PC/Linux platforms there are a variety of CPU choices. We believe that the Athlon CPUs are the most cost effective, and we purchased new test systems for the Athlon CPU to perform benchmarks for comparison to the more expensive Opteron systems. Benchmarks on the 36-km domain showed that the cheaper Athlon system's performance was very similar to that of the Opteron system.

Increased computational and input/output load from running multiple model simulations and increasing domain size have continued to increase the network traffic associated with the modeling effort. During 2004 we purchased a new high-speed network switch to reduce problems resulting from network congestion. We also continued to experiment with system configurations to attempt to reduce network congestion and improve system I/O performance.

As of February 2005, we continue to experience problems with CMAQ jobs crashing in simulations using multiple CPUs. Usually this occurs when a CMAQ job fails to start after the completion of a previous day's simulation. This is caused by communication failure between CPUs on different machines. Jobs using one or two CPUs run without difficulty, but jobs using four or more CPUs will fail to restart on average about 10% of the time. This requires considerable effort to monitor and manually restart CMAQ jobs when they fail to start. This problem may occur only on the UCR cluster, perhaps because of the large number of CPUs and/or the amount of disk storage in the cluster, and the resulting heavy load on net communications. Other groups have not reported this problem, so it is likely that states or tribes will not experience it, but it is a possibility worth noting here.

We expect that computer hardware will need to be upgraded and expanded before doing large numbers of emissions sensitivity simulations during 2005. Hardware needs will depend on the number of model simulations to be performed and whether we run only the 36-km model or both the 36-km and 12-km models. We believe that the RMC's current computing facilities are sufficient to handle the 36-km modeling and a limited number of 12-km simulations. Additional CPUs will be needed if we perform a large number of 12-km simulations. We will need additional data storage for modeling control strategies during 2005.

3.3 Status of Task 1 Deliverables

Table 3-1 gives the status of each Task 1 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 3-1. Status of the Task 1 deliverables.

Deliverable	Status
Biweekly Modeling Forum (MF) conference call	Ongoing. Switched to a monthly MF call and a monthly RMC project management call in October 2004.
Quality Assurance Project Plan (QAPP)	Completed first draft in September 2004. Revised version completed in December 2004.
Monthly project reports	Combined into a single interim report for January through September 2004. Monthly reports began in August 2004; see http://pah.cert.ucr.edu/aqm/308/progress_reports04.shtml .
Periodic web site updates	Web site has been periodically updated with reports, Power-Point files, QA products, and evaluation results; see http://pah.cert.ucr.edu/aqm/308/ .
MM5, emissions, and CMAQ data files	Datasets are available via portable disk drives.

4. Task 2: Test, Improve, Quality Control, Obtain External Peer Review, and Finalize 36-km and 12-km MM5 Simulations for Eventual Use in CMAQ

To support CMAQ visibility modeling for the §308 SIPs/TIPs, the RMC has carried out MM5 simulations for the entire year of 2002 on grids with resolutions of 36 km and 12 km. In this section, we first describe the process through which the optimal MM5 model configuration was determined. We then give an overview of the performance of the final WRAP 2002 annual 36-km and 12-km simulations.

4.1 Introduction

4.1.1 Task history

In the fall of 2003, we made an initial MM5 run for the year 2002 on the RPO Unified Continental 36-km Modeling Grid domain. The model configuration for this run was based on a prior 2002 MM5 application undertaken by the Iowa Department of Natural Resources (IDNR) (Matthew Johnson, IDNR, personal communication, 2003), which was in turn set according to the optimal MM5 physics options that resulted from an in-depth sensitivity project carried out by IDNR and the Lake Michigan Air Directors Consortium (LADCO). While the IDNR simulations used MM5 version 3.5, the applications carried out for the WRAP used the latest version of the model (v3.6.1) available at the end of 2003. Additional modifications to the physics configuration and application methodology were made for the WRAP simulation based on the latest information from EPA, IDNR, LADCO, and others. First, we opted to use the Reisner 2 mixed-phase cloud microphysics package (Reisner et al., 1998), according to suggestions from EPA/ORD. Second, the INTERPPX option, which allows for continuous soil moisture initialization from one run segment to the next, was not used, based on poor performance reported by IDNR and LADCO.

The initial 2002 36-km WRAP simulation (referred to hereafter as Run 0) results showed that MM5 performed better in the central and eastern U.S. than in the West, and generally performed better in winter than in summer (Morris et al., 2004a; Kembell-Cook et al., 2004). In the western U.S., the amplitude of the diurnal temperature cycle was persistently underestimated during the summer, especially in the Southwest. In the desert Southwest, the humidity was greatly overestimated during the summer as well, and there was a pronounced cold bias. Some of these problems appeared to be linked to the excessive simulated precipitation generated by MM5 during the summer, especially in the Southwest. This can have serious repercussions for CMAQ modeling, since too much rain can “wash out” pollutants, while the too cool, humid, and cloudy environment may lead to incorrect pollutant chemistry and aerosol thermodynamics. Temperature and humidity problems overshadowed the surface wind performance, which was not particularly good, but was likely affected by smaller-scale topographic influences that are not well represented even at the finer 12-km resolution. Wind performance improved quickly with height

above the surface, suggesting that regional transport speeds/directions were reasonably represented.

In April 2004, we undertook initial sensitivity tests for a five-day period in July 2002 for the RPO Unified domain in an attempt to find alternative MM5 configurations that would improve the poor summertime performance at 36 km. Furthermore, in-depth analyses were conducted to compare our performance against 36-km MM5 runs made for the Visibility Improvement – State and Tribal Associations of the Southeast (VISTAS) RPO, and against operational Eta Data Assimilation System (EDAS) fields. From these analyses, we found that the use of the Kain-Fritsch II scheme (as in the VISTAS 2002 MM5 modeling) improved, but did not entirely solve, the precipitation overprediction problem. We also found that removal of soil moisture nudging improved temperature and humidity performance for the short summertime tests. The evaluation of the EDAS fields used in the MM5 four-dimensional data assimilation (FDDA) revealed that EDAS did not exhibit the summertime cold, wet bias in the Southeast, so the bias was not introduced by the FDDA. From these initial tests, we identified a new model configuration for the 36-km run (referred to as Run 5) for new annual 2002 simulations, and updated the WRAP MM5 modeling protocol to reflect this (see Table 4-1). (“Analysis FDDA” and “observational FDDA” are defined in Section 4.2.)

Table 4-1. MM5 configurations from original (Run 0) and modified (Run 5) MM5 runs.*

Run ID	LSM	PBL	Cumulus	Micro-physics	Analysis FDDA		Obs FDDA	Soil Moisture Nudging
					3-D	Surface		
Run 0	PX	ACM	KF	Reisner 2	W/T/H	W/T/H	None	Yes
Run 5	PX	ACM	KF II	Reisner 2	W/T/H	W/T/H	None	No

*Abbreviations used in this table: LSM = land-surface model; PBL = planetary boundary layer; FDDA = four-dimensional data assimilation; obs = observational; PX = Pleim-Xiu; ACM = Asymmetric Convective Model; KF = Kain-Fritsch; W/T/H = wind/temperature/humidity.

Although the configuration identified in the new MM5 modeling protocol did improve humidity, temperature, and precipitation performance over the short July test period (especially where improvement was needed most), the desert Southwest continued to exhibit unsatisfactory levels of precipitation and humidity. As stated above, these issues will likely play crucial roles in CMAQ performance.

These initial MM5 sensitivity simulations attempted to identify a better-performing 36-km MM5 simulation that could be used to simulate all of 2002 but retain the Pleim-Xiu (PX) land-surface model (LSM) and the Asymmetric Convective Model (ACM) planetary boundary layer (PBL) options. When results of the Run 5 model performance were presented at the May 24-25, 2004, national RPO modeling meeting in Denver, CO (Emery et al., 2004), there were still concerns about the 2002 MM5 model performance in the western U.S. Thus, WRAP requested that the RMC perform further MM5 sensitivity tests to identify a better-performing configuration, including investigating (1) alternative LSM/PBL configurations to PX/ACM and (2) the possibility

of using different MM5 configurations for different times of year. After the performance issues at 36-km resolution had been addressed, we could then turn our attention to MM5's performance on the WRAP nested 12-km grid.

4.1.2 Summary of approach

During the summer of 2004, we carried out additional 36-km MM5 test simulations in an attempt to further improve MM5 performance on that grid. The latest available version of MM5 (v3.6.2) was used. Since the most severe problems for the initial WRAP 2002 MM5 annual simulation were the wet bias and precipitation overestimation in summer, we first investigated these issues for the five-day July test period (July 1-5, 2002) on the 36-km grid to maximize computational efficiency. We tested four physics options: (1) the cumulus parameterization; (2) the LSMs; (3) the PBL models; and (4) FDDA.

The first group of tests focused on the cumulus parameterization, which is the major MM5 component responsible for the overstated summertime rainfall. Most of the summer rainfall in the U.S. is due to convective clouds; stratiform rain produced by midlatitude cyclones is a smaller fraction of the total rainfall in summer than in winter. We examined the performance of the Kain-Fritsch II, Betts-Miller, and Grell cumulus schemes.

Next, we conducted a series of tests using different combinations of PBL and LSM options. In other MM5 applications around the country, including in California, we have achieved good model performance using the historically standard five-layer slab model as well as the NOAA LSM. Our choices for PBL models include the Eta scheme, the ACM, the Blackadar scheme, and our "modified" Medium-Range Forecast (MRF) model (M-MRF). The standard MRF available with MM5 is known to contain deficiencies that lead to overestimates of mixing depth and diurnal phase lags in wind speed due to overestimates of surface momentum flux. Our simple modifications have been shown to fix these problems (ATMET, 2003).

In the past, we have avoided performing MM5 sensitivity tests that altered the Pleim-Xiu/ACM LSM/PBL configuration because it is recommended by EPA and it has been shown by other RPOs (e.g., VISTAS) to provide the best overall meteorological model performance and best CMAQ performance (Olerud and Sims, 2003; Morris et al., 2004b). Also, it allows the use of the Pleim-Xiu dry deposition scheme in CMAQ, which is technically superior and performs better than the alternative (Wesely scheme). However, because most of the MM5 Pleim-Xiu tests to date have focused on the eastern U.S., and given the importance of the LSM/PBL scheme to MM5 performance, we tested alternative LSM/PBL schemes to see if they would provide better performance in the western United States.

Once the cumulus and LSM/PBL schemes had been selected, we performed a series of experiments to determine the best FDDA configuration. Finally, because the above sensitivity tests were done for July only, we ran 5-d segments in winter, spring, and fall to assess whether the performance showed improvement in seasons other than summer. Once we had an optimal configuration, we went back and tested it against the original MM5 run from the initial WRAP 2002 36-km modeling (Table 4-1, Run 0), and also against our interim Run 5 configuration from Table 4-1. We then examined the non-WRAP subdomains to determine how the new set of physics options affected MM5's performance in the eastern U.S.

After settling on a configuration for the 36-km annual run, we turned our attention to MM5's performance on the WRAP nested 12-km grid. Further sensitivity tests at this resolution were undertaken, allowing for the possibility that the 36-km physics options might differ from those selected for the 12-km run. Sections 4.2 through 4.6 provide details on each step of the approach just discussed.

4.2 Additional 36-km MM5 Sensitivity Tests

Table 4-2 shows the additional 36-km MM5 sensitivity tests discussed above that were used to identify a better MM5 configuration for simulating meteorology in the western U.S. These sensitivity tests differed in the choice of LSM, PBL scheme, cumulus parameterization, explicit cloud microphysics, and type and level of FDDA. Below are the various schemes tested in this study. No soil moisture nudging was performed for any of the runs.

- *LSMs*: NOAH; Pleim-Xiu (PX); five-layer slab
- *PBL Schemes*: Eta; modified MRF (M-MRF); Asymmetric Convective Model (ACM); Blackadar
- *Cumulus Schemes*: Betts-Miller (BM); Grell; Kain-Fritsch II (KF II)
- *Cloud Microphysics Schemes*: simple ice; Reisner 2
- *FDDA*: W = wind; T = temperature; H = humidity. "Analysis FDDA" refers to analysis (grid) nudging; "observational FDDA" indicates that FDDA is used to nudge the model solution toward observational data at individual measurement sites.

Table 4-2. Summary of additional MM5 sensitivity tests.

Run ID	LSM	PBL	Cumulus	Micro-physics	Analysis FDDA		Obs FDDA
					3-D	Surface	
Run 1a	NOAH	Eta	Betts-Miller	Simple ice	W/T/H	W/T/H	None
Run 1ba	NOAH	M-MRF	Betts-Miller	Reisner 2	W/T/H	W/T/H	None
Run 1bb	NOAH	M-MRF	Betts-Miller	Reisner 2	W/T/H	W/T/H	W
Run 2a	Pleim-Xiu	ACM	Betts-Miller	Reisner 2	W/T/H	W/T/H	None
Run 2aa	Pleim-Xiu	ACM	Betts-Miller	Reisner 2	W/T/H	W	None
Run 2ac	Pleim-Xiu	ACM	Betts-Miller	Reisner 2	W/T/H	W/T/H	W/T/H
Run 2ad	Pleim-Xiu	ACM	Betts-Miller	Reisner 2	W/T/H	W	W
Run 2ae	Pleim-Xiu	ACM	Betts-Miller	Reisner 2	W/T/H	W	W
Run 2b	Pleim-Xiu	ACM	Grell	Reisner 2	W/T/H	W/T/H	None
Run 3a	5-layer	Blackadar	Betts-Miller	Simple ice	W/T/H	W/T/H	None
Run 3b	5-layer	M-MRF	Betts-Miller	Reisner 2	W/T/H	W/T/H	None

4.3 Analysis Procedures

We conducted the MM5 sensitivity test evaluation by examining the surface performance statistics using the METSTAT evaluation software package developed by ENVIRON, and by comparing the output MM5 total (convective + large-scale) precipitation fields with gridded observed precipitation amounts. Observed precipitation data came from the Climate Prediction Center (CPC) gridded precipitation amount dataset, available from the National Weather Service (NWS) CPC web site at <http://www.cpc.ncep.noaa.gov/products/precip/realtime/retro.shtml>.

The CPC daily precipitation amounts are on a grid that covers the U.S. mainland at a resolution of $0.25^\circ \times 0.25^\circ$, and are ramped down to zero immediately offshore. The advantage of this field is that it has a reasonably high resolution, which is especially important when it comes to resolving the effects of orography on precipitation over the western U.S. We calculated the performance statistics for surface wind, temperature, and humidity using METSTAT with the NCAR ds472 surface observations dataset.

Our analysis is organized around a type of scatterplot called “soccer plots,” developed by ENVIRON, that display average performance statistics for each subdomain for the modeled time period. Subdomain definitions are shown in Figure 4-1; Table 4-3 lists the METSTAT subdomain numbers shown in Figure 4-1 and the corresponding abbreviations used in the discussions below. Soccer plots usually plot average bias versus error for a meteorological variable. Model performance benchmarks or goals also plotted on the soccer plot are used to show whether the performance of the variable meets the goal. In the following subsections, soccer plots are shown for wind speed bias versus wind speed root mean squared error (RMSE), temperature bias versus temperature error, and humidity bias versus humidity error. In each plot, a solid line indicates the benchmark. The benchmarks, developed by Emery and Tai (2001), were based upon the evaluation of more than 30 MM5 and Regional Atmospheric Modeling System (RAMS) meteorological simulations in support of air quality applications performed in the last few years, as reported by Tesche et al. (2002). A data point that falls inside the box represents a model run that meets the performance benchmark. Perfect model performance is indicated by a data point at (0,0); the closer a data point is to the origin, the better the model’s performance. We emphasize that the benchmarks are not used as acceptance/rejection criteria of the MM5 model simulation. Rather, they put the MM5 model performance into perspective and allow the identification of potential problems in the MM5 fields.

Table 4-3. METSTAT subdomain abbreviations.

METSTAT Subdomain	Name Abbreviation	METSTAT Subdomain	Name Abbreviation
1	PacNW	7	GreatLakes
2	SW	8	OhioVal
3	North	9	SE

METSTAT Subdomain	Name Abbreviation	METSTAT Subdomain	Name Abbreviation
4	DesertSW	10	NE
5	CenrapN	11	MidAtl
6	CenrapS		

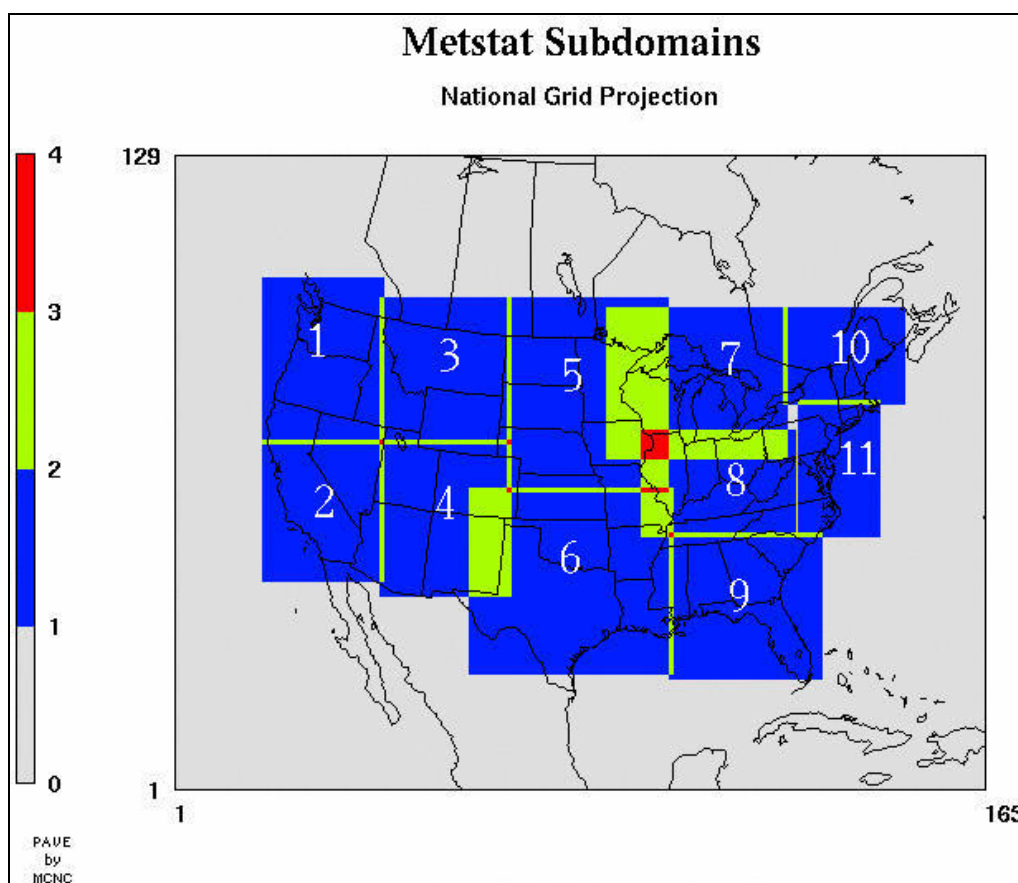


Figure 4-1. Definition of METSTAT subdomains.

4.4 MM5 Sensitivity Test Results

4.4.1 Cumulus parameterization sensitivity test

We began by testing MM5's sensitivity to the choice of cumulus parameterization. The original 2002 MM5 run (Run 0) used the Kain-Fritsch scheme. Because results from VISTAS 36-km MM5 modeling showed improved surface fields relative to Run 0 using Kain-Fritsch II, KF II

was the first scheme we tested (Run 5). Next, we compared runs that used the Grell (Run 2b) and Betts-Miller (Run2a) parameterizations to Run 5. All of these runs were made using the PX/ACM LSM/PBL schemes, the Reisner 2 cloud microphysics scheme, W/T/H analysis nudging at the surface and aloft, and no FDDA nudging to observations (“obs nudging”).

Figure 4-2a summarizes the wind performance for the July 2002 test period. All three cumulus schemes show a low wind speed bias. For the SW, PacNW, and North subdomains, the Grell scheme has a smaller error than the other schemes, and is similar in bias. In the DesertSW subdomain, the Betts-Miller scheme slightly outperforms the others in both bias and error, but all three schemes are far from the benchmark for DesertSW.

Figure 4-2b shows the results for temperature. All three schemes show a general cold bias. The Betts-Miller scheme has the smallest overall bias, and does slightly better than the Grell scheme for error. The KF II scheme has the smallest error, except in the PacNW subdomain, in which it is an outlier. The Betts-Miller scheme has the best overall temperature performance. It has the smallest bias, and although it has a slightly larger error than the KF II scheme for DesertSW, SW, and North, it does significantly better than KF II in the Pacific Northwest.

The humidity performance is shown in Figure 4-2c. Here again, the Betts-Miller scheme shows the best overall performance. For the SW and PacNW subdomains, the performance of the three schemes is comparable, but the Betts-Miller scheme is clearly better for the North and DesertSW subdomains.

Figure 4-3 is a plot of observed versus MM5 precipitation for the modeled time period. All three runs are too wet across the northern United States. Kain-Fritsch II has a strong wet bias, particularly in the SW and DesertSW subdomains, and also underpredicts the precipitation maximum over Texas. Both the Grell and Betts-Miller schemes produce a maximum over Texas, although they translate it to the southwest of the observed location. Over the southwestern U.S., the Betts-Miller precipitation field is closer to the observations than that from Grell, which generates too much rain in this region. Based on the improvement in performance over the Southwest and Texas, we concluded that the Betts-Miller scheme produced the best simulation of precipitation for this time period.

Overall, of the three cumulus packages tested, Betts-Miller was the best-performing scheme for temperature, humidity, and precipitation. We therefore selected this scheme and used it in all subsequent runs as we continued with further sensitivity tests.

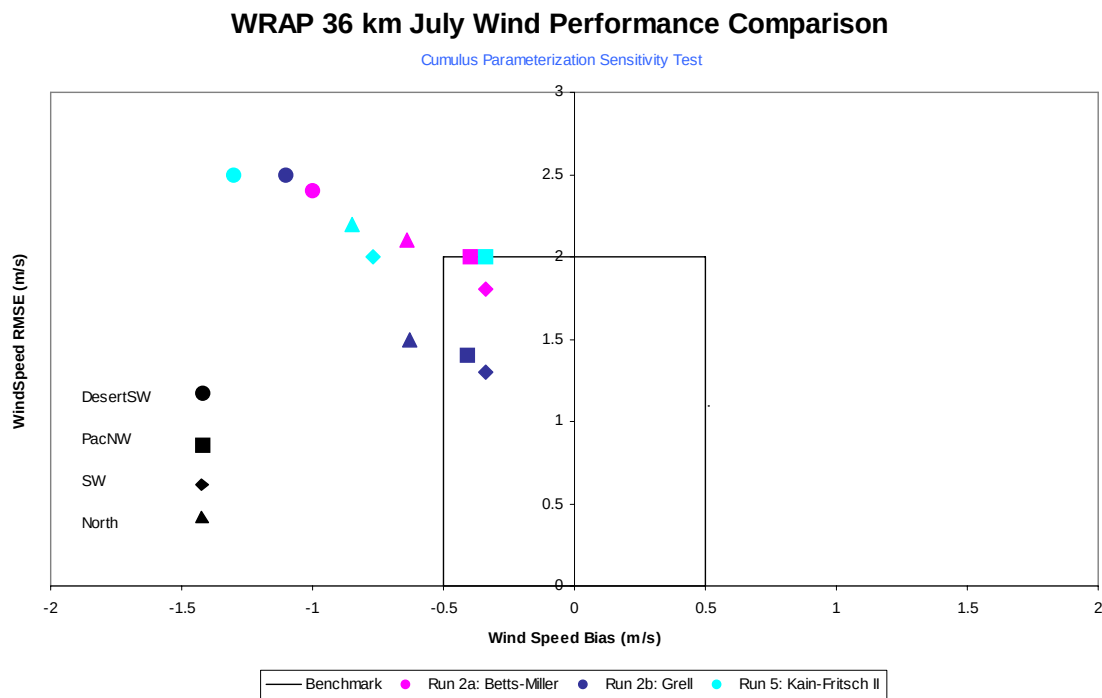


Figure 4-2a. Wind soccer plot for cumulus parameterization sensitivity test.

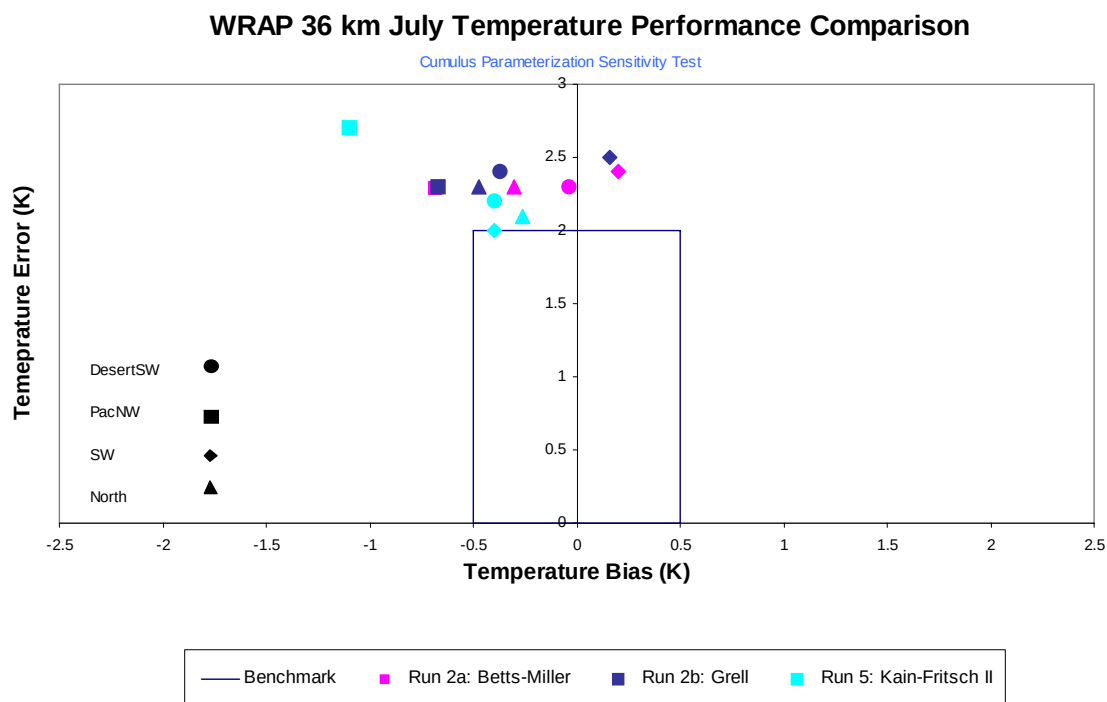


Figure 4-2b. Temperature soccer plot for cumulus parameterization sensitivity test.

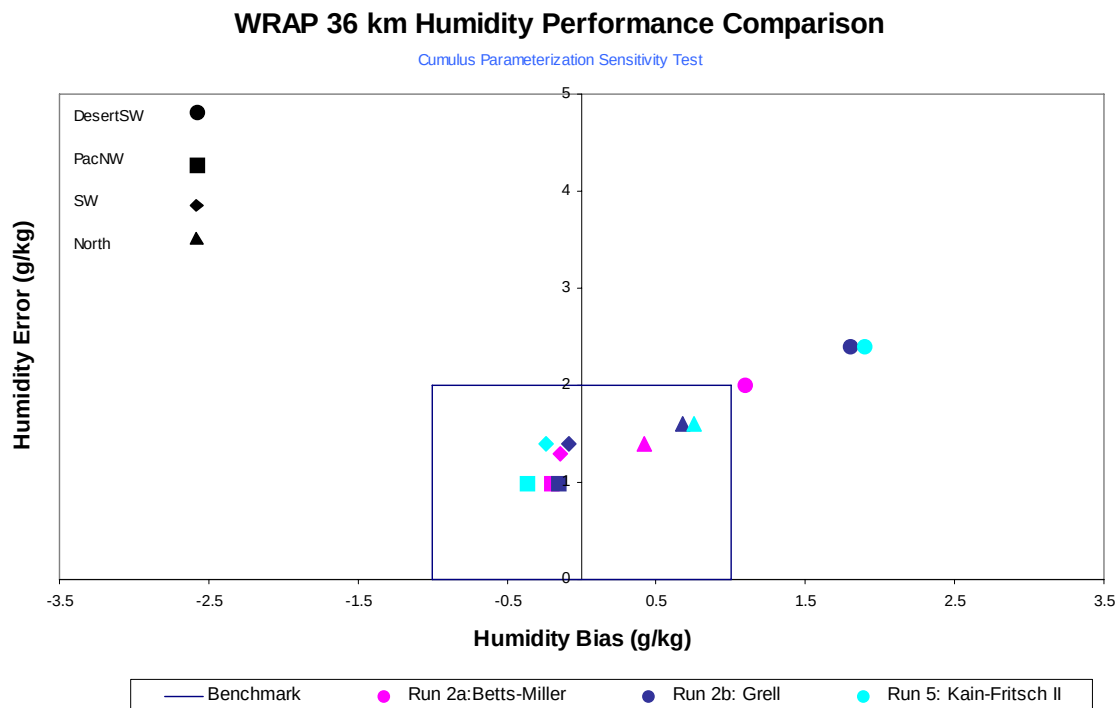


Figure 4-2c. Humidity soccer plot for cumulus parameterization sensitivity test.

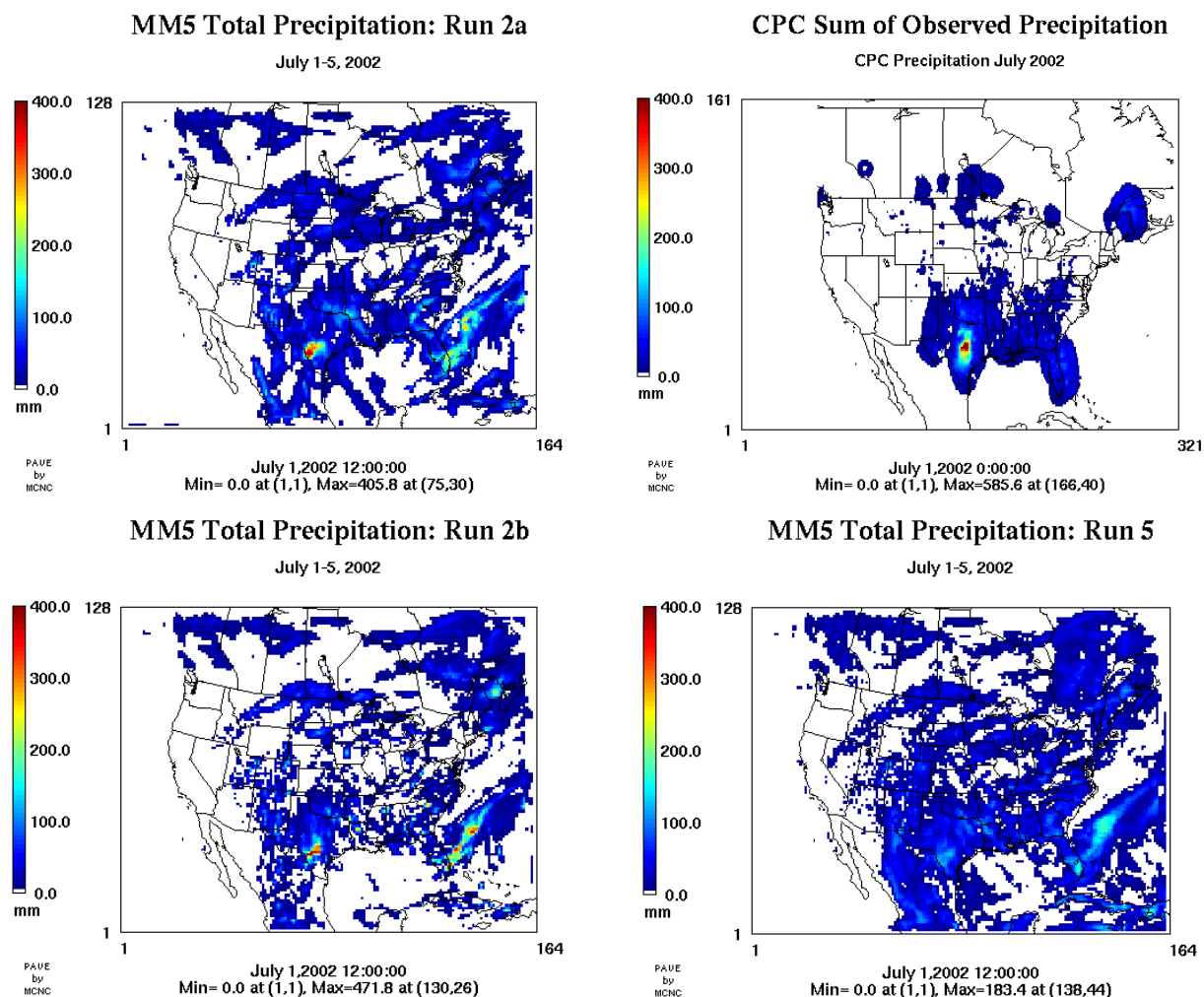


Figure 4-3. Precipitation comparison for the cumulus parameterization sensitivity test. Run 2a (top left): Betts-Miller; Run 2b (bottom left): Grell; Run 5 (bottom right): Kain-Fritsch II. Observed is shown at top right.

4.4.2 LSM/PBL sensitivity test

Next, we tested the LSM and PBL parameterizations. All of the runs described in this section used the Betts-Miller cumulus parameterization, W/T/H analysis nudging at the surface and aloft, and no obs nudging. We began by comparing the NOAH LSM (Run 1ba) with the five-layer model (Run 3b). In both runs, the modified MRF (M-MRF) PBL scheme and the Reisner 2 cloud microphysics scheme were used.

Figure 4-4a shows the wind performance for the Runs 1ba and 3b LSM sensitivity test.* Both the five-layer and NOAH runs show a low wind speed bias, with the bias more pronounced in the

*Note that Figures 4-4a through 4-4c include results for more than just these two runs. The other runs are discussed later in the text. The same is true for Figure 4-5.

five-layer case. For both runs, the SW and PacNW subdomains lie within the benchmark, while North and DesertSW do not. The NOAH run performs better for all subdomains except for the DesertSW. For DesertSW, the NOAH run has a slightly smaller bias, but a larger error.

The LSM temperature comparison is shown in Figure 4-4b. Both runs have a cold bias, but the bias is remarkably pronounced for the NOAH run in the PacNW and North subdomains. The error is smaller for all subdomains in the five-layer run, as is the bias in PacNW and North. For the SW and DesertSW subdomains, the NOAH run has a smaller bias, but larger error. Overall, the five-layer model temperature performance was an improvement over that of the NOAH run.

Figure 4-4c shows the humidity performance for these runs. There is an overall wet bias, except in the SW subdomain. For humidity, the NOAH run meets the performance goal, while the five-layer run lies entirely outside the benchmark. The NOAH run performs better in the North and PacNW than in the SW and DesertSW subdomains.

The precipitation performance is shown in Figure 4-5. Run 1ba does slightly better here, producing less rain over the desert Southwest states than does run 3b; Run 1ba is therefore closer to the observed rainfall field than Run 3b.

Overall, the NOAH model outperformed the five-layer model. The five-layer model introduces a large positive humidity bias in the DesertSW and SW subdomains, which is one of the main problems from the original Run 0 that we were trying to ameliorate in this study. Having eliminated the five-layer LSM model from further consideration, we then compared the NOAH/M-MRF combination (Run 1ba) with the run that used the PX/ACM configuration (Run 2a), also in Figures 4-4 and 4-5.

Figure 4-4a displays the wind comparison for the NOAH/M-MRF and PX/ACM runs. The two runs show equivalent performance for error, and the NOAH/M-MRF run has a smaller overall bias. For temperature (Figure 4-4b), neither run meets the performance benchmark, but the PX/ACM run is a clear improvement in both bias and error over the NOAH/M-MRF run. The cold bias is far more pronounced in the NOAH/M-MRF run for the PacNW and North subdomains.

For humidity (Figure 4-4c) there is not much difference between the two runs, except in DesertSW, where PX/ACM has a higher bias and error. For precipitation, the PX/ACM run shows some slight improvement over the NOAH/M-MRF case over the southwestern U.S. The intensity of the maximum over Texas is less well simulated in the PX/ACM run, however. Performance is roughly equivalent elsewhere.

Overall, there was no single factor that made it easy to select one LSM/PBL scheme over the other. As there was no significant improvement in going to the NOAH/M-MRF configuration, we decided to use the PX/ACM configuration because it allows the use of the Pleim-Xiu dry deposition algorithm in subsequent CMAQ modeling, is endorsed by EPA, and allows consistency with the other RPOs.

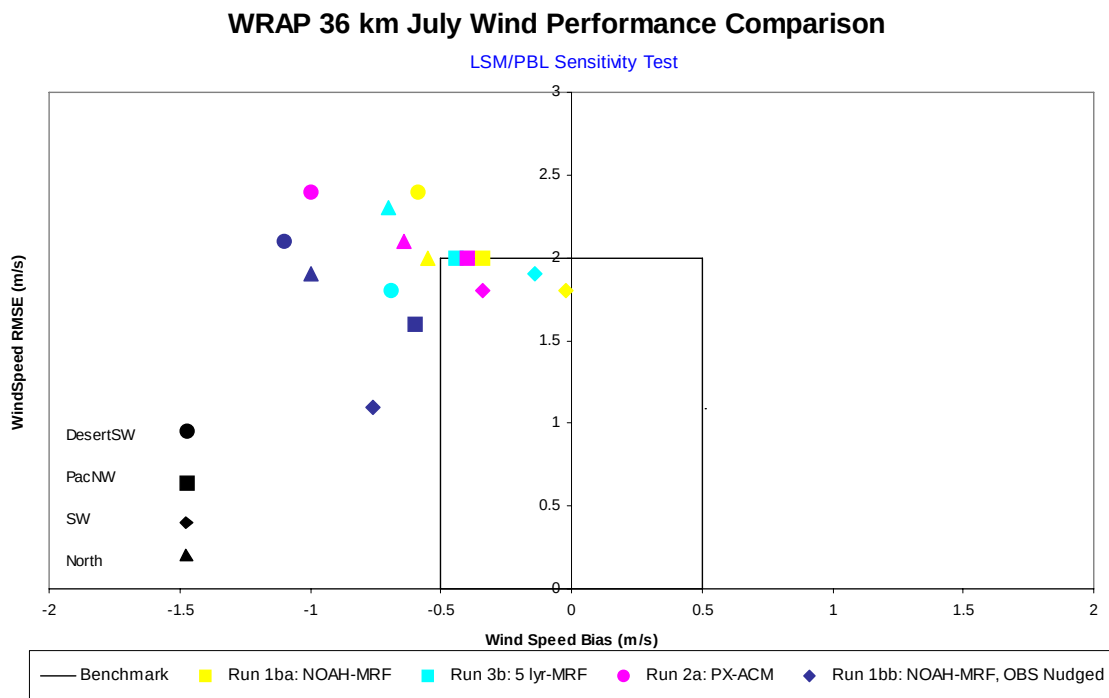


Figure 4-4a. Wind soccer plot for LSM/PBL parameterization sensitivity test.

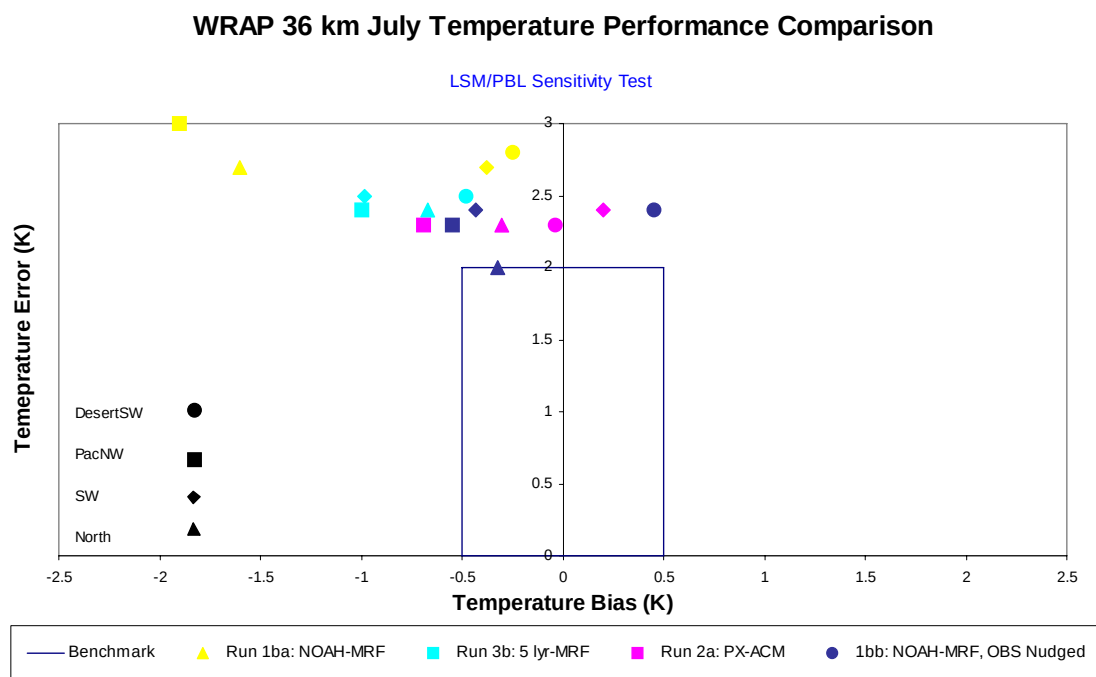


Figure 4-4b. Temperature soccer plot for LSM/PBL parameterization sensitivity test.

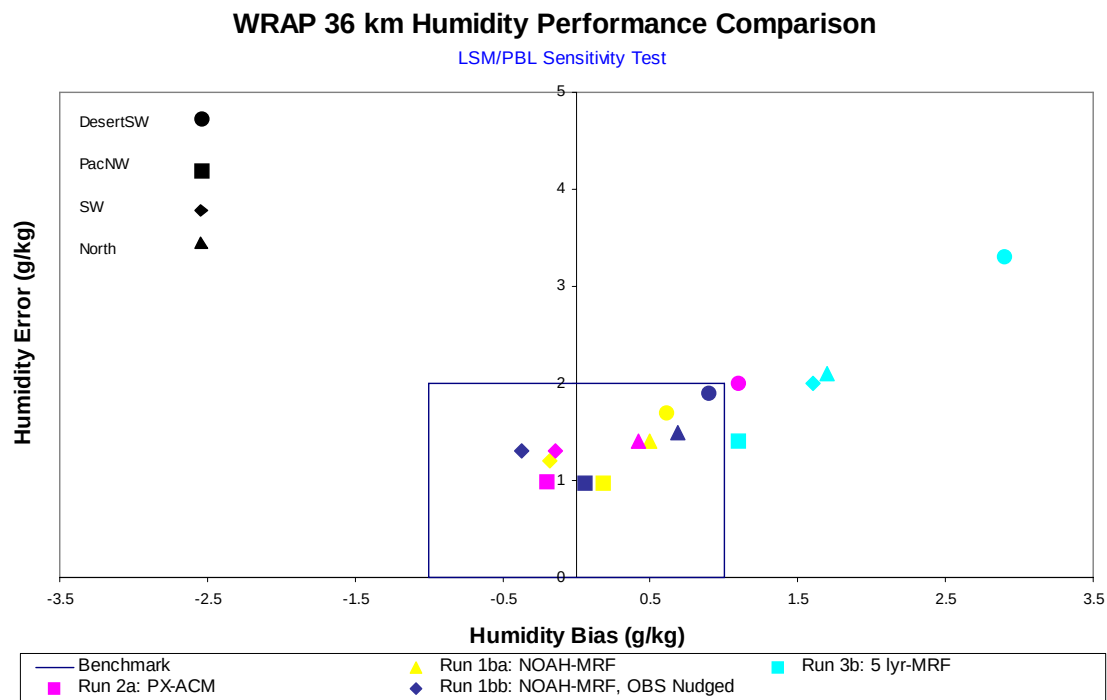


Figure 4-4c. Humidity soccer plot for LSM/PBL parameterization sensitivity test.

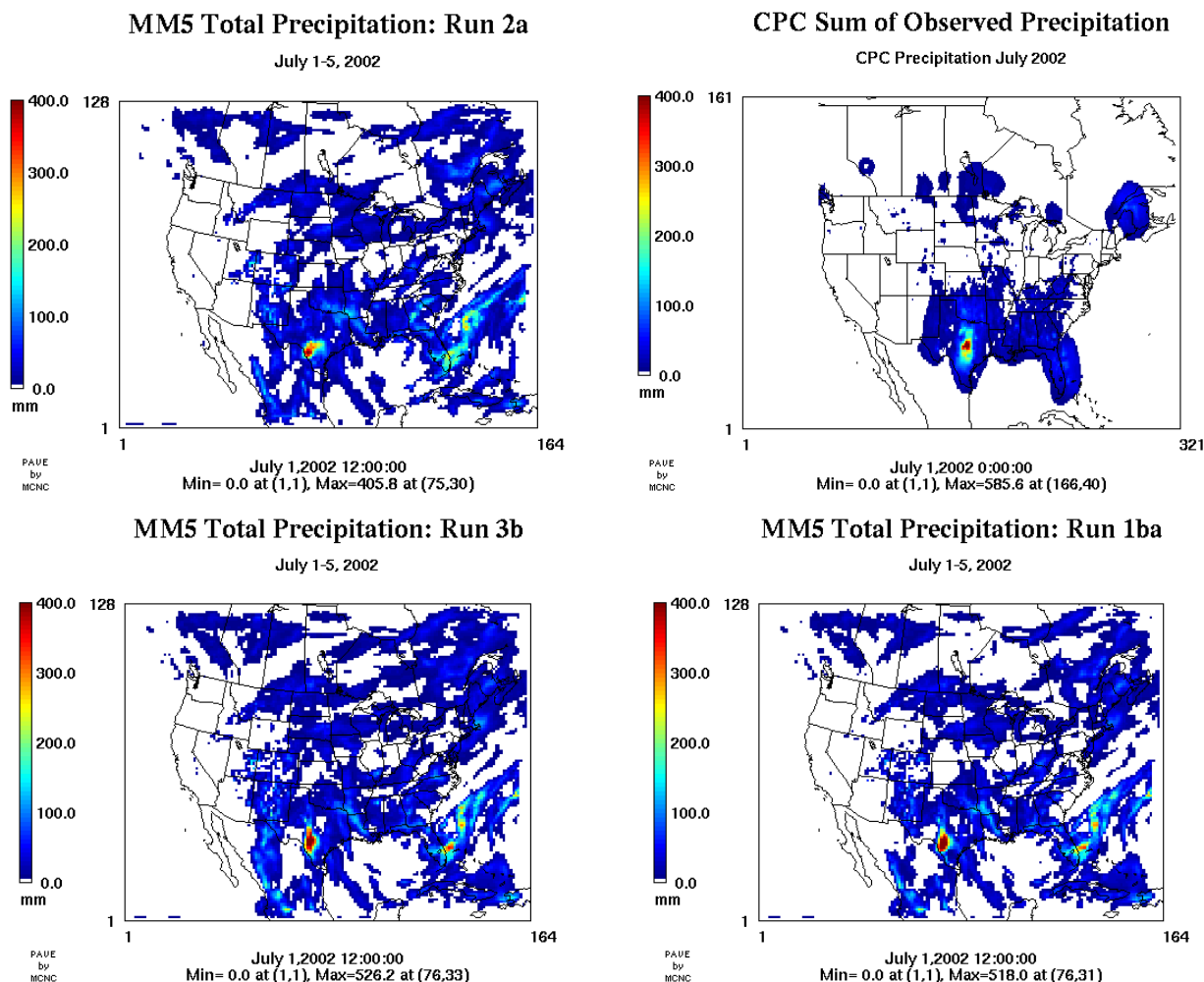


Figure 4-5. Precipitation comparison for the LSM/PBL parameterization sensitivity test.
Run 2a (top left): PX/ACM; Run 3b (bottom left): 5-layer/M-MRF; Run 1ba (bottom right): NOAH/M-MRF. Observed is shown at top right.

4.4.3 FDDA sensitivity test

Having selected a cumulus parameterization and an LSM/PBL combination, we turned to the FDDA configuration. The runs discussed in this section (2aa, 2ac, 2ad, and 2ae) differ only in their FDDA (see Table 4-2 for the run specifications); all use the PX/ACM, Betts-Miller, and Reisner 2 schemes and W/T/H analysis nudging aloft.

Figure 4-6a compares the wind performance for the runs with different FDDA configurations. For all runs, all subdomains except PacNW (2a and 2aa) and SW (2a) lie outside the benchmark. There is low wind speed bias for all runs and all subdomains. Run 2a shows the smallest bias, while 2ac has the lowest overall error. It is difficult to say which runs exhibit the best wind performance based on this figure. Figure 4-6b shows the wind direction error versus the wind speed RMSE. In this figure, the effects of obs nudging on the surface wind field are apparent.

Runs that had obs nudging (2ac, 2ad, and 2ae) lie together closer to the benchmark than the runs that were not obs nudged (2aa).

For temperature (Figure 4-6c), Run 2ae clearly shows the best performance. All subdomains but one are within the benchmark; Run 2ae also has the smallest bias and error. For humidity (Figure 4-6d), performance is comparable among the runs, and all subdomains except DesertSW lie within the benchmark. Differences in the precipitation fields for all the FDDA sensitivity runs were small (not shown) and did not help to distinguish among the runs in terms of performance.

On the basis of its superior temperature performance and wind performance, which were similar to those of the best-performing runs, Run 2ae was determined to have the best FDDA configuration.

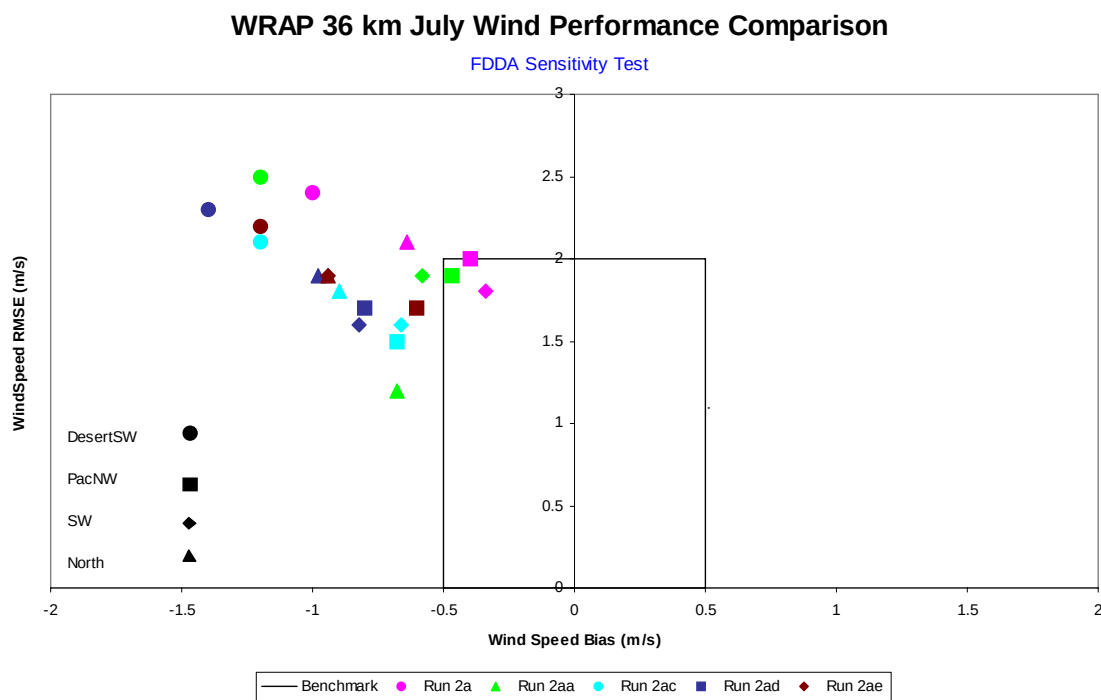


Figure 4-6a. Wind speed soccer plot for FDDA configuration sensitivity test.

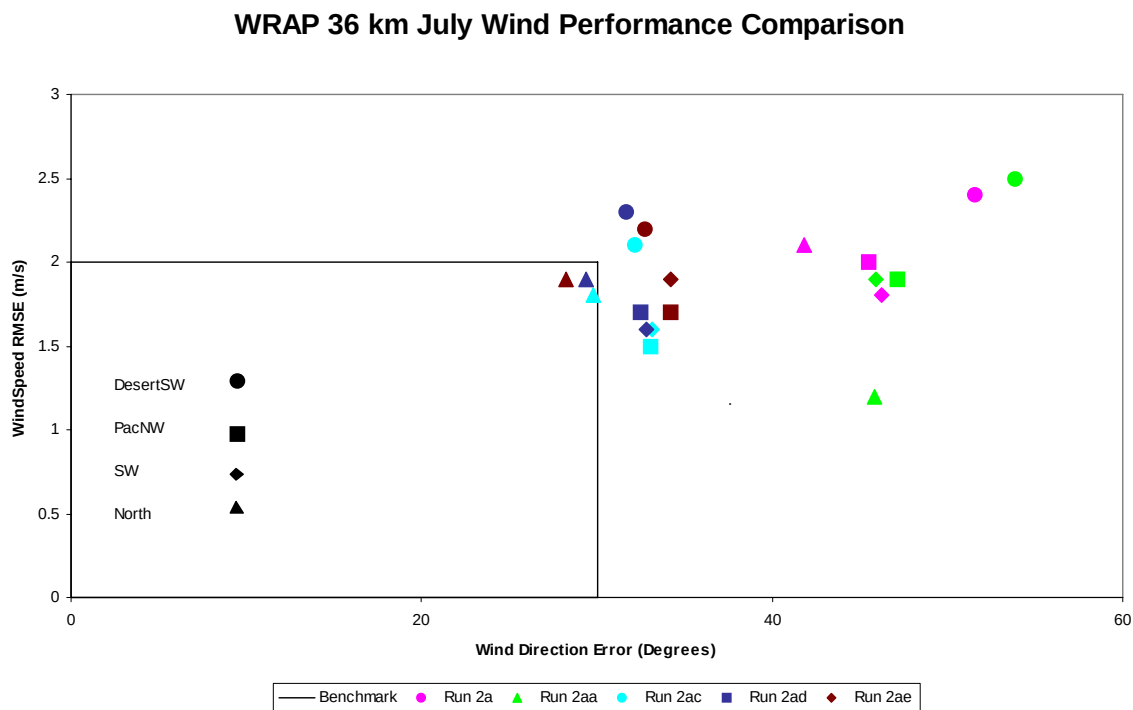


Figure 4-6b. Wind speed/direction soccer plot for FDDA configuration sensitivity test.

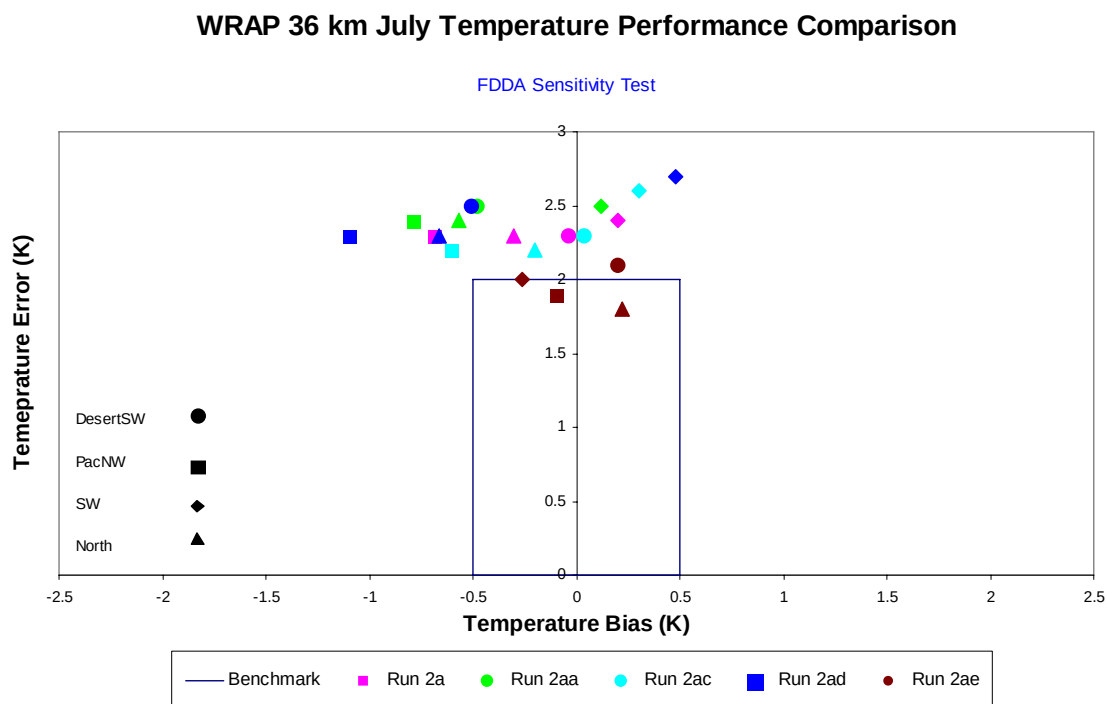


Figure 4-6c. Temperature soccer plot for FDDA configuration sensitivity test.

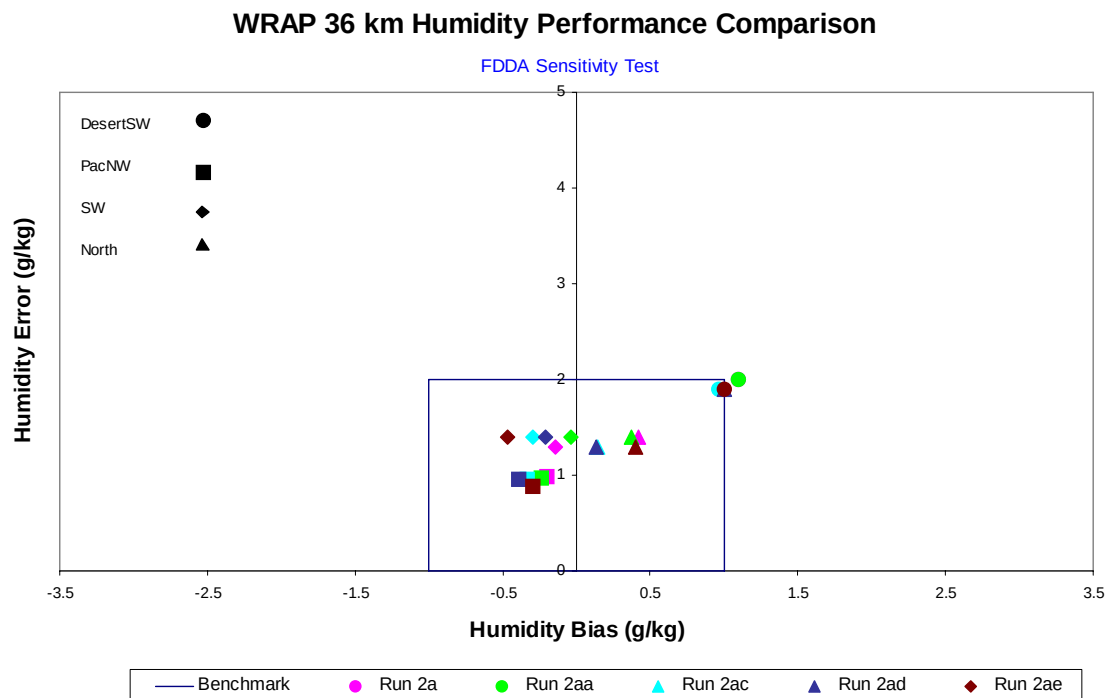


Figure 4-6d. Humidity soccer plot for FDDA configuration sensitivity test.

Next, to allow for the possibility that nudging the NOAH/M-MRF case might cause significant improvement, we made another run (Run 1bb), which was identical to Run 2ae except that the NOAH/M-MRF LSM/PBL scheme was used instead of PX/ACM. The results are shown in Figures 4-7a through 4-7c, with the more weakly nudged Run 1ba included to show the effects of nudging. For wind speed bias and error, Run 1bb (NOAH) is a slight improvement over Run 2ae (PX), except for the SW subdomain, for which NOAH shows marked improvement over PX. For temperature, Run 2ae (PX) had a smaller bias and error than the other runs (NOAH). For humidity and precipitation, there is no run that clearly performed better than the others. We selected Run 2ae (PX, with W/T/H analysis nudging at the surface and W observational nudging) as the best-performing run overall for July 2002, because the temperature performance is deemed to be more important than the wind performance, given that the terrain in the western U.S. may prevent good agreement between modeled and observed surface winds at 36-km resolution.

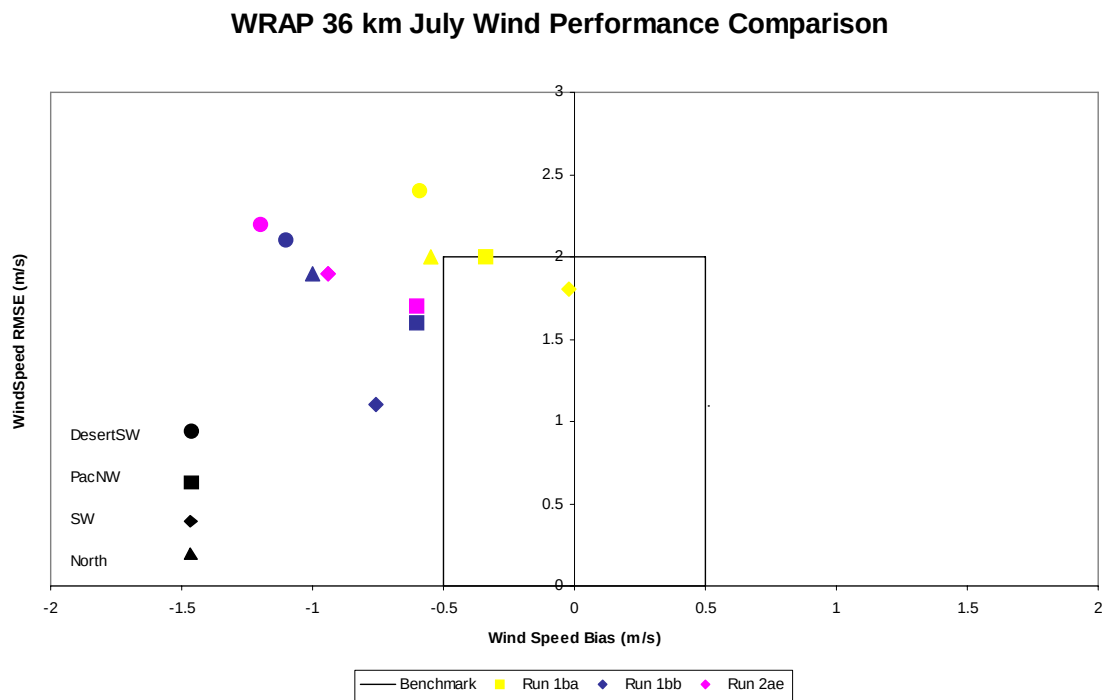


Figure 4-7a. Wind soccer plot for NOAH/M-MRF nudging sensitivity test.

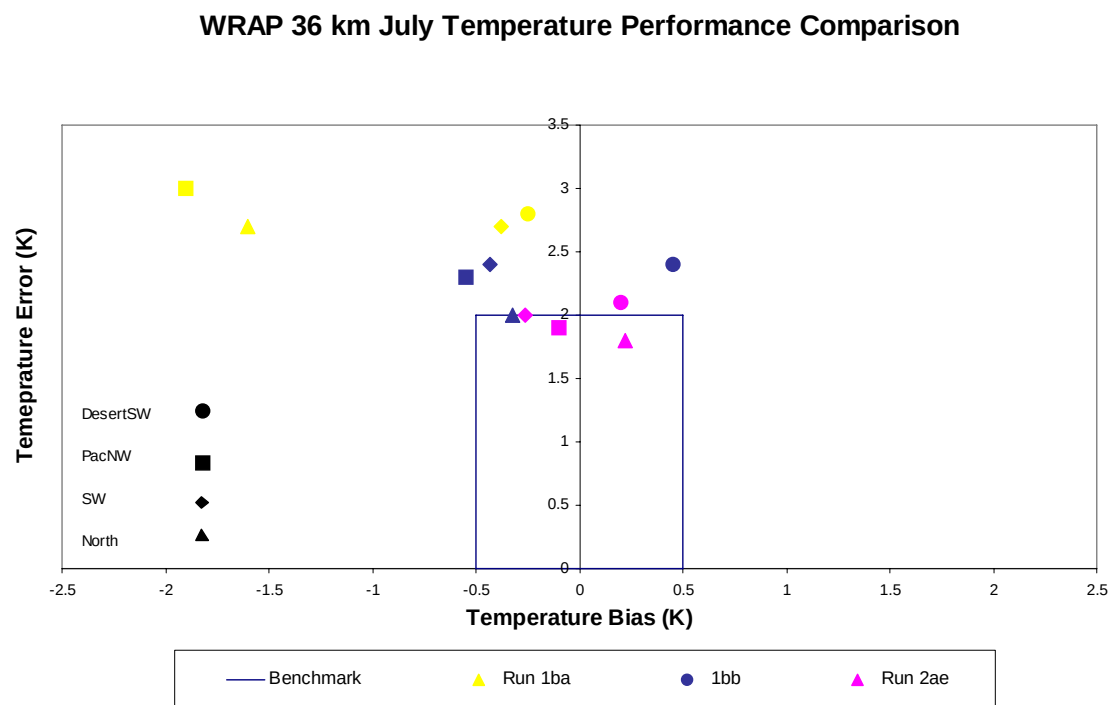


Figure 4-7b. Temperature soccer plot for NOAH/M-MRF nudging sensitivity test.

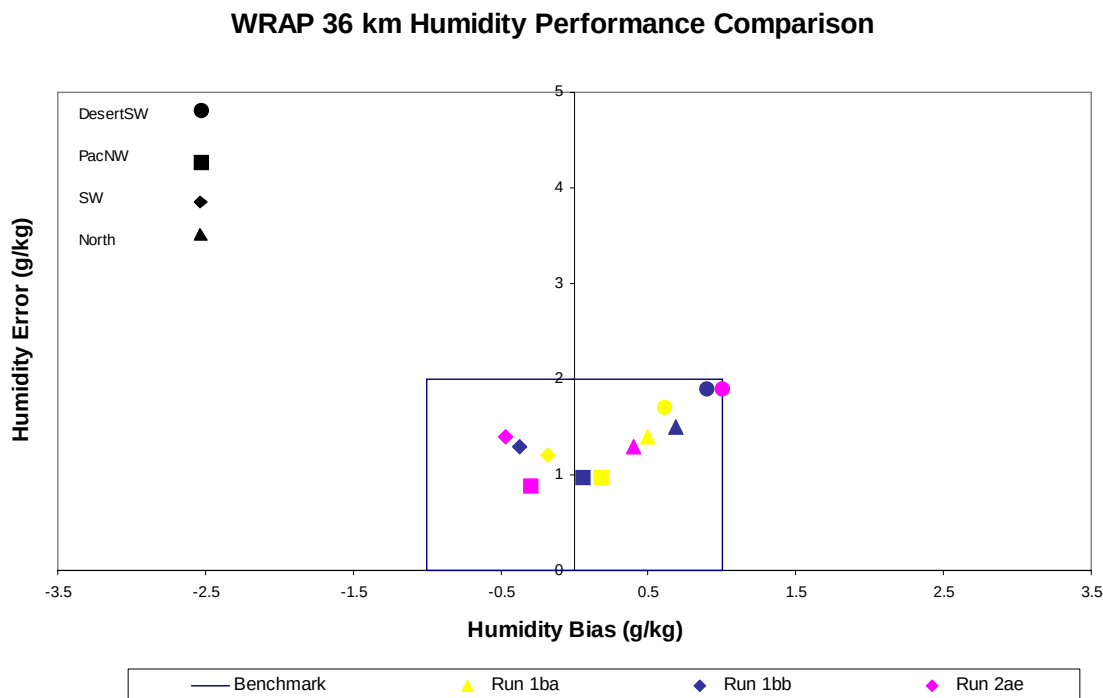


Figure 4-7c. Humidity soccer plot for NOAA/M-MRF nudging sensitivity test.

4.4.4 Tests in other seasons

Having determined a better MM5 configuration based on the July sensitivity tests, we then moved to other parts of the year, leaving open the possibility that we may use a different MM5 configuration for different times of year for the final year-long 2002 simulation. The two best-performing runs overall for July (Runs 2ae and 1bb) were run for 5-d periods in January, April, and October, representing the winter, spring, and fall seasons.

Figures 4-8a through 4-8f show the performance of Runs 2ae and 1bb during the four 5-d runs representing the four seasons. We begin by comparing the wind performance of the two runs for all four seasons (Figures 4-8a,b). For January, performance in the PacNW, SW, and DesertSW is similar, while Run 1bb shows significant improvement in the North subdomain over Run 2ae. In both April and October, Run 1bb has generally lower bias and error, with the four subdomains clustered closer to the benchmark than in Run 2ae. In July, Run 1bb has a smaller bias, while Run 2ae has a smaller error. This is true for all subdomains except PacNW, for which Run 2ae has a smaller bias than Run 1bb. Overall, then, Run 1bb performs better for wind throughout the year, with the points clustered closer to the benchmark. Note, however, that all points lie outside the benchmark for both simulations except for January PacNW and North for Run 1bb.

For temperature (Figures 4-8c,d) in January, Run 2ae has a smaller bias and error for North and DesertSW. For SW, performance is similar, and for PacNW, Run 1bb has a smaller bias and error. In April, Run 1bb does better; in Run 2ae, PacNW and North have a strong cold bias and lie far outside the benchmark. In July and October, Run 2ae performs better, with most of the

subdomains situated within the benchmark, while in Run 1bb all subdomains lie in a halo around the benchmark.

For humidity (Figures 4-8e,f), performance between the two runs is comparable. The precipitation performance (not shown) was similar enough that differences in the precipitation fields were not useful in choosing between the two runs.

Figures 4-9a through 4-9c compare the observed precipitation (Figure 4-9a; for the U.S. only) versus estimated precipitation for Runs 2ae and 1bb (Figures 4-9b,c) for the four 5-d seasonal periods. There is good agreement between the observed and estimated precipitation in January. Both MM5 runs overstate the extent of the precipitation in April and July, but agree with the observations fairly well in October. The precipitation performance for Runs 2ae at 1bb is nearly identical.

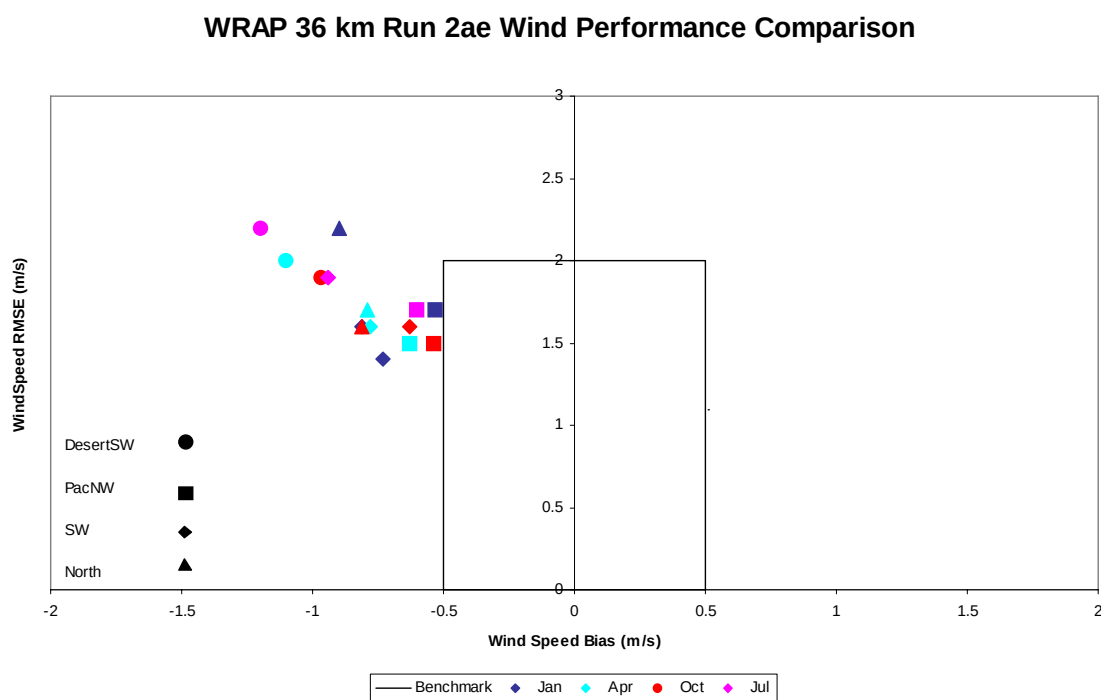
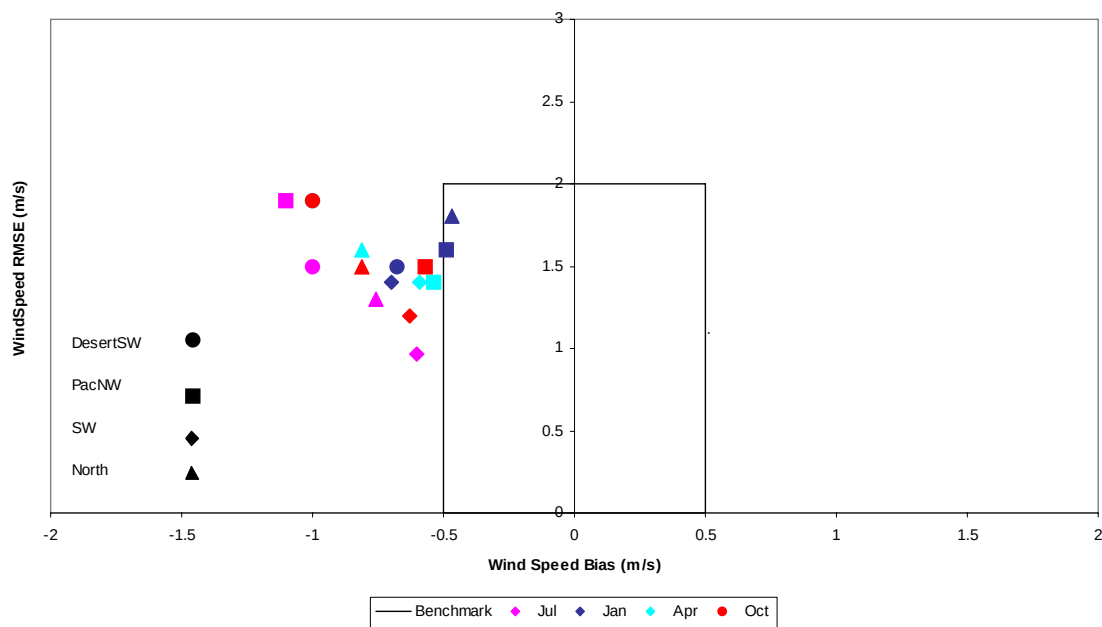


Figure 4-8a. Wind soccer plot for Run 2ae seasonal test.

WRAP 36 km Run 1bb Seasonal Wind Performance Comparison



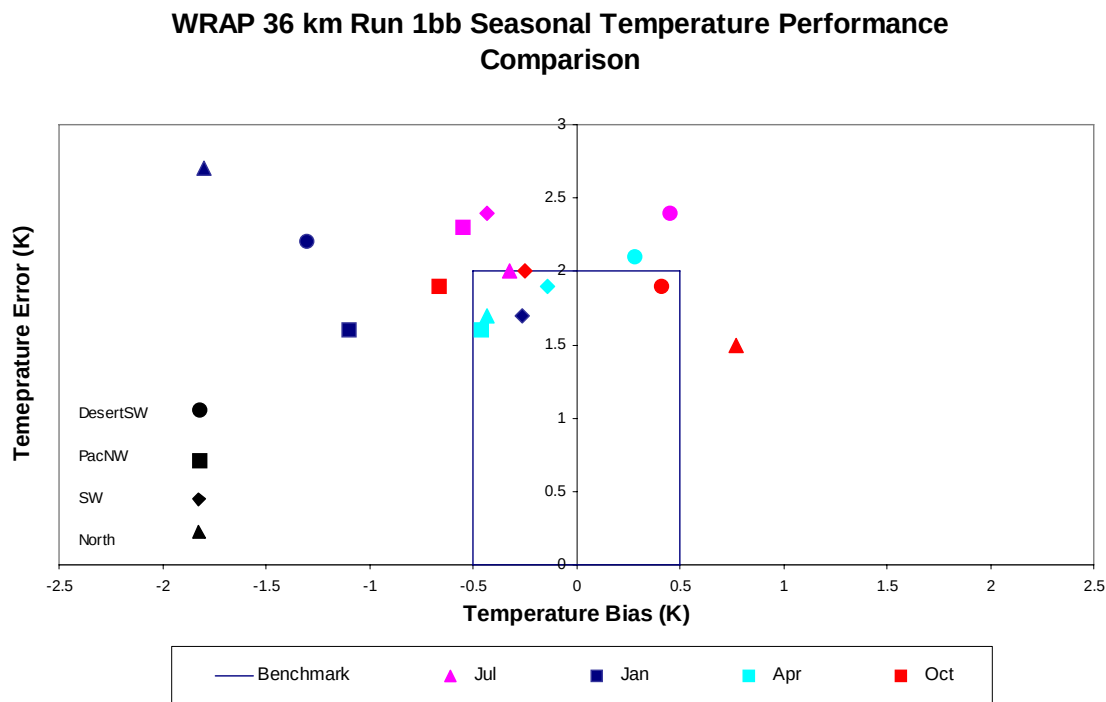


Figure 4-8d. Temperature soccer plot for Run 1bb seasonal test.

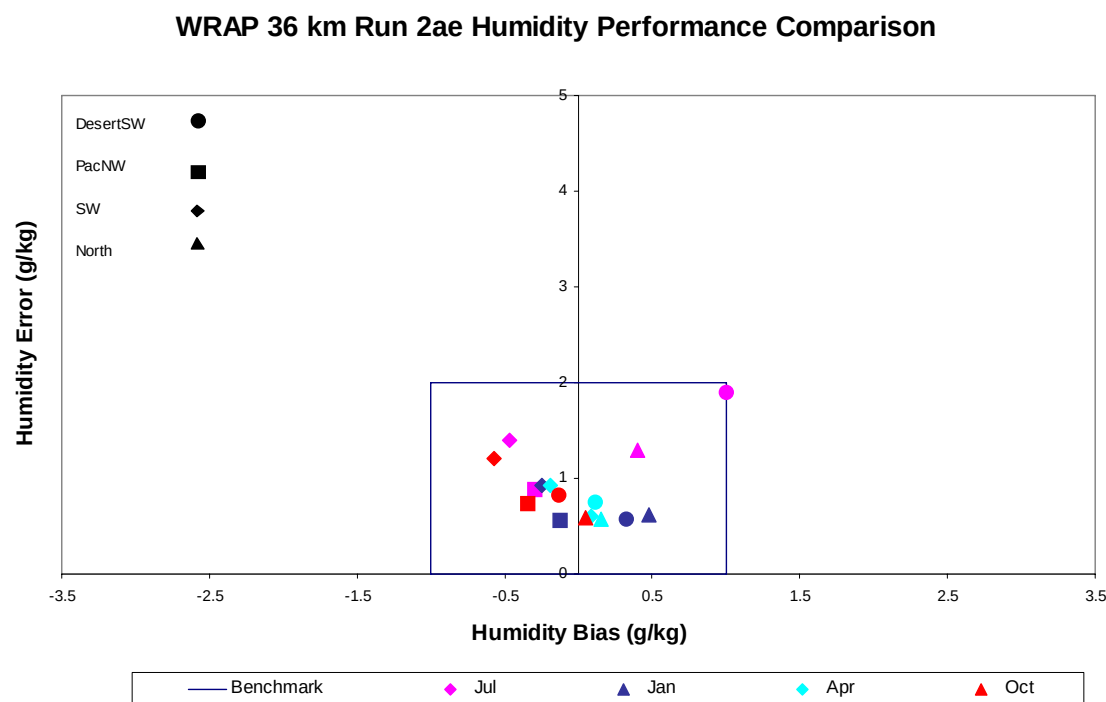


Figure 4-8e. Humidity soccer plot for Run 2ae seasonal test.

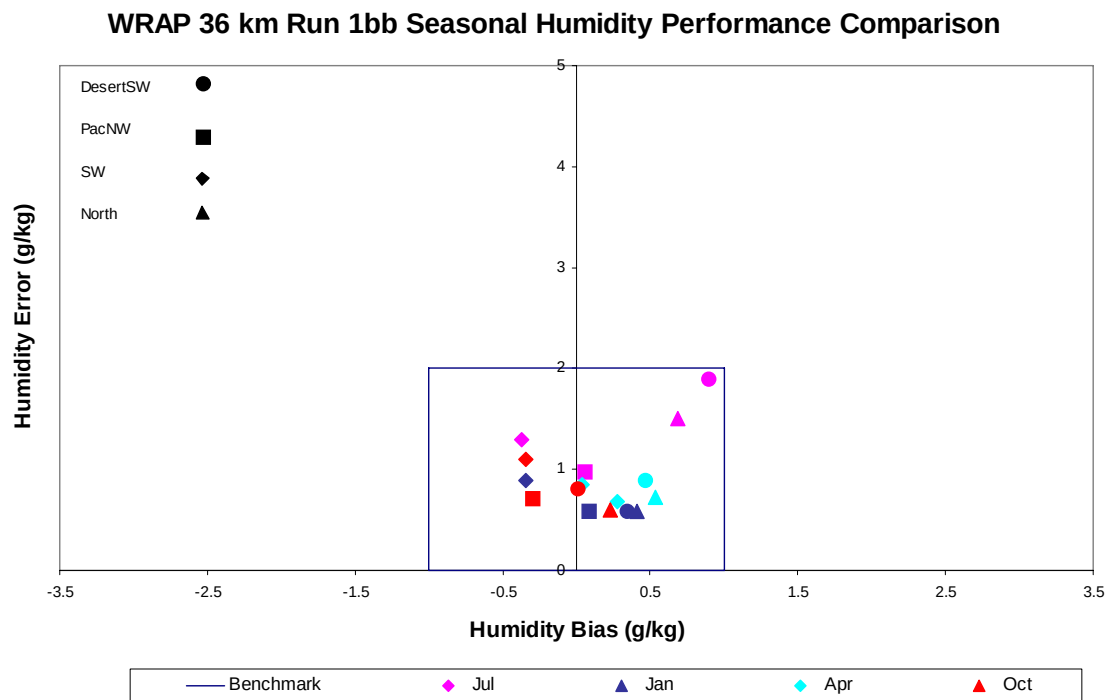


Figure 4-8f. Humidity soccer plot for Run 1bb seasonal test.

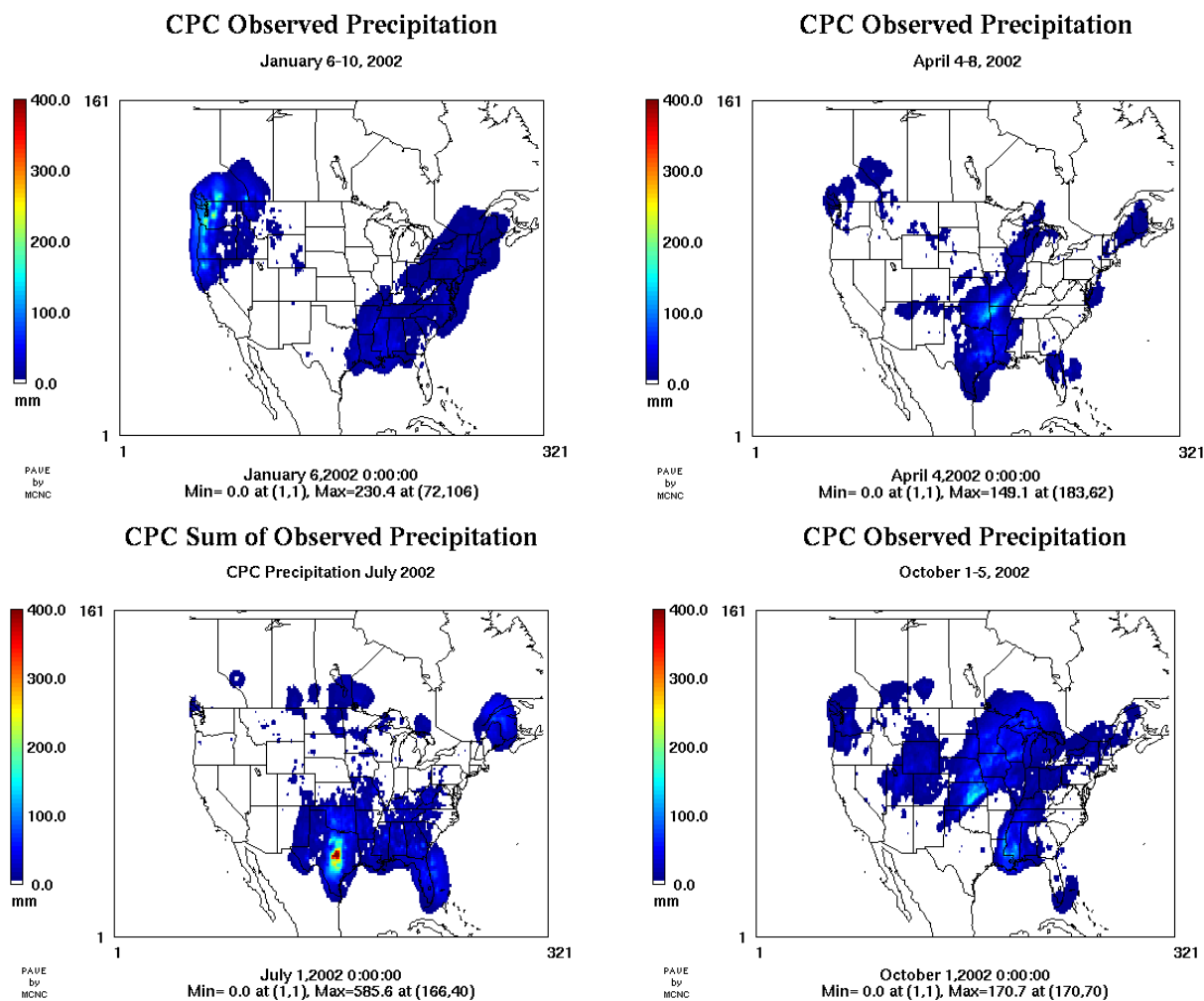


Figure 4-9a. CPC observed precipitation for the five-day modeled segment in each season.

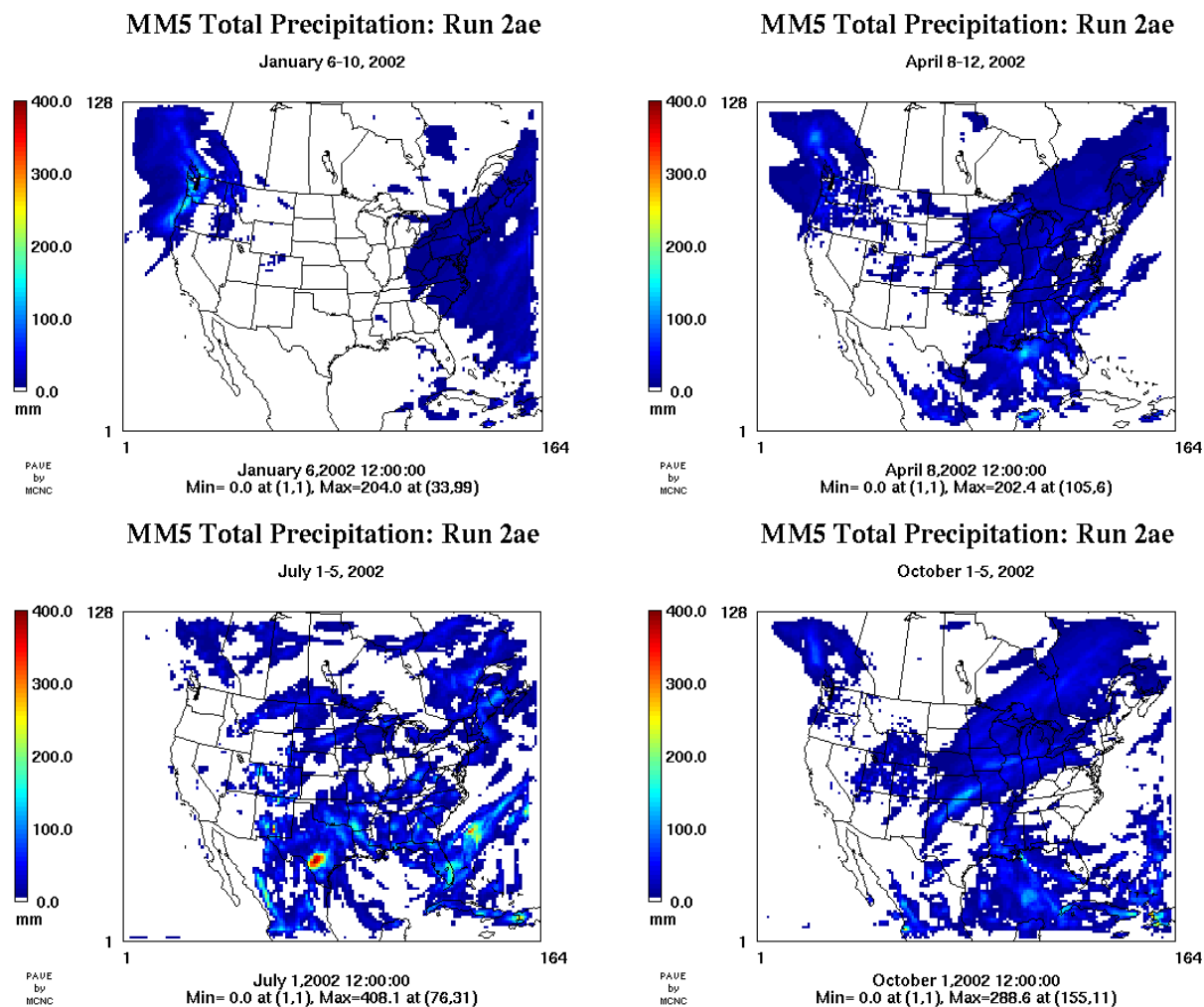


Figure 4-9b. Seasonal precipitation test for Run 2ae (PX).

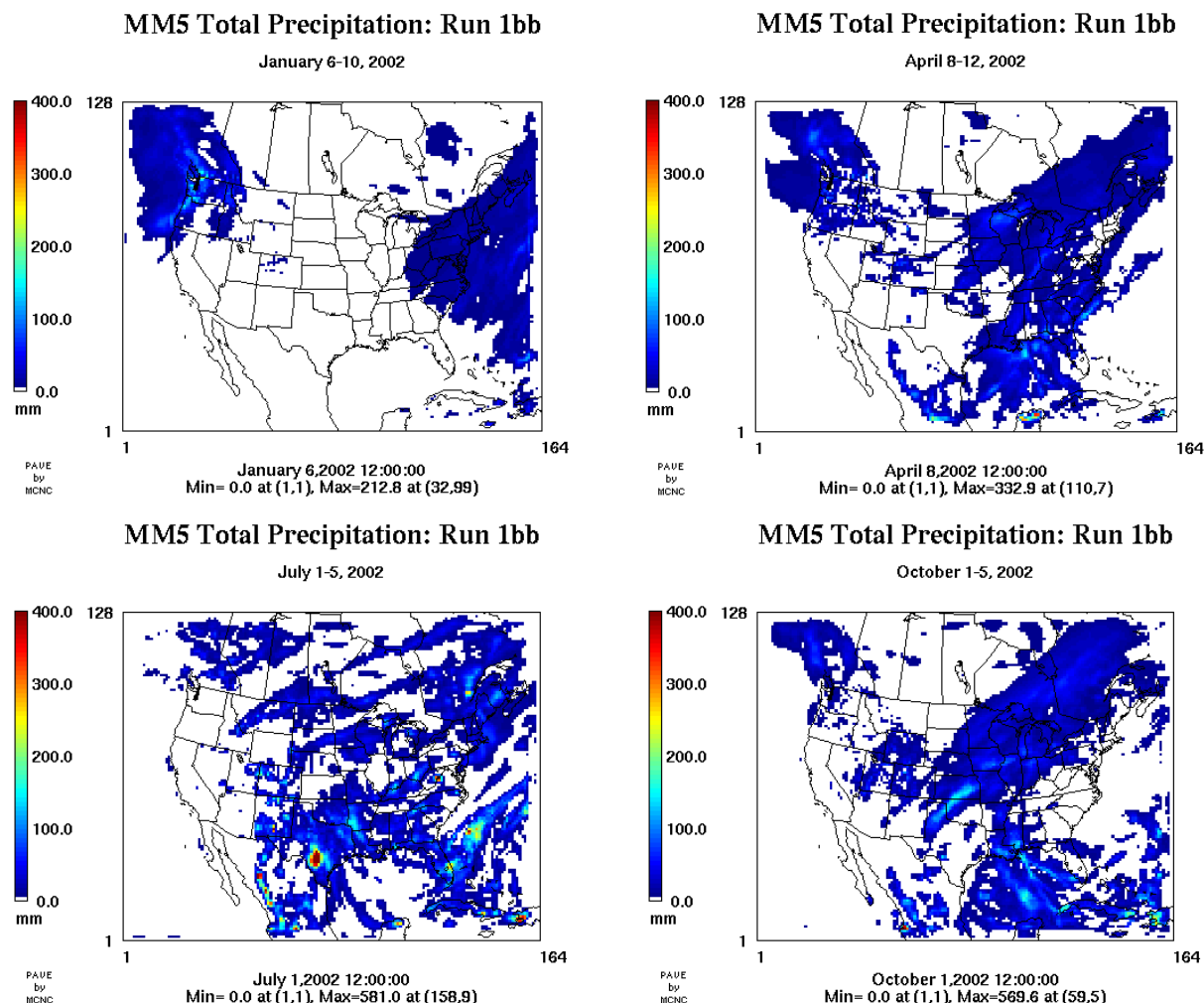


Figure 4-9c. Seasonal precipitation test for Run 1bb (M-MRF).

4.4.5 Selection of best-performing run

The regional haze events critical for WRAP CMAQ modeling tend to occur in the summer. We therefore selected Run 2ae, which gave better temperature performance during the summer, as the best-performing run overall. In the July simulation, the winds and humidity were comparable between Runs 2ae and 1bb. The performance improvement in Run 1bb in January and April was insufficient reason to switch the LSM/PBL scheme in winter/spring because the improvement brought only one additional subdomain point into the benchmark, and there was no improvement in temperature or humidity. We therefore chose to stay with PX/ACM throughout the year to get the best summer simulation and to allow the use of the Pleim-Xiu dry deposition algorithm in CMAQ throughout the year.

4.5 Summary of Results for the WRAP Region, and Performance in Other Subdomains

4.5.1 Summary of WRAP region results

A graphical representation of the differences between the initial MM5 run (Run 0) (Morris et al., 2004a; Kemball-Cook et al., 2004), the interim run (Run 5) (Emery et al., 2004), and the final run (Run 2ae) is shown in Figures 4-10 through 4-12. Figure 4-10a shows the wind bias and error for all three runs. For the DesertSW subdomain, there is improvement in both bias and error as we progress from Run 0 through Run 2ae. For the other three subdomains, as we move from Run 0 to Run 5, there is a reduction in error and an increase in the low wind speed bias. All points but one (Run 0, PacNW) lie outside the benchmark. Figure 4-10b, which shows wind direction bias and gross error, indicates that Run 2ae also produces improvements in the wind direction field relative to Runs 0 and 5.

For temperature (Figure 4-10c), all subdomains but DesertSW now lie within the benchmarks for Run 2ae, and that run is clearly the best-performing run for both error and bias in all subdomains. The most noticeable change in going from Run 0 to Run 2ae is that DesertSW is no longer an outlier, but now lies close to the benchmark for error, and within it for bias.

For humidity (Figure 4-10d), all subdomains now lie within the benchmark. Again, DesertSW has gone from being an outlier, whose wet bias left it far wide of the benchmark, to falling within the benchmark. For North, going from Run 0 to Run 5 and from Run 5 to Run 2ae brings the subdomain inside the benchmark. For SW, Run 2ae is an improvement in error but not in bias.

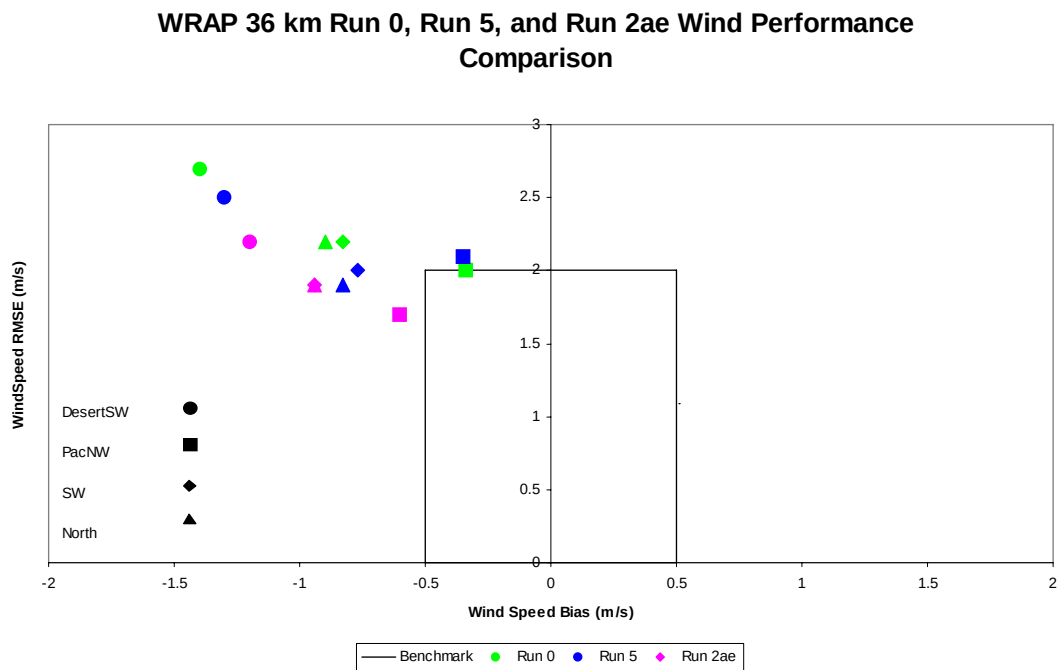


Figure 4-10a. Wind speed soccer plot for comparison of original (Run 0), interim (Run 5), and final (Run 2ae) 2002 MM5 runs.

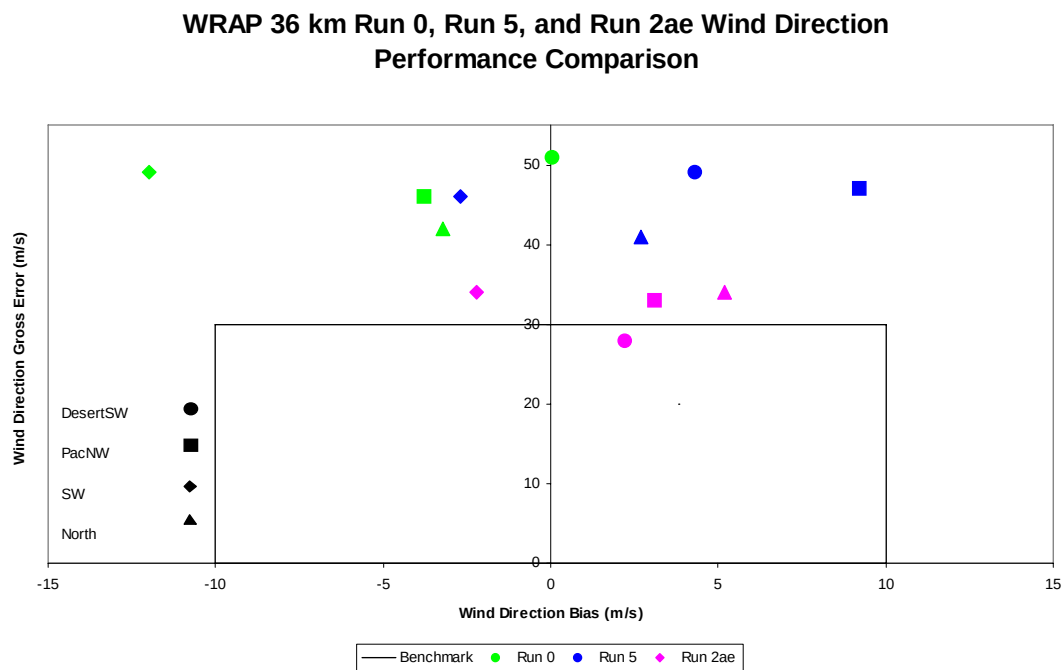


Figure 4-10b. Wind direction soccer plot for comparison of original (Run 0), interim (Run 5), and final (Run 2ae) 2002 MM5 runs.

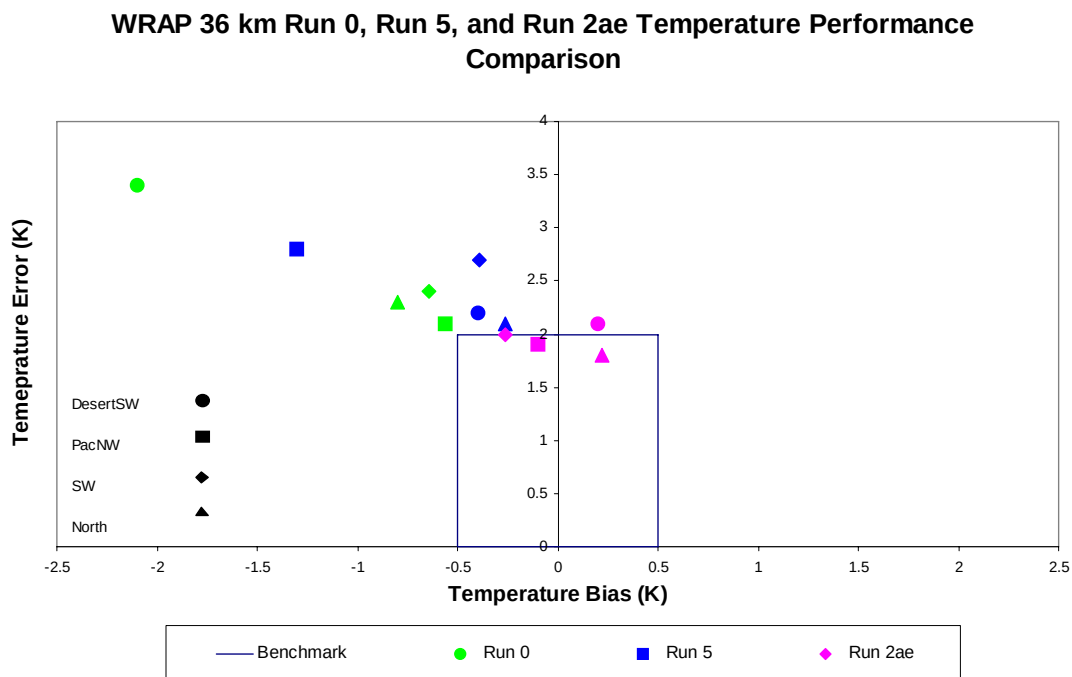


Figure 4-10c. Temperature soccer plot for comparison of original (Run 0), interim (Run 5), and final (Run 2ae) 2002 MM5 runs.

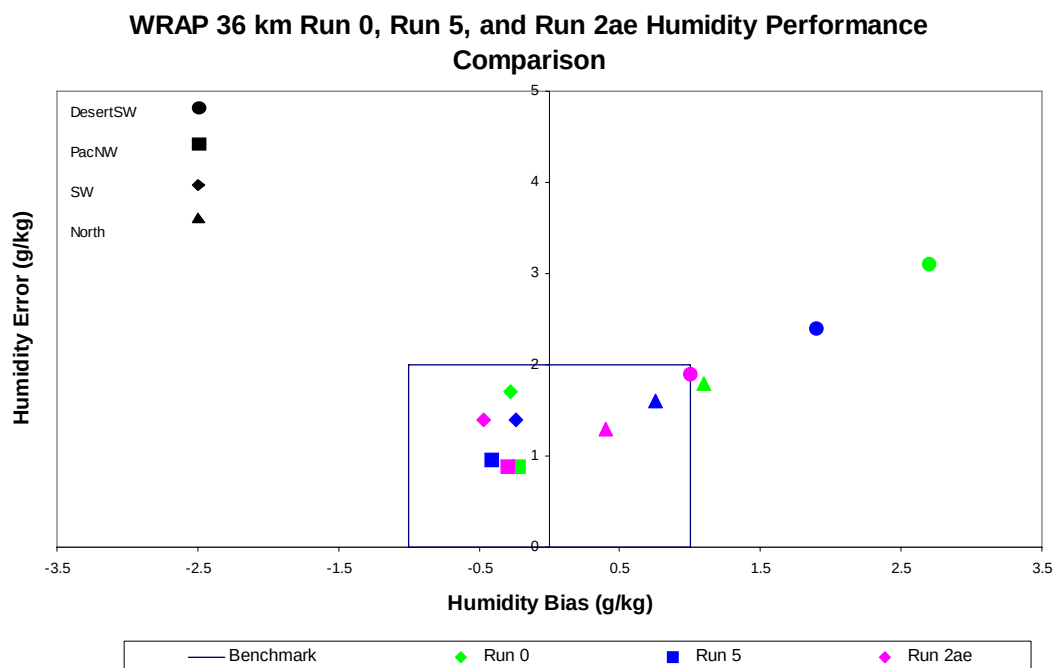


Figure 4-10d. Humidity soccer plot for comparison of original (Run 0), interim (Run 5), and final (Run 2ae) 2002 MM5 runs.

Figures 4-11a and 4-11b are time series of predicted (MM5) and observed temperature for Run 0 and Run 2ae. In Run 0, the amplitude of the predicted diurnal temperature cycle is smaller than in the observations. This was attributed to the presence of excess water at the surface, indicated by the wet bias in DesertSW (Figure 4-10d) and the excessive precipitation seen in Run 0 in Figure 4-12. Since water has a higher specific heat than soil, the presence of excess water at the surface tends to damp the amplitude of daily temperature rise and fall. There is a marked improvement in Run 2ae; the amplitude of the diurnal cycle more nearly matches that of the observations, and the substantial cold bias of Run 0 has been replaced by a slight warm bias.

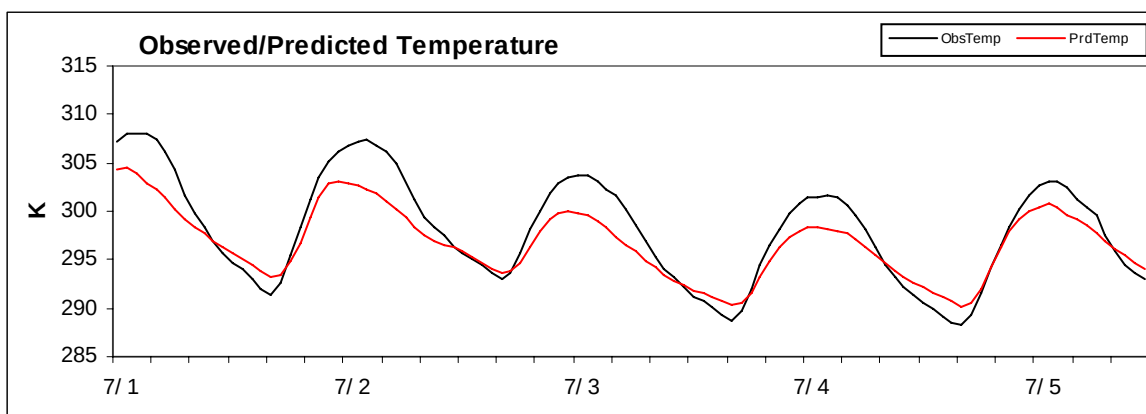


Figure 4-11a. July 1-5, 2002, MM5 predicted versus observed surface temperature time series for Run 0.

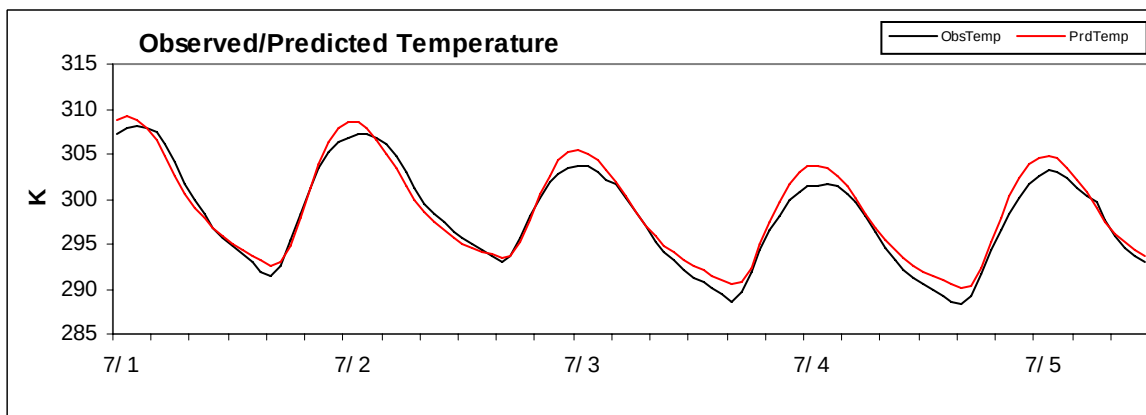


Figure 4-11b. July 1-5, 2002, MM5 predicted versus observed surface temperature time series for Run 2ae.

The precipitation field for Run 2ae is notable for its improvement over Runs 0 and 5 (Figure 4-12). The general overprediction of precipitation is less severe in Run 2ae than in the other two runs. The WRAP subdomains in particular see rainfall amounts from Run 2ae that are closer to

observed; this is reflected in the humidity soccer plot (Figure 4-10d), which shows a reduction of the wet bias in the DesertSW seen in Runs 0 and 5. The observed precipitation maximum over Texas is simulated reasonably well in Run 2ae, but is underpredicted in Runs 0 and 5. These precipitation patterns suggest that the Betts-Miller scheme is simulating the buildup and release of convective available potential energy (CAPE) more accurately than the Kain-Fritsch schemes, which seem to be discharging CAPE too soon and causing more widespread, less intense rainfall.

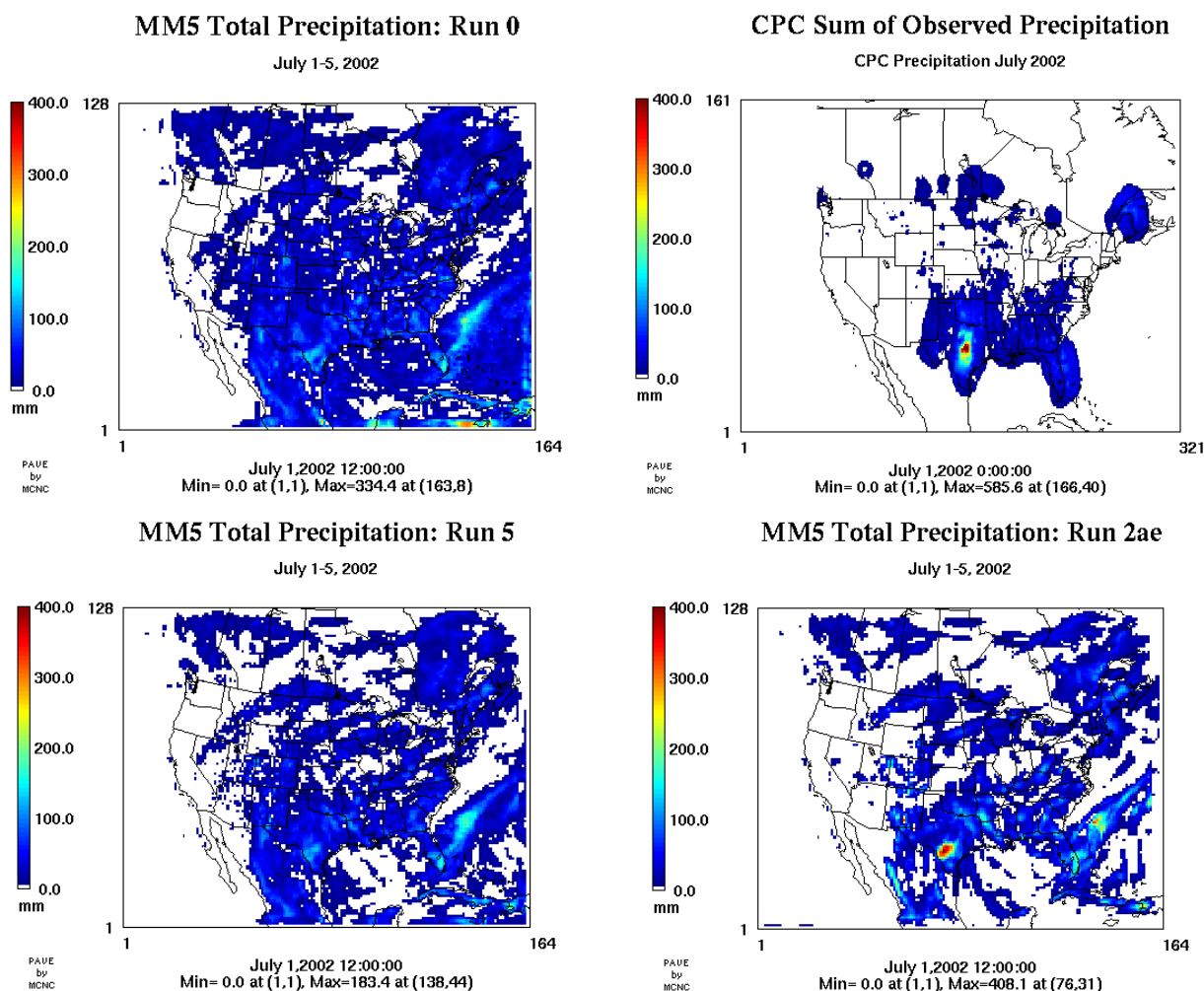


Figure 4-12. Precipitation comparison for July 2002 for original (Run 0), interim (Run 5), and final (Run 2ae) MM5 runs. Observed is shown at top right.

Table 4-4 summarizes the change in surface model performance evaluation (MPE) statistics, moving from the original WRAP 2002 annual run (Run 0) through the interim version (Run 5) to the final version (Run 2ae) in the western subdomains. There is significant improvement from Run 0 to Run 2ae. Of particular note are the increases in the humidity indexes of agreement (IOAs) in SW and DesertSW. These two subdomains had a substantial deficiency in the original

run, with a large wet bias. Note that the wet bias in the DesertSW subdomain has been more than halved in going from Run 0 to Run 2ae. The gross humidity error is also greatly reduced in these two subdomains. PacNW and SW also show improvement in humidity gross error, but show a slight degradation in bias performance. Overall, the new Run 2ae model configuration resulted in a greatly improved simulation of humidity over the western U.S.

Table 4-4. Surface model performance evaluation statistics summary.

Statistic	Bench mark	DesertSW Runs			North Runs			PacNW Runs			SW Runs		
		0	5	2ae	0	5	2ae	0	5	2ae	0	5	2ae
Wind spd bias	<±0.5	-1.47	-1.30	-1.22	-0.90	-0.85	-0.94	-0.34	-0.35	-0.59	-0.82	-0.77	-0.94
Wind spd RMSE	<2.0	2.69	2.51	2.21	2.32	2.2	1.88	1.97	2.05	1.67	2.16	1.98	1.85
Wind spd IOA	≥0.6	0.55	0.57	0.70	0.72	0.73	0.83	0.67	0.65	0.77	0.68	0.70	0.77
Wind dir bias	<±10	0.05	4.79	3.13	-3.22	6.23	2.19	-3.75	9.23	5.18	-11.85	-2.28	-2.23
Wind dir gross error	<30	50.5	50.3	32.8	42.2	43.4	28.3	45.9	46.6	34.2	49.3	47.3	34.2
Temp bias	<±0.5	-2.07	-0.4	0.2	-0.8	-0.26	0.22	-0.56	-1.28	-0.10	-0.64	-0.39	-0.26
Temp gross error	<2	3.42	2.19	2.07	2.32	2.09	1.77	2.14	2.8	1.86	2.37	2.72	2.02
Temp IOA	≥0.8	0.89	0.96	0.96	0.94	0.95	0.97	0.94	0.89	0.96	0.95	0.99	0.97
Humidity bias	<±1	2.73	1.90	1.00	1.08	0.75	0.40	-0.23	-0.41	-0.30	-0.28	-0.24	-0.47
Humidity gross error	<2	3.14	2.40	1.91	1.80	1.60	1.30	0.92	0.96	0.88	1.72	1.41	1.42
Humidity IOA	≥0.6	0.65	0.75	0.80	0.73	0.79	0.83	0.70	0.69	0.72	0.62	0.73	0.77

There is also a reduction in the cold bias that was apparent in Run 0. In DesertSW, the cold bias that was originally -2.1°C drops to 0.2°C in Run 2ae. Reductions in the cold bias are also seen in the other subdomains. Likewise, temperature error is reduced in all subdomains, although not enough to bring it entirely within the performance benchmark. Corresponding improvements are seen in the temperature IOA. Finally, the wind speed and wind direction bias and error generally exhibit improved model performance from initial Run 0 to final Run 2ae.

4.5.2 Tests in other subdomains

The tests described above focused on the western U.S., and the final configuration was selected on the basis of those results. Optimizing the MM5 configuration for the western U.S. may cause degradation of performance in other parts of the country, however. To investigate this, we compared model performance in the non-WRAP subdomains for Run 0, Run 5, and Run 2ae. Example results are presented for several of the subdomains; all results are available in the task interim report (<http://pah.cert.ucr.edu/aqm/308/docs.shtml>).

Figure 4-13a displays the wind performance comparison. Run 2ae is clearly the best of the three runs here, with a lower error than Run 0 or Run 5 for all subdomains. For MidAtl, CenrapN, and

NE, Run 2ae also has the smallest bias (note that the point for CenrapN coincides with the point for MidAtl for Run 2ae). For the CenrapS subdomain, Run 2ae has a smaller bias than Run 0, but a slightly larger bias than Run 5. For the OhioVal subdomain, the bias for Run 0 and Run 2ae is identical, and is slightly larger than that of Run 5.

For temperature (Figure 4-13b), Run 2ae has lower or equal error for all subdomains, and a smaller bias for MidAtl and CenrapS. For the other subdomains, the bias in 2ae is slightly larger than in Run 5, but still falls well within the benchmark. All points show a warm bias in Run 2ae, which is a shift from Run 0, for which all subdomains have a cold bias. Run 5 shows the subdomains equally split between warm and cold biases.

For humidity (Figure 4-13c), Run 2ae shows improvement over Runs 0 and 5 for all subdomains, lowering or eliminating the wet bias seen in Runs 0 and 5. Changes in error are less pronounced, but where they occur, Run 2ae has a smaller error.

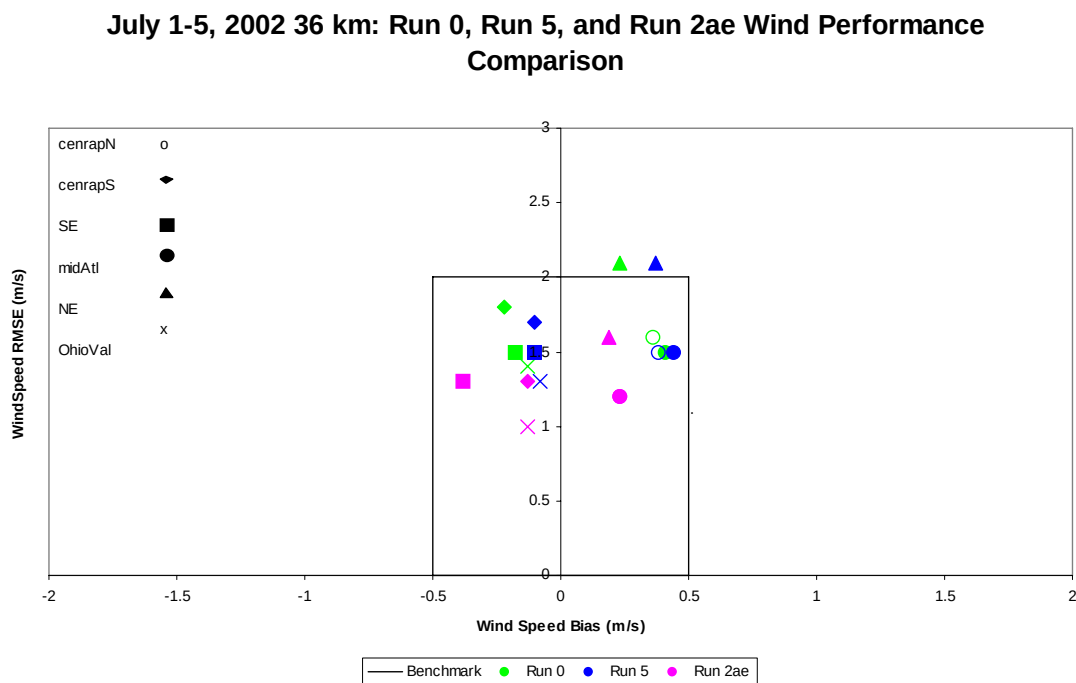


Figure 4-13a. Wind soccer plot for comparison of original (Run 0), interim (Run 5), and final (Run 2ae) 2002 MM5 runs for subdomains outside WRAP.

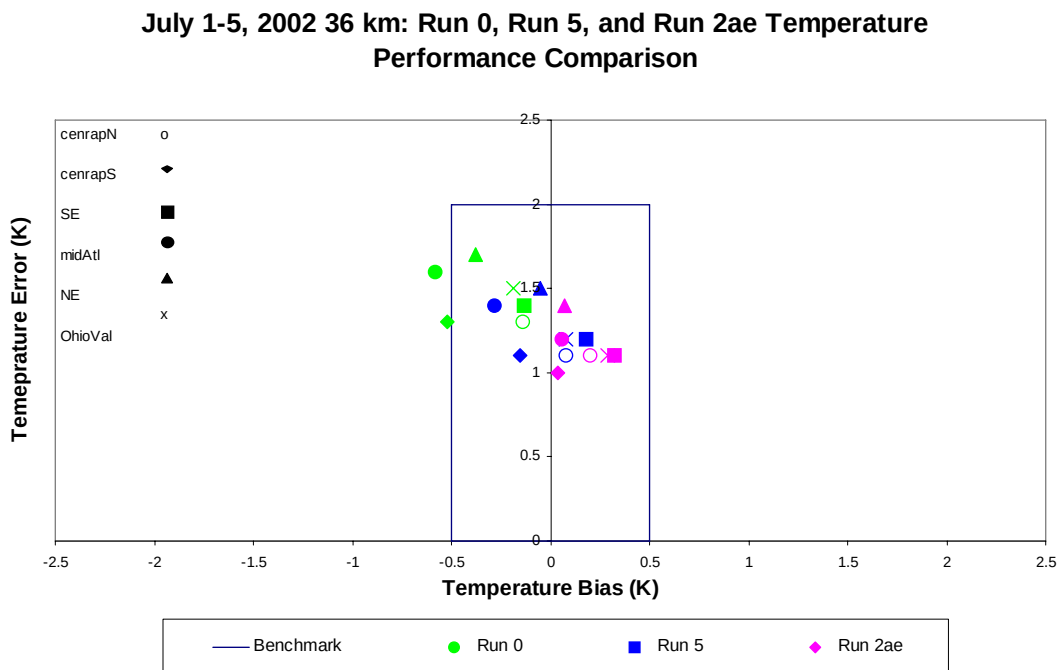


Figure 4-13b. Temperature soccer plot for comparison of original (Run 0), interim (Run 5), and final (Run 2ae) 2002 MM5 runs for subdomains outside WRAP.

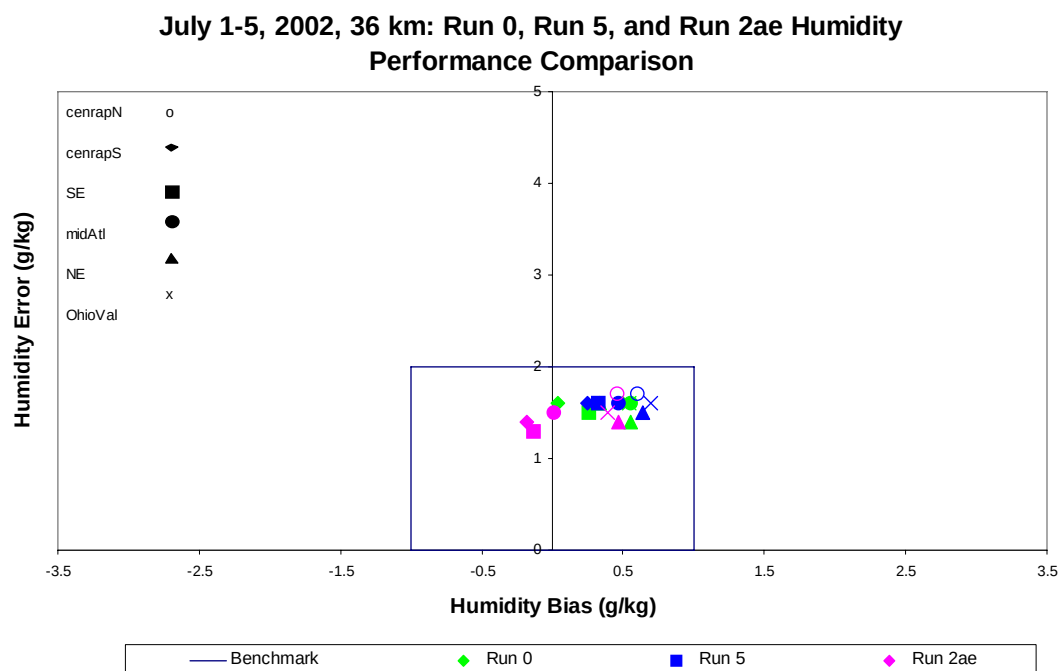


Figure 4-13c. Humidity soccer plot for comparison of original (Run 0), interim (Run 5), and final (Run 2ae) 2002 MM5 runs for subdomains outside WRAP.

4.6 Additional 12-km MM5 Sensitivity Tests

Having settled on a better MM5 configuration for the 36-km grid, we turned our attention to the WRAP 12-km grid. Reviewers of the MM5 sensitivity study report titled “MM5 Sensitivity Studies to Identify a More Optimal MM5 Configuration for Simulating Meteorology in the Western U.S.” (Kemball-Cook et al., 2004) raised concerns about the use of the Betts-Miller scheme at 12-km resolution. We therefore ran several tests to evaluate the effect of different cumulus parameterizations on the 12-km domain using the final “Run 2ae” configuration. At the 12-km scale, the problem of cumulus parameterization is not well posed, as there is no clear spectral gap between the resolved grid-scale process and the scale of the parameterized process (Arakawa and Chen, 1987). Molinari (1993) suggests that parameterization of cumulus convection for grid resolutions of 2 to 20 km cannot be addressed with either a fully explicit method or a hybrid parameterization approach. However, our ultimate goal of doing visibility modeling with CMAQ required us to be pragmatic and configure MM5 in a physically reasonable way that produces the most accurate representation of the 2002 meteorology. Our plan for the 12-km-grid cumulus scheme, therefore, was to conduct several sensitivity tests to determine which cumulus scheme (or alternatively, no cumulus scheme at all) gives the best performance in terms of rainfall and surface temperature, humidity, and wind. The sensitivity tests were conducted for the modeling period July 1-5, 2002, and are summarized in Table 4-5. The runs are identically configured except for the choice of cumulus parameterization, and, in the case of Run BM0a, the surface obs nudging and surface analysis nudging.

Table 4-5. Summary of cumulus sensitivity tests on the 12-km grid.

Run ID	36-km Cumulus	12-km Cumulus	Analysis FDDA		Obs FDDA
			3-D	Surface	
BM	Betts-Miller	Betts-Miller	W/T/H	W/T/H	W
BM0	Betts-Miller	None	W/T/H	W/T/H	W
BM0a	Betts-Miller	None	W/T/H	W	W
KF	Kain-Fritsch	Kain-Fritsch	W/T/H	W/T/H	W
KFII	Kain-Fritsch II	Kain-Fritsch II	W/T/H	W/T/H	W

Figure 4-14a shows the soccer plot for the wind performance on the 12-km grid for the above five MM5 runs. The BM and BM0 runs have the smallest biases in all four subdomains, and slightly larger errors. BM0a represents a degradation in performance relative to BM and BM0. For wind, then, the BM and BM0 runs give the best performance, and are too similar to one another to say which of the two is preferable. For temperature (Figure 4-14b), the KF run is a clear outlier. KFII and the BM simulations give approximately equivalent performance in terms of temperature. For humidity (Figure 4-14c), the BM and BM0 runs are a clear improvement over KF and KFII. Run BM0a offers a slight improvement over BM and BM0 for the DesertSW and North subdomains.

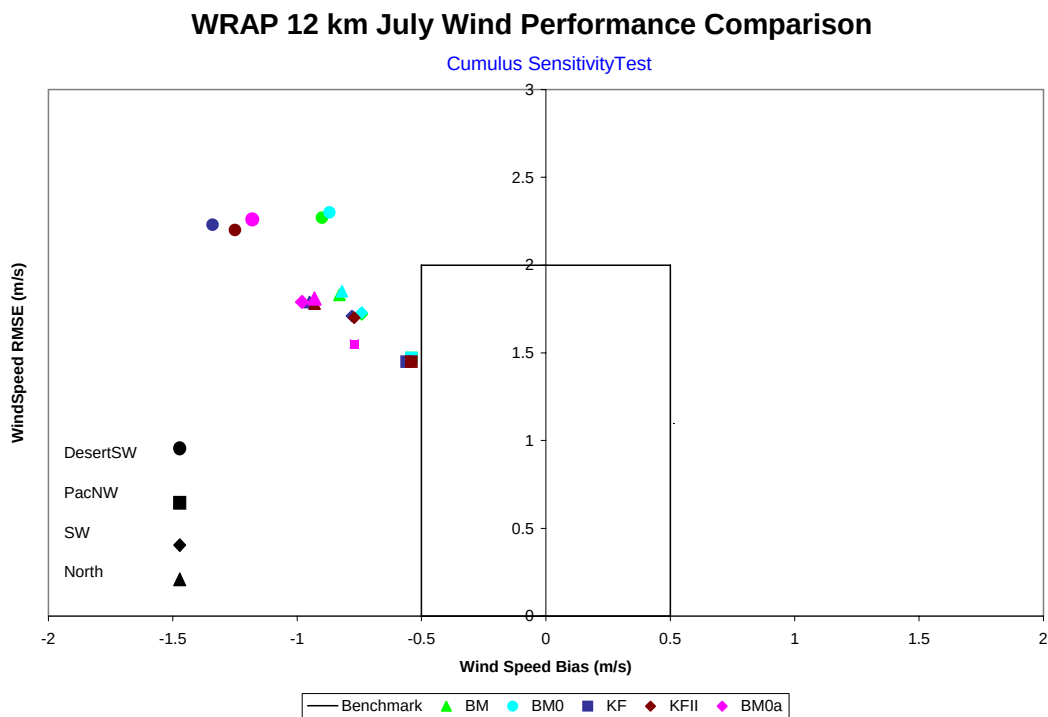


Figure 4-14a. Wind soccer plot for cumulus sensitivity test on 12-km grid.

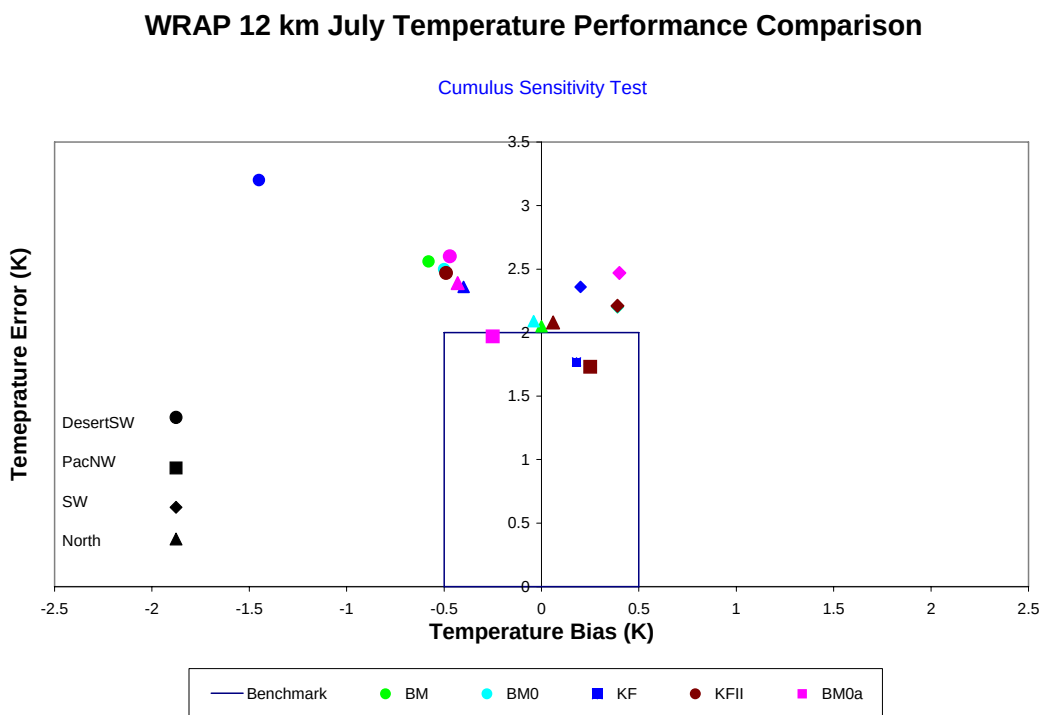


Figure 4-14b. Temperature soccer plot for cumulus sensitivity test on 12-km grid.

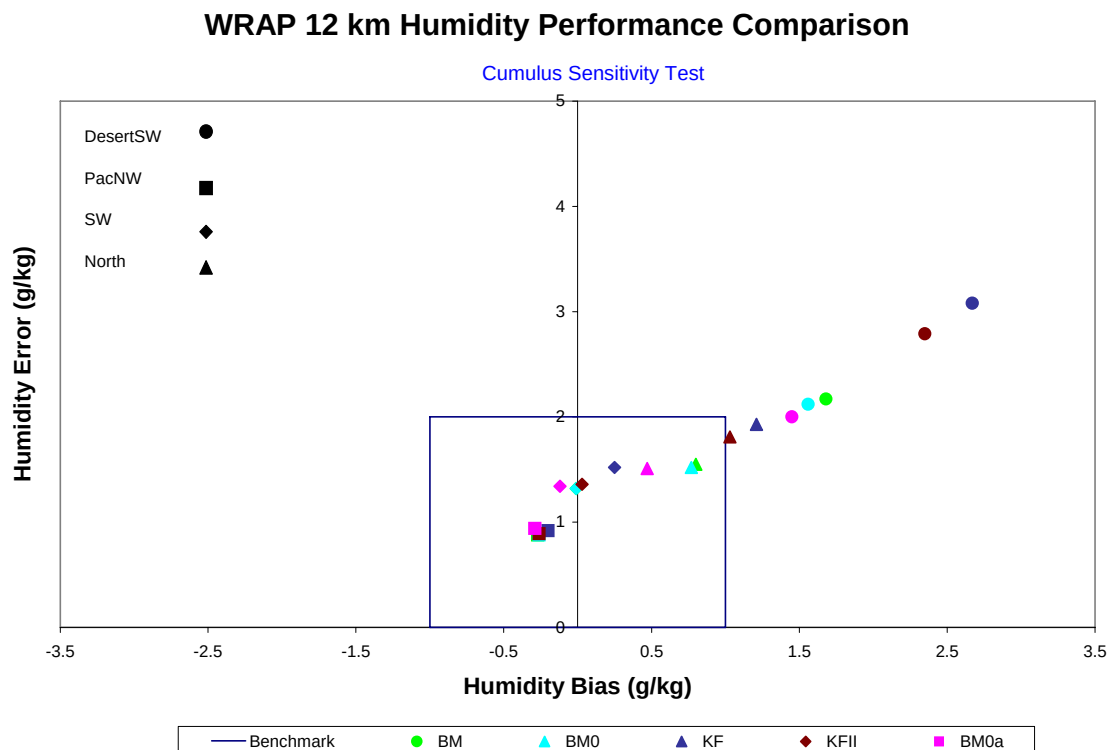


Figure 4-14c. Humidity soccer plot for cumulus sensitivity test on 12-km grid.

On balance, the BM and BM0 runs produced the best performance out of all the simulations tested on the 12-km grid, with BM0a producing slightly degraded but comparable performance relative to BM and BM0. Based on peer reviewer comments on the document “MM5 Sensitivity Studies to Identify a More Optimal MM5 Configuration for Simulating Meteorology in the Western U.S.,” we chose BM0a. The reason for this choice is the concern raised by the reviewers regarding surface analysis nudging of temperature and humidity. While this type of nudging can improve the surface statistics (making the run look better on the soccer plot), it can cause a degradation in the aloft simulation by adversely affecting the modeled stability.

The BM0a configuration was then used for the annual 2002 MM5 simulation to support WRAP’s regional haze modeling. This final MM5 simulation was conducted using the RPO Unified domain 36-km grid combined with the WRAP nested 12-km grid (this type of nested-grid simulation is referred to from here forward as a “36/12-km” simulation). The WRAP modeling protocol (ENVIRON and UCR, 2004) was updated to reflect the new model configuration.

4.7 Evaluation of the Final WRAP 2002 MM5 36/12-km Annual Run

After rerunning the MM5 36/12-km 2002 annual simulation, we compared the 36-km run’s performance with that of the initial WRAP_0 run (referred to as Run 0 above) as well as with two additional 36-km continental-scale annual runs performed by the CENRAP and VISTAS

RPOs. We evaluated the performance of each model run in replicating the evolution of observed winds, temperature, humidity, precipitation, and boundary layer morphology to the extent that resources and data availability allowed. This served as an assessment of the reliability of the new WRAP run's 36-km meteorological fields in adequately characterizing the state of the atmosphere and for serving as (1) boundary conditions for the 12-km regional-scale WRAP domain MM5 run and (2) the meteorological driver for the CMAQ 36-km continental-scale run. Finally, we evaluated the final 12-km WRAP run and assessed its suitability for providing meteorological conditions for the proposed 12-km CMAQ application. This work is discussed in the WRAP MM5 final report available at http://pah.cert.ucr.edu/aqm/308/mm5_reports04.shtml.

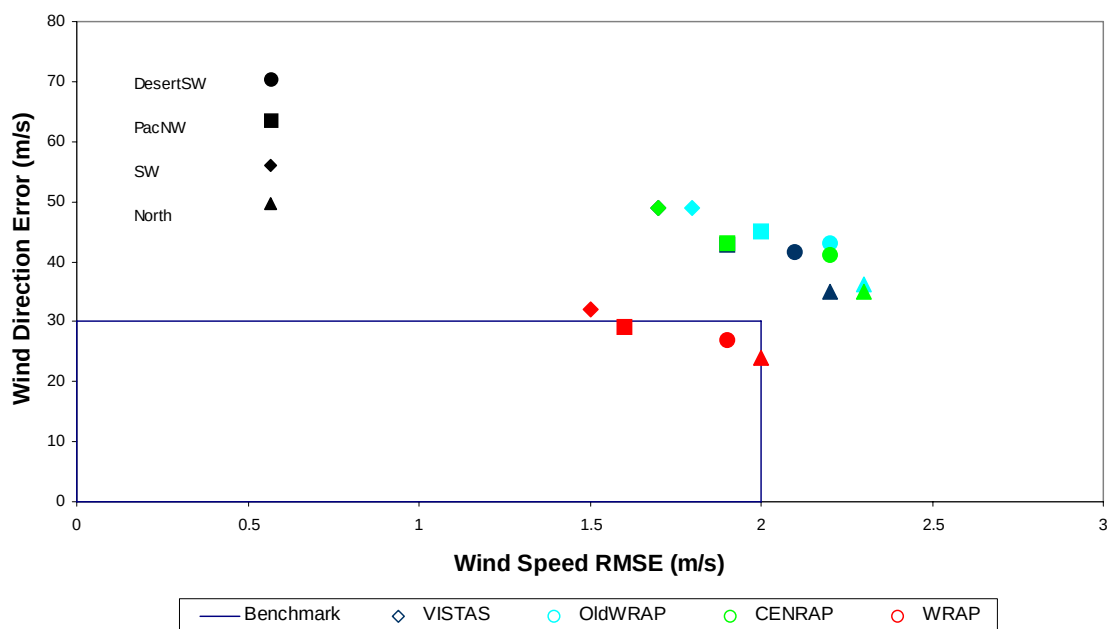
4.7.1 METSTAT Surface Evaluation

The starting point for the analysis of the new 2002 36-km MM5 runs was an assessment of the surface statistics for wind, temperature, and humidity using METSTAT. Soccer plots were generated and evaluated for each month of 2002. For brevity, we include only January (Figures 4-15 through 4-17) and July (Figures 4-18 through 4-20) in this report. MM5's performance was qualitatively different during summer and winter, with the spring and fall seasons serving as transitional periods between winter and summer. January and July were found to be representative of MM5's performance during the winter and summer seasons. The model's spring statistical performance was similar to that of fall. The main strengths and weaknesses of the 2002 MM5 runs are captured in the January and July plots. For each of those months, we show a soccer plot for the subdomains in the western U.S. (the WRAP region) and a second soccer plot for the central and eastern U.S. This is done to reduce the amount of data shown on one plot to a manageable level, and also because MM5's performance was qualitatively different between the western U.S. and the rest of the country. A detailed analysis is given in the final report (link listed above). Here, we list the major results of the analysis.

Summary of the Annual Cycle in MM5 Surface Performance:

- For temperature and humidity, the best-performing run overall was VISTAS; it had no outliers and had no serious performance problems at any particular time or subdomain.
- For wind, the best-performing run was the new WRAP run. There was not much difference in wind performance among the other three runs (WRAP_0, CENRAP, VISTAS).
- For wind, there is not much variation in performance in the east or the west over the course of the annual cycle, although the wind direction error is smaller in winter than in summer. The wind direction RMSE does not vary significantly over the course of the year for any of the four runs.

CENRAP / VISTAS / WRAP January Wind Performance Comparison Over the Western U.S.



CENRAP / VISTAS / WRAP January Wind Performance Comparison Over the Central and Eastern U.S.

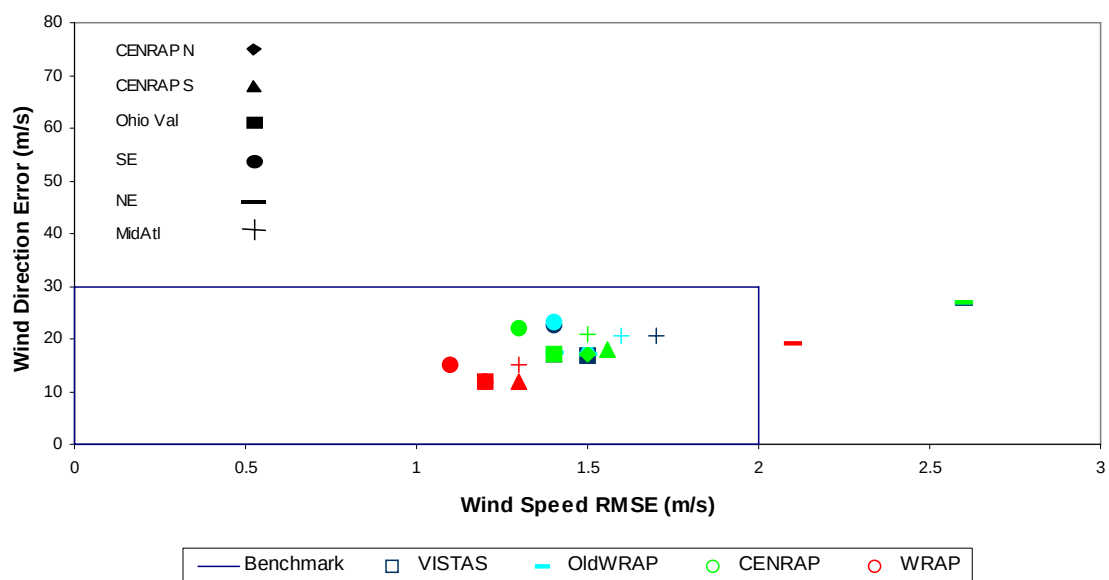
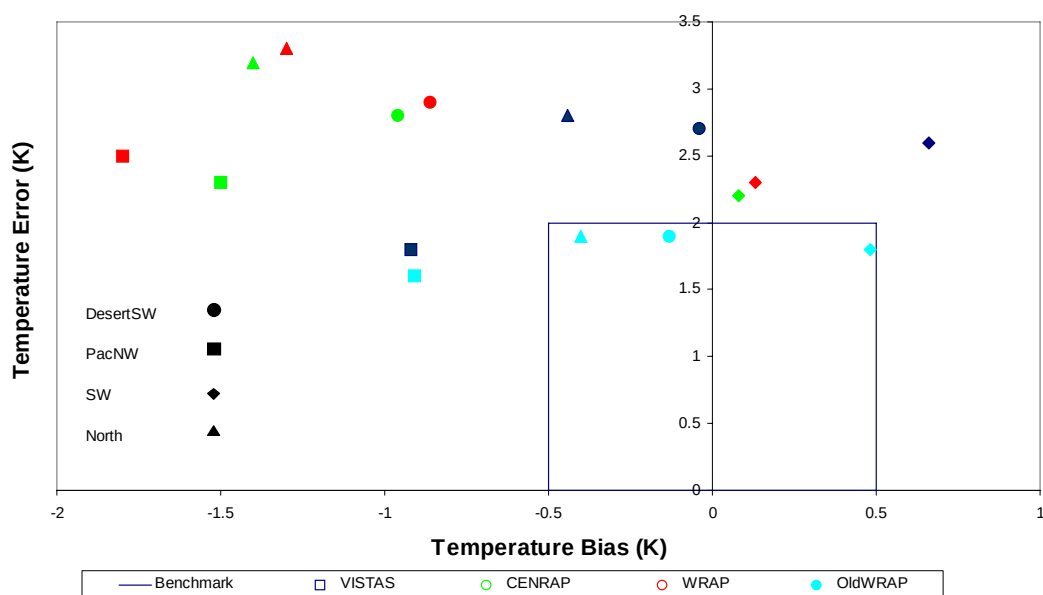


Figure 4-15. 36-km surface wind performance soccer plot for January for western U.S. (top) and central and eastern U.S. (bottom)

CENRAP / VISTAS / WRAP January Temperature Performance Comparison Over Western U.S.



CENRAP / VISTAS / WRAP January Temperature Performance Comparison over Central and Eastern U.S.

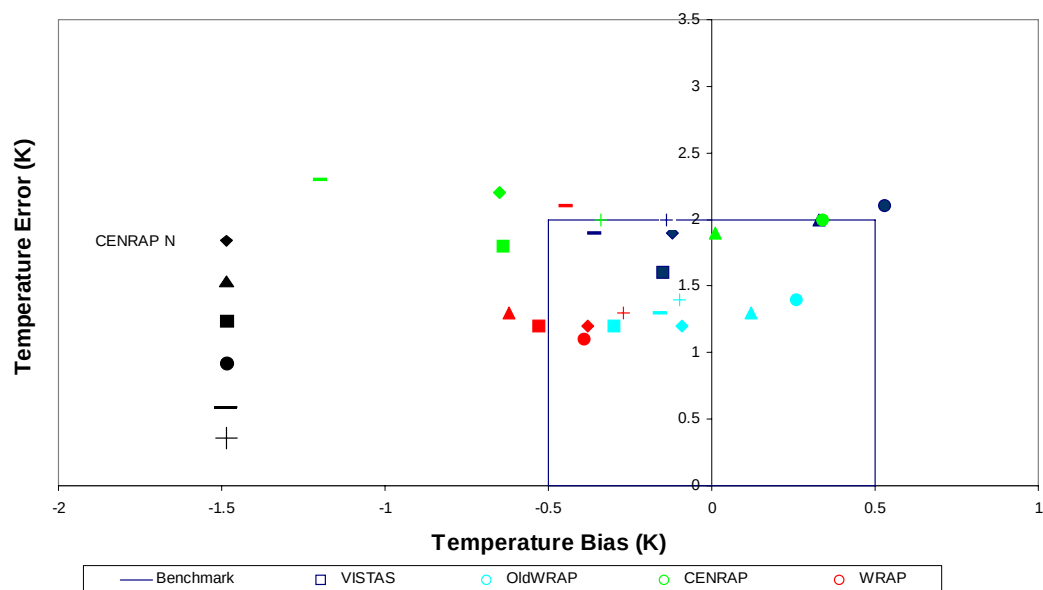
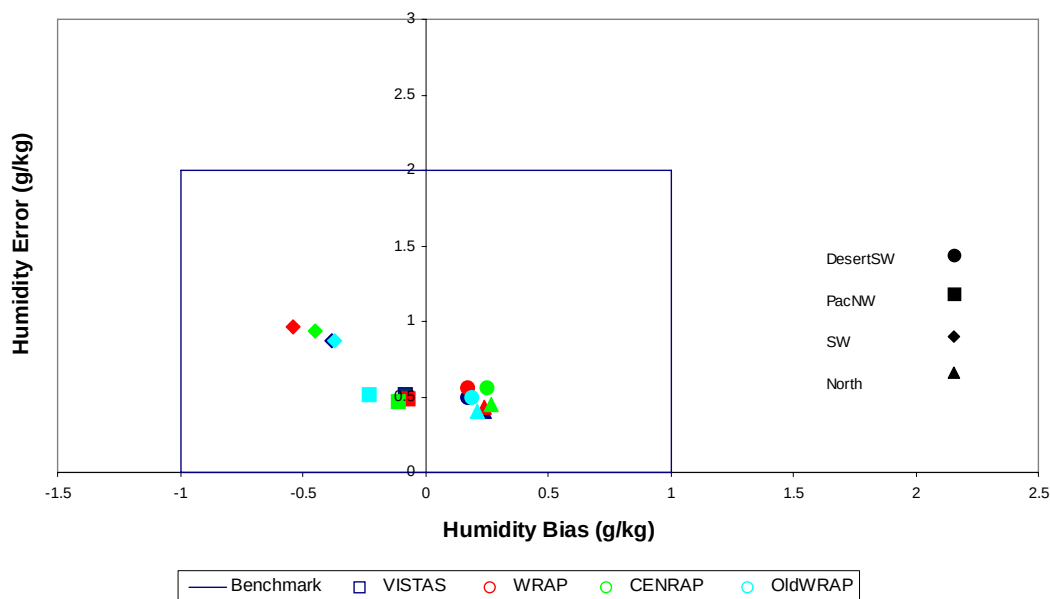


Figure 4-16. 36-km surface temperature performance soccer plot for January for western U.S. (top) and central and eastern U.S. (bottom).

CENRAP / VISTAS / WRAP January Humidity Performance Comparison Over the Western U.S.



CENRAP / VISTAS / WRAP January Humidity Performance Comparison Over the Central and Eastern U.S.

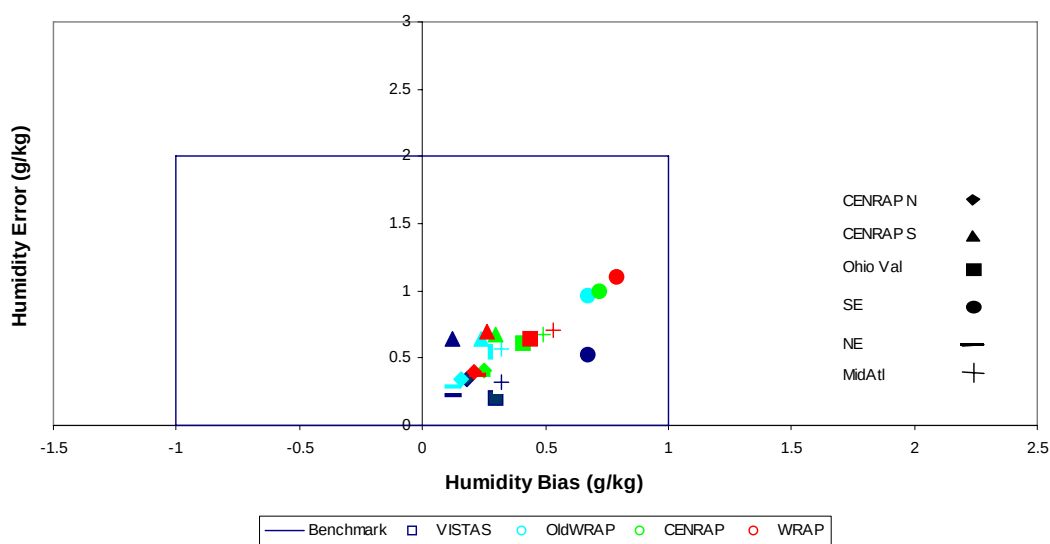


Figure 4-17. 36-km surface humidity performance soccer plot for January for western U.S. (top) and central and eastern U.S. (bottom).

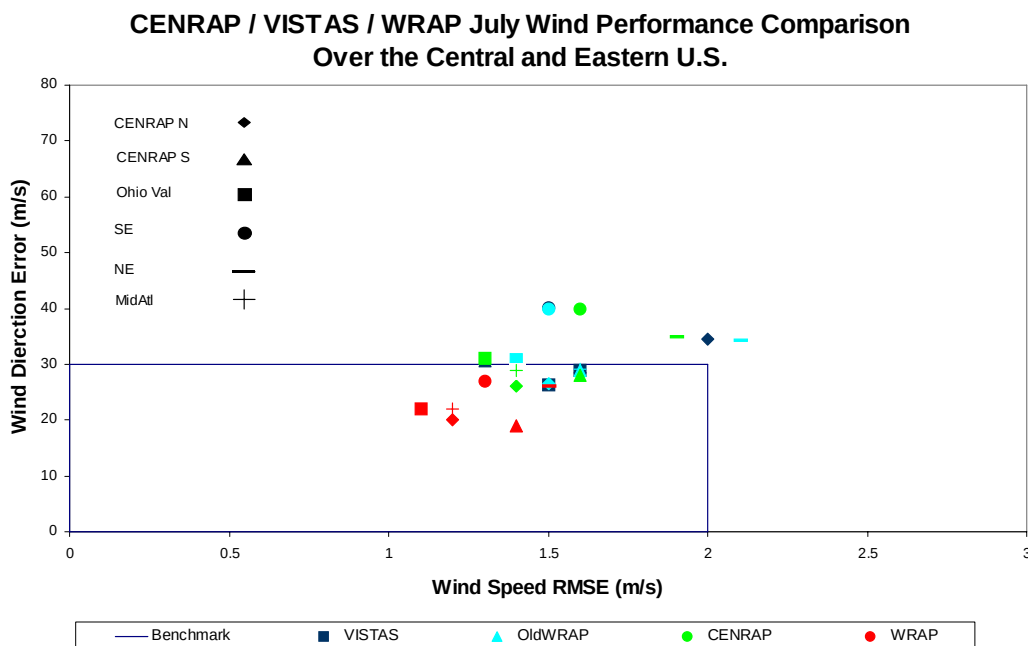
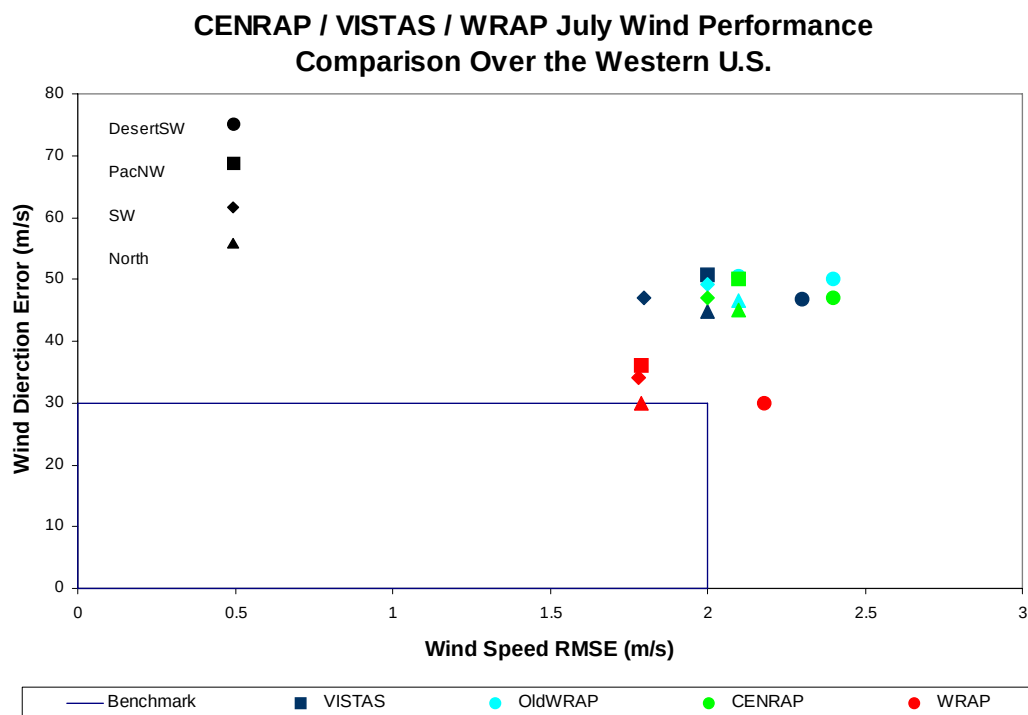


Figure 4-18. 36-km surface wind performance soccer plot for July for western U.S. (top) and central and eastern U.S. (bottom).

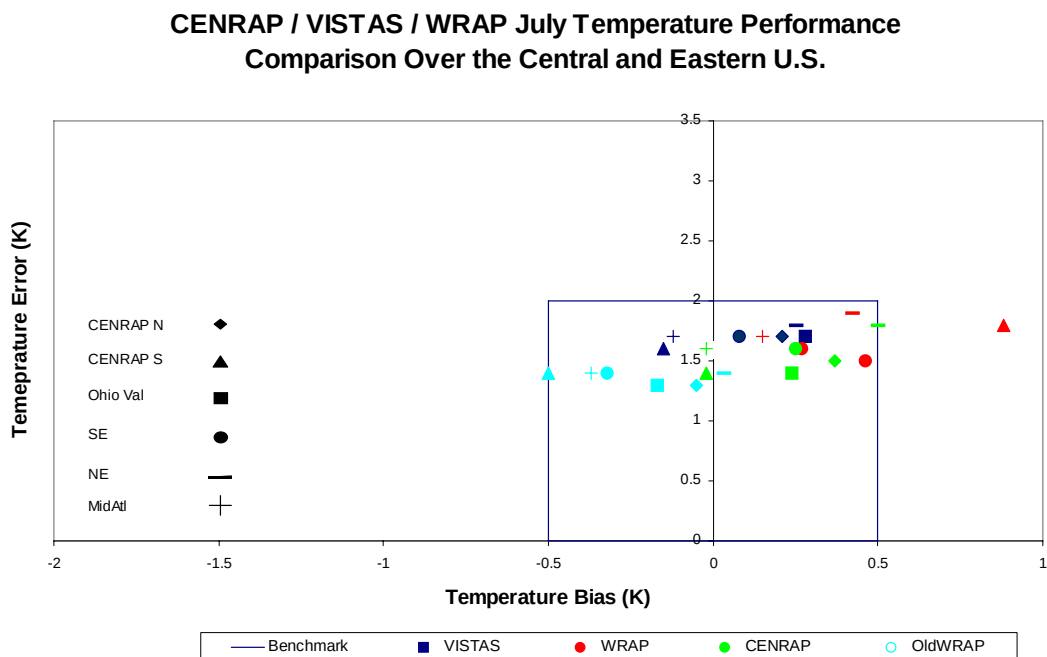
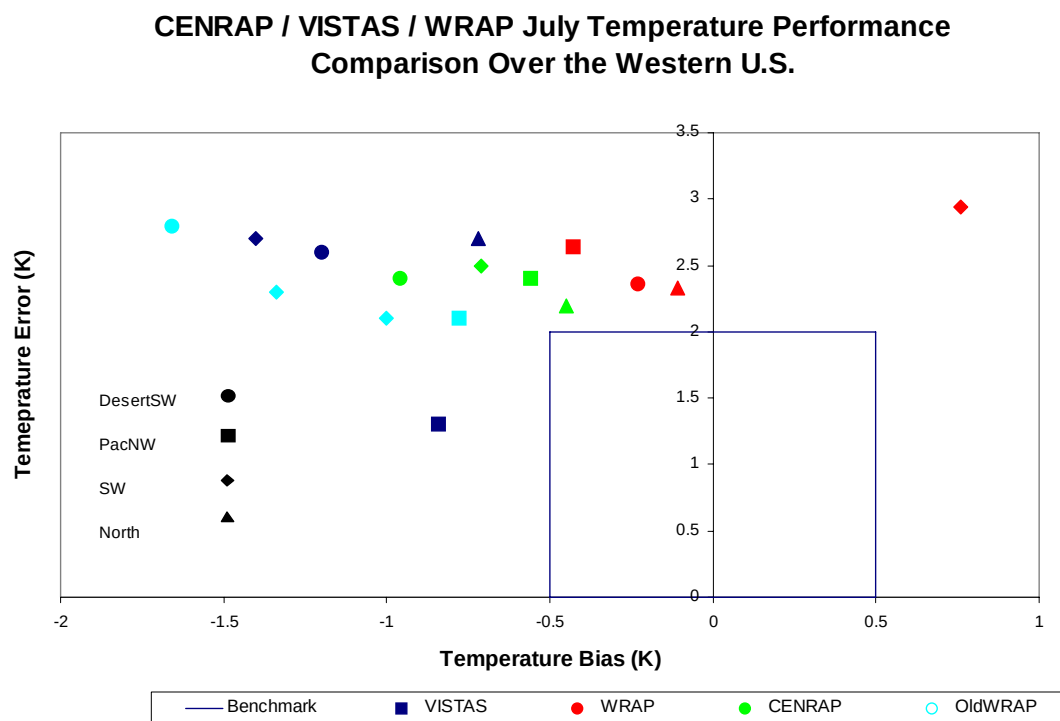


Figure 4-19. 36-km surface temperature performance soccer plot for July for western U.S. (top) and central and eastern U.S. (bottom).

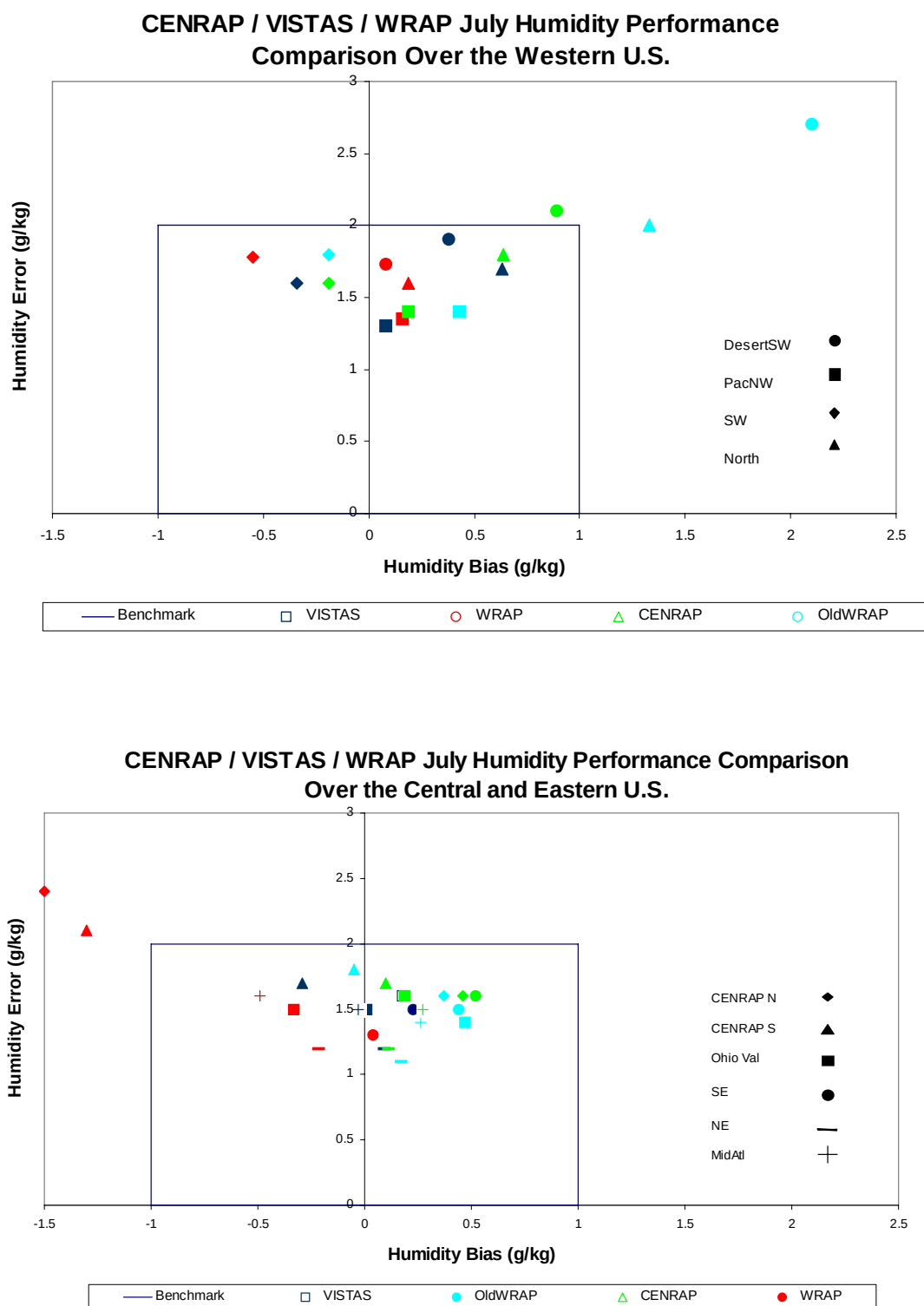


Figure 4-20. 36-km humidity performance soccer plot for July for western U.S. (top) and central and eastern U.S. (bottom).

Summary of the Annual Cycle in MM5 Surface Performance (continued):

- For temperature in the west, all runs except the nudged WRAP_0 run lie outside the benchmark (except for the SW and PacificNW subdomains, which lie barely within the benchmark in December). Performance is much better in the east than in the west.
- The new WRAP run had a less accurate surface temperature simulation than WRAP_0, which used analysis nudging of surface temperature.
- For temperature in the east, all or nearly all of the subdomains lie within the benchmark during most months.
- Humidity performance was generally within the benchmarks for all regions for all runs except the WRAP_0 run.
- For humidity, in the west, performance is best in winter and deteriorates as summer approaches. The culprit is the humidity error, not the bias, except for the WRAP_0 run outliers in July in the North and DesertSW subdomains.
- Except for SW, all western subdomains have a wet bias in July. This is likely related to excess simulated precipitation.
- For eastern subdomains, humidity performance is comparable to western subdomains, as was true for wind.
- The new WRAP run showed significant improvement in July humidity performance in the west relative to the WRAP_0 run, but does worse in the east. We can attribute both of these changes in performance to reduction in rainfall and therefore surface moisture that we get in going from the Kain-Fritsch cumulus scheme to the Betts-Miller scheme

4.7.2 Precipitation Evaluation

Next, we evaluated the precipitation fields in the VISTAS, CENRAP, WRAP_0, and new WRAP 2002 36-km MM5 runs. We examined the annual cycle in the monthly rainfall totals in the MM5 runs and compare them to observed monthly rainfall totals (Figures 4-21 and 4-22).

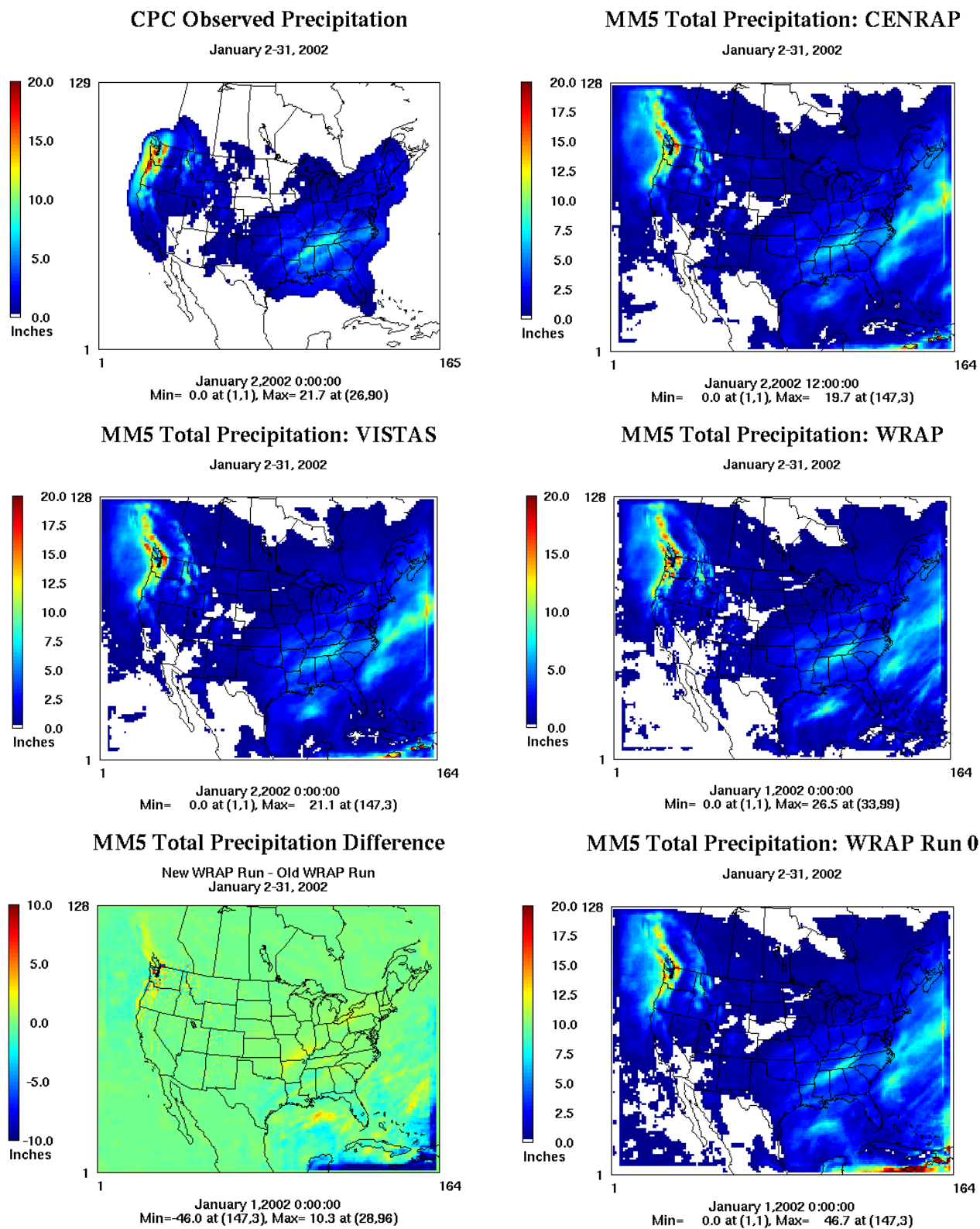


Figure 4-21. January observed and modeled precipitation.

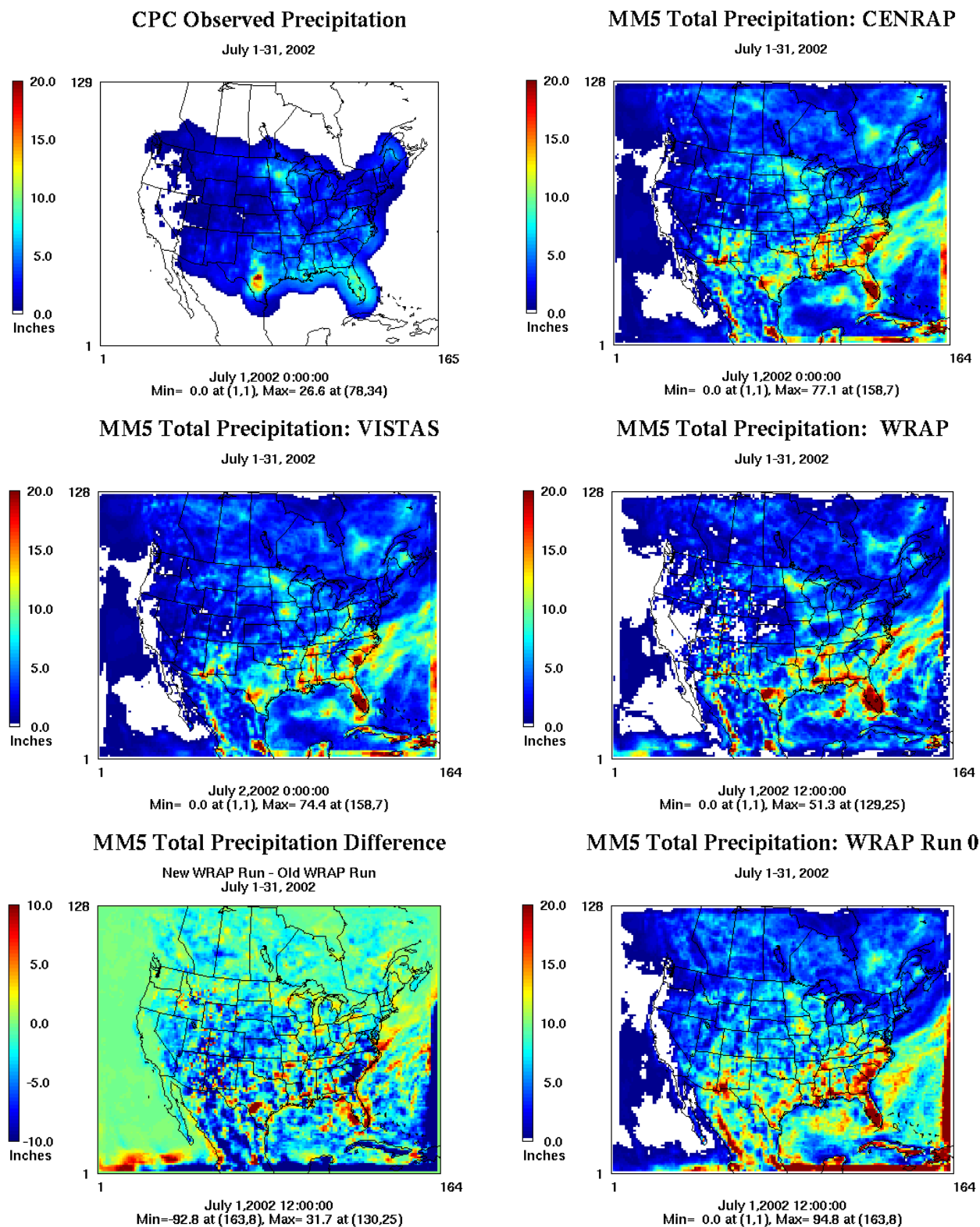


Figure 4-22. July observed and modeled precipitation.

In summary, differences among the four 36-km MM5 runs in terms of precipitation performance were relatively small. All four runs were able to reproduce many of the major stratiform (i.e., resolved at grid-scale) precipitation features, and all four had difficulty with convective precipitation. This is to be expected, given that convection is a subgrid-scale phenomenon whose parameterization is poorly understood. The biggest difference among the four simulations came in July; in the western U.S., the overestimation of precipitation was smallest in the new WRAP run, but the new WRAP run also overpredicted convective rainfall in the southeastern United States. These changes are clearly related to the use of a different type of cumulus scheme in the new WRAP run than in the other three runs. For the purposes of WRAP visibility modeling, the new WRAP run is clearly an improvement over the WRAP_0 run, and has more accurate precipitation fields in the western U.S. in both summer and winter.

4.7.3 Upper-Air Evaluation

To assess whether MM5 is simulating the vertical structure of the atmosphere with reasonable accuracy in the four 36-km runs, we compared model temperature and dew point soundings with those from a limited number of radiosonde stations. We focused on the months of January and July, as these two months were at the extremes of good and poor model performance at the surface.

For the months of January and July, a radiosonde station was selected from each subdomain, and the 00Z and 12Z observed and modeled soundings from each day were compared for the CENRAP, VISTAS, WRAP_0, and WRAP runs. 12Z and 00Z soundings were analyzed in order to examine differences between stable (nocturnal) and unstable (daytime) conditions (00Z and 12Z are 4pm PST/7pm EST and 4am PST/7am PST, respectively). In the following discussion, we summarize the general features of the upper-air soundings found in the extended analysis of January and July. By looking at two months for a limited number of stations, we had a manageable amount of sounding data to analyze, but we caution that it would be unwise to place too much confidence in generalizing these results from two months of data from 11 stations to the entire MM5 domain and the entire year. We summarize the results of the upper-air analysis below:

- In both January and July, the CENRAP and VISTAS runs were better able to simulate PBL temperature inversions than were the two WRAP runs. Figure 4-23 shows the 12Z sounding for Spokane, WA (OTX) for July 2, 2002. The CENRAP and VISTAS runs both underestimate the strength of the inversion, but the problem is worse in the WRAP_0 and new WRAP runs.
- CENRAP and VISTAS dew point temperature profiles were generally closer than that of WRAP_0 to the observed profile, and these two runs were better able to handle extreme excursions in temperature and dew point profiles in the lower troposphere.
- The new WRAP run tended to have a more accurate dew point profile than the WRAP_0 run at 12Z, and a temperature profile that was less accurate near the surface, which is reasonable given the lack of surface temperature analysis nudging the new WRAP run.

- Because of the analysis nudging of surface temperature, the WRAP_0 surface temperature was generally closer than CENRAP or VISTAS to the observed surface temperature, but profiles above surface were less accurate in WRAP_0 than in CENRAP or VISTAS.
- For July soundings with a deep, convecting boundary layer, CENRAP and VISTAS frequently better reproduced the observed temperature inversion at the top of the PBL, while the WRAP_0 run showed a smoother decrease of temperature with increasing altitude. This problem is somewhat ameliorated in the new WRAP run. Figure 4-24 shows the observed and simulated soundings for 00Z on July 16 at Midland, TX. The observed sounding shows a deep, dry adiabatic convecting layer with an inversion at 700 mb. Both the CENRAP and VISTAS runs simulate an inversion just above 700 mb, although it is weaker than the observed inversion. The WRAP_0 temperature sounding shows temperature decreasing smoothly with increasing altitude, with no inversion. The new WRAP run still does not manage to produce an inversion, but does a better job of approximating the temperature profile immediately above the observed inversion.
- The new WRAP run has a more accurate surface pressure than any of the other three runs. This improvement in the surface pressure in the new WRAP run seems to be a general feature of this run, and was noted in both summer and winter soundings. It is unclear what caused this improvement.
- During winter, there was not much difference between the new and old WRAP runs. What differences there were occurred near the surface. The WRAP_0 run tended to have a more accurate temperature profile near the surface, due to its surface analysis nudging. Because cumulus convection is not as active during the winter, the surface temperature differences predominated in winter. There was generally little change in the dew point profile in winter.
- In summer, there were larger differences between the new and old WRAP runs stemming from the difference in parameterization of cumulus convection. Although there was a deterioration in the temperature profile near the surface in the new WRAP run (due to turning off surface temperature nudging), the dew point profile was often more accurate in the new WRAP run.
- Overall, the upper-air profiles in the CENRAP and VISTAS runs were very similar to one another, and both of these runs had some marked differences with the two WRAP runs (i.e., success at simulating low-level nocturnal inversions or the PBL top inversion). It is possible that the differences between the two WRAP runs and the other two runs may be attributed to the different explicit moisture schemes.

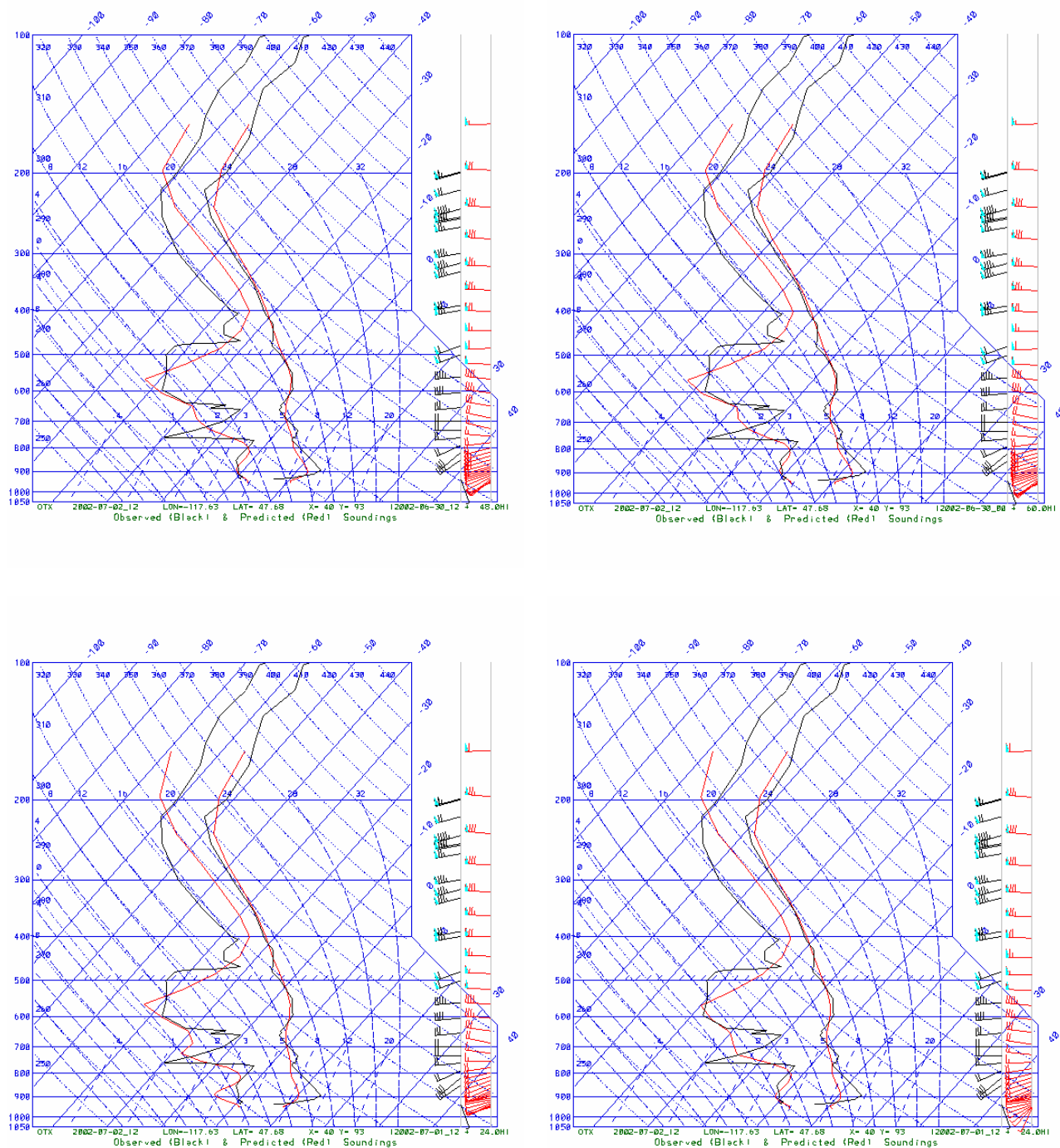


Figure 4-23. July 2, 2002, 12Z Sounding for Spokane, WA.
Upper left-hand panel: CENRAP; upper right-hand panel: VISTAS;
lower left-hand panel: WRAP_0; lower right-hand panel: new WRAP.

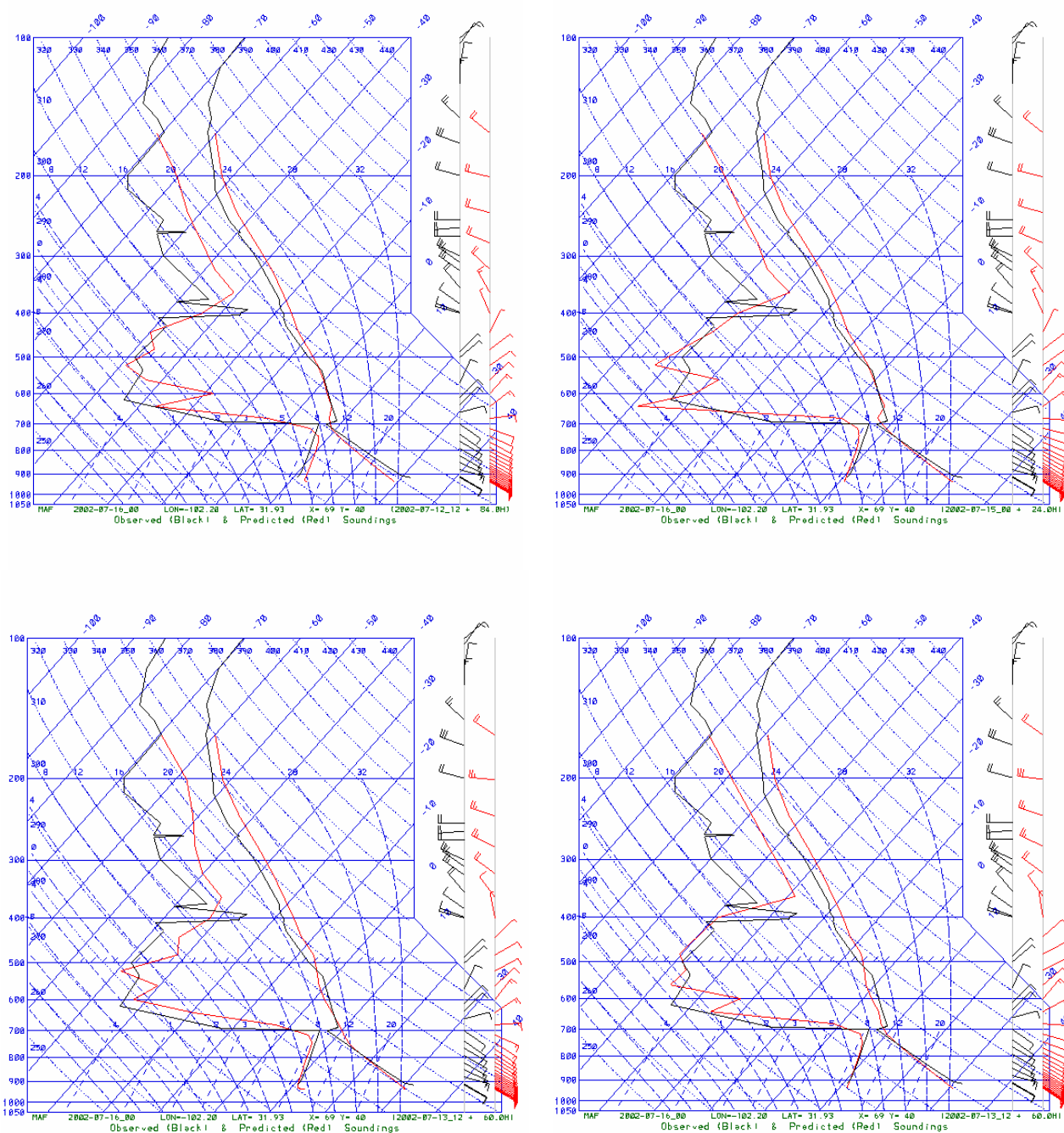


Figure 4-24. July 16, 2002, 00Z Sounding for Midland, TX.
Upper left-hand panel: CENRAP; upper right-hand panel: VISTAS;
lower left-hand panel: WRAP_0; lower right-hand panel: new WRAP.

4.7.4 12-km METSTAT Surface Performance Evaluation

Next, we assessed the performance of the 2002 12-km MM5 run. The evaluation of the MM5 surface meteorological variables using METSTAT is presented first, followed by a comparison of the CPC observed and MM5 predicted precipitation patterns.

As in the analysis of the 36-km run, soccer plots were generated and evaluated for each month of the year 2002 for the 12-km grid. On these soccer plots, we also include for reference the data from the 36-km run, so that we can see the effects on performance of running at higher resolution and with different cumulus parameterization (none, in the case of the 12-km run). As in the 36-km run, MM5's performance was qualitatively different during summer and winter, with the spring and fall seasons serving as transitional periods between winter and summer. January and July were found to be representative of MM5's performance during the winter and summer seasons. For brevity, we include only January and July in this report. The main strengths and weaknesses of the 2002 12-km MM5 run are captured in the January plots (Figures 4-25 through 4-27) and July plots (Figures 4-28 through 4-30). For both months, we show a soccer plot for the subdomains in the western U.S. (the 12-km WRAP region). The subdomain definitions are the same as those used in the 36-km run.

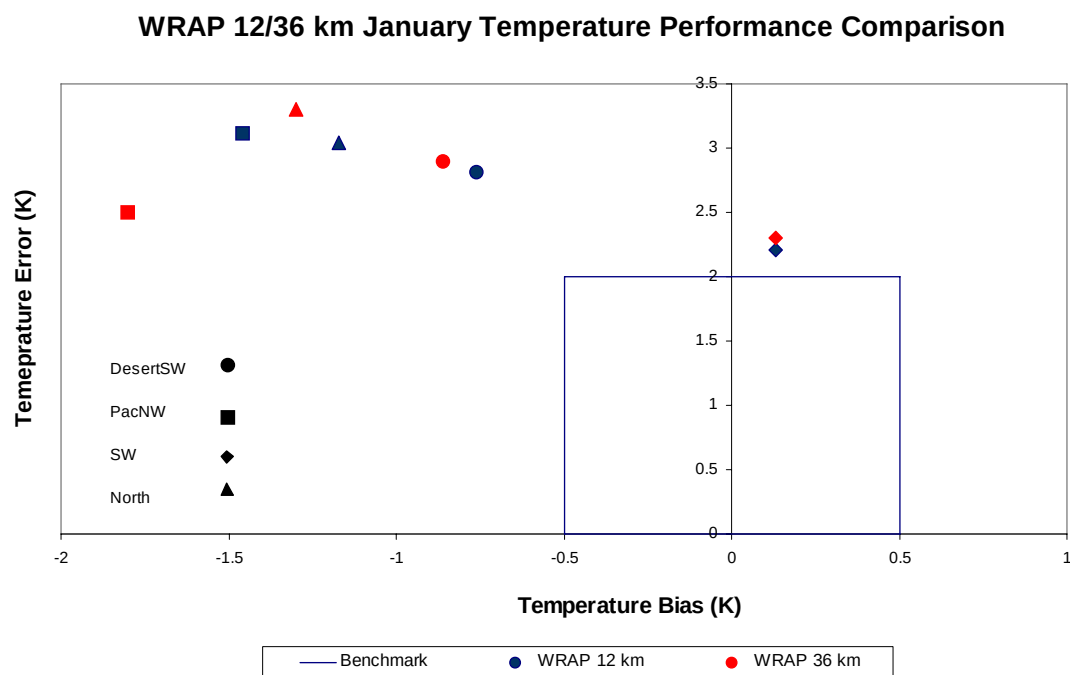


Figure 4-25. 12/36-km surface temperature performance soccer plot for January for the WRAP region.

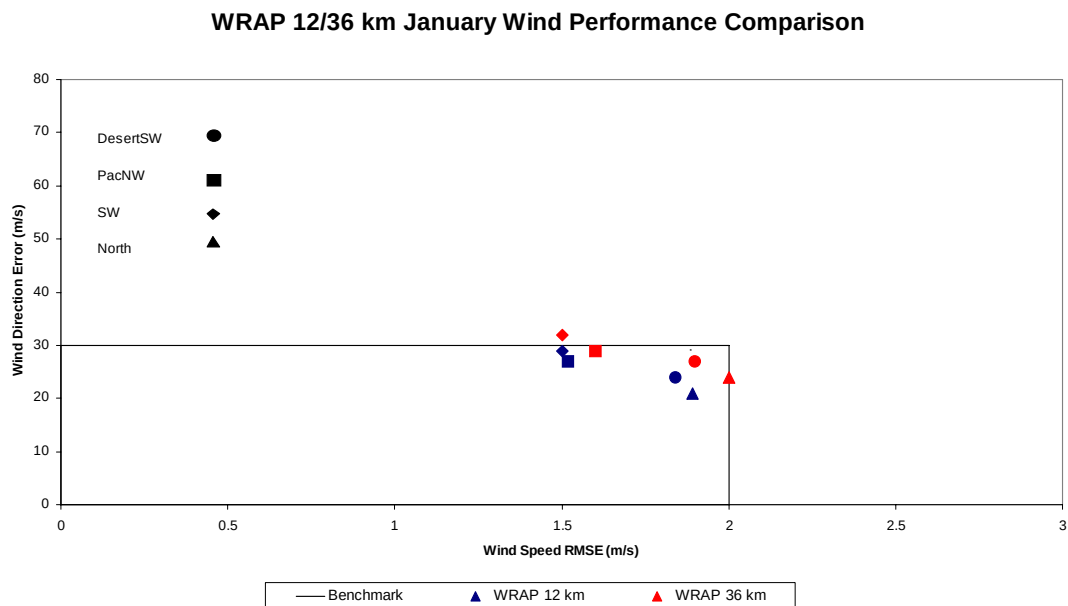


Figure 4-26. 12/36-km surface wind performance soccer plot for January for the WRAP region.

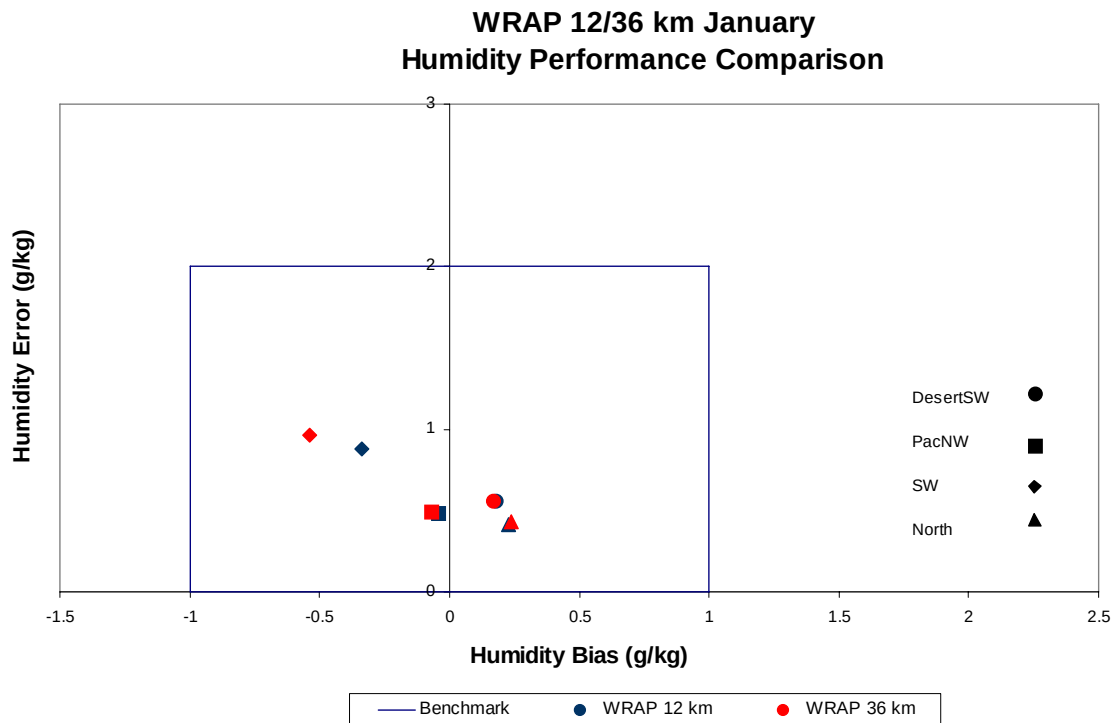


Figure 4-27. 12/36-km surface humidity performance soccer plot for January for the WRAP region.

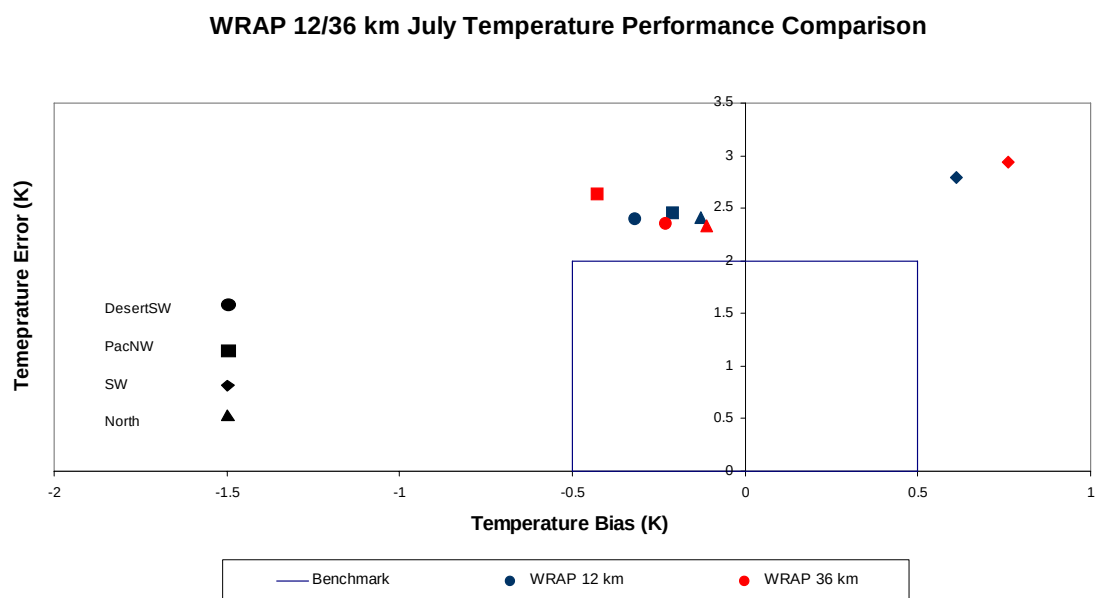


Figure 4-28. 12/36-km surface temperature performance soccer plot for July for the WRAP region.

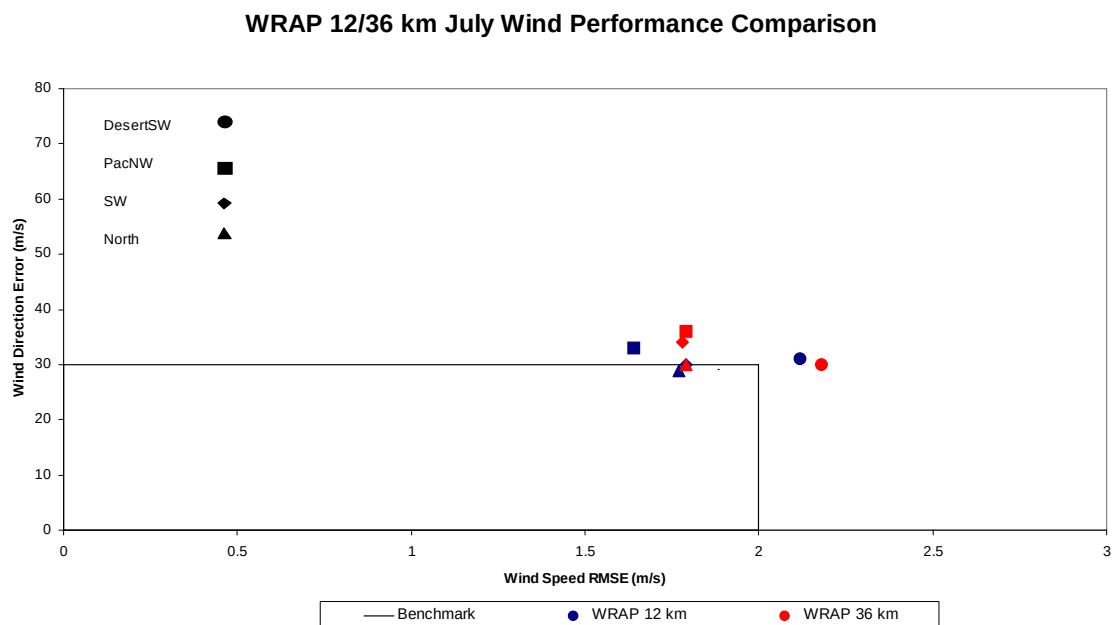


Figure 4-29. 12/36-km surface wind performance soccer plot for July for the WRAP region.

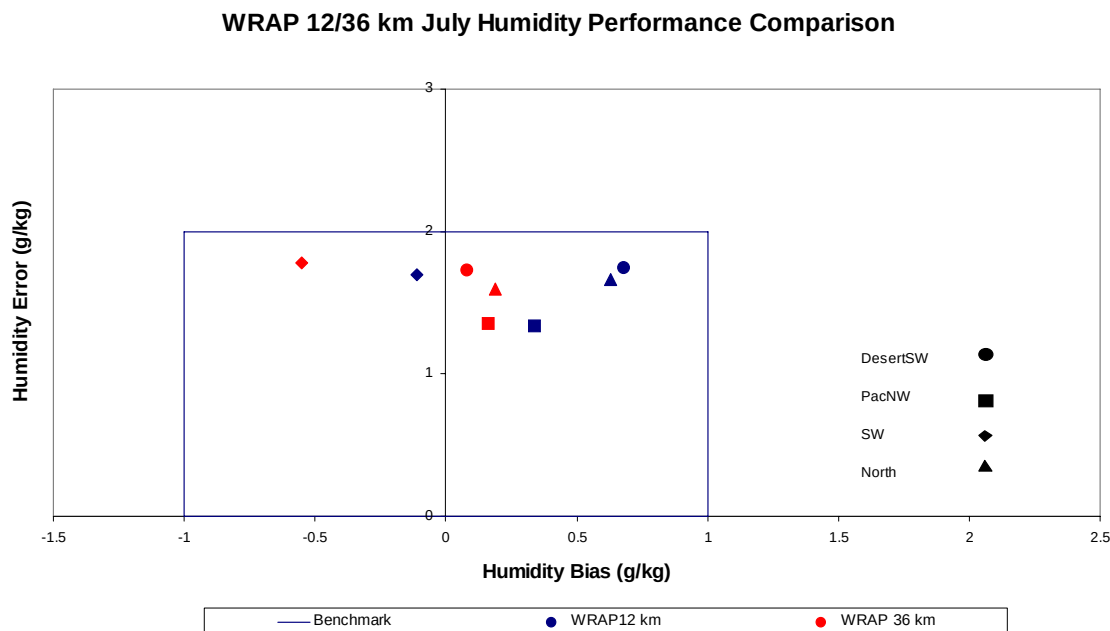


Figure 4-30. 12/36-km surface humidity performance soccer plot for July for the WRAP region.

We summarize the results of the 12-km analysis below:

- January: For temperature (Figure 4-25), all subdomains fall outside the benchmark for both the 36-km and 12-km runs. For the North, SW, and DesertSW subdomains, the 12-km run offers a small improvement in performance, but not enough to move the subdomains significantly closer to the benchmark.
- January: For all four subdomains, the 12-km wind and humidity performance (Figures 4-26 and 4-27) falls within the benchmark and is a slight improvement over the 36-km performance.
- July: The soccer plot for temperature (Figure 4-28) shows that the bias for the PacificNW, North, and DesertSW subdomains is now within the benchmark. Although the temperature error is not within the benchmark for these three subdomains, it has been reduced relative to the error in January. This is a significant improvement in performance relative to the WRAP_0 36-km and 12-km runs, and is a result of the new WRAP run configuration's optimization for improvement of the July humidity and temperature performance.
- July: Very small improvements are seen in the July 2002 wind speed and wind direction model performance using the 12-km over the 36-km grid (Figure 4-29).
- July: For humidity (Figure 4-30), all subdomains fall within the benchmark. This is in marked contrast to the WRAP_0 run (not shown), where a strong wet biases occurred in

the North and DesertSW subdomains due to excessive convective rainfall in those regions.

The METSTAT surface analysis shows that the 12-km run is within or near performance benchmarks for wind and humidity over the annual cycle of 2002, but the temperature results fall outside the bias benchmark. It is possible that this is due to terrain resolution effects. The new 12-km WRAP is a significant improvement in terms of its surface performance relative to the WRAP_0 12 km run.

4.7.5 12-km Precipitation Performance Evaluation

In this section, we evaluate the precipitation performance of the 2002 12-km MM5 run. The original WRAP_0 run had a strong positive precipitation bias over the WRAP region on both the 36-km and 12-km grids. In tandem with the 36-km sensitivity tests described in Kemball-Cook et al. (2004b), a second series of sensitivity tests was performed on the 12-km grid to identify a more optimal configuration for that domain. The best choice for cumulus scheme turned out to be no cumulus parameterization, as discussed in Section 2. Figures 4-31a through 4-31j show a comparison of the observed CPC precipitation and the MM5-predicted precipitation over the course of the new WRAP 2002 12-km simulation.

In January (Figures 4-31a and 4-31b), the agreement between the overall predicted and observed pattern is reasonably good. MM5 picks up the precipitation maxima over the mountain ranges in the Pacific Northwest, although rainfall amounts are too high over both ranges. There is excessive precipitation in the CenrapN and North regions, and MM5 underpredicts the rainfall over the central California coast. In March (Figure 4-31c and 4-31d), the model again overpredicts the rainfall over the mountain ranges of the Pacific Northwest. Aside from this, however, MM5 shows impressive skill.

As we move from winter to summer and convective rainfall becomes more important, MM5's forecast skill deteriorates. Figure 4-31e and Figure 4-31f show the observed and modeled precipitation for July. Although MM5 does a reasonable job with the SW and PacNW subdomains, where little or no rain falls, there is a general overprediction of rainfall. This is consistent with the wet bias seen in the surface humidity soccer plot for July (Figure 4-30) for all subdomains except SW. In general, the model does a good job with the overall precipitation pattern, but individual maxima are overpredicted. The model is running with no convective parameterization. This means that in order for convection to occur, the entire 12-km grid column must saturate and be unstable. In the real world, convective updrafts tend to be smaller than 12 km across. This may mean that it is relatively difficult for modeled convection to be initiated, and it becomes unrealistically intense when it does occur because an unphysical amount of instability has been allowed to build up in the convecting grid cell.

As fall arrives, and the partitioning of rainfall moves toward an increase in the stratiform component, MM5's performance improves. Figures 4-31g and 4-31h show the observed and modeled precipitation for October. In October, the model underestimates precipitation in the banded features over the CenrapS region, but otherwise agrees reasonably well with observations.

MM5's December performance (Figures 4-31i and 4-31j) is similar to that of January. The model simulates the overall pattern of precipitation over the Pacific Northwest, but overestimates the intensity of the maxima. As in January, precipitation over the North and CenrapN sub-domains is overestimated. Otherwise, the model does a good job of simulating the December precipitation field.

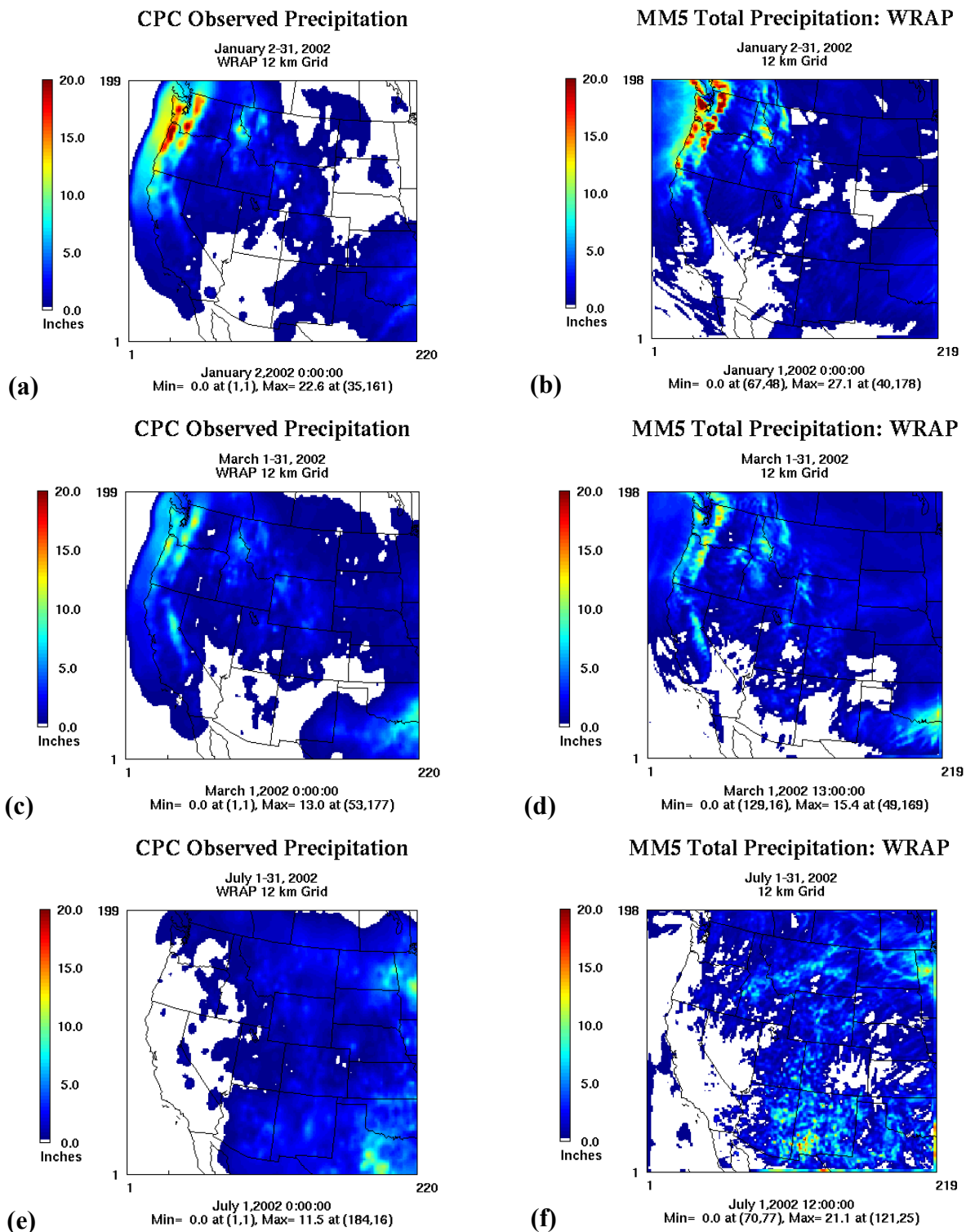


Figure 4-31. Annual cycle in 12-km MM5 precipitation. (a) January CPC observed precipitation. (b) January MM5 predicted total precipitation. (c) March CPC observed precipitation. (d) March MM5 predicted total precipitation. (e) July CPC observed precipitation. (f) July MM5 predicted total precipitation. (figure continued on next page)

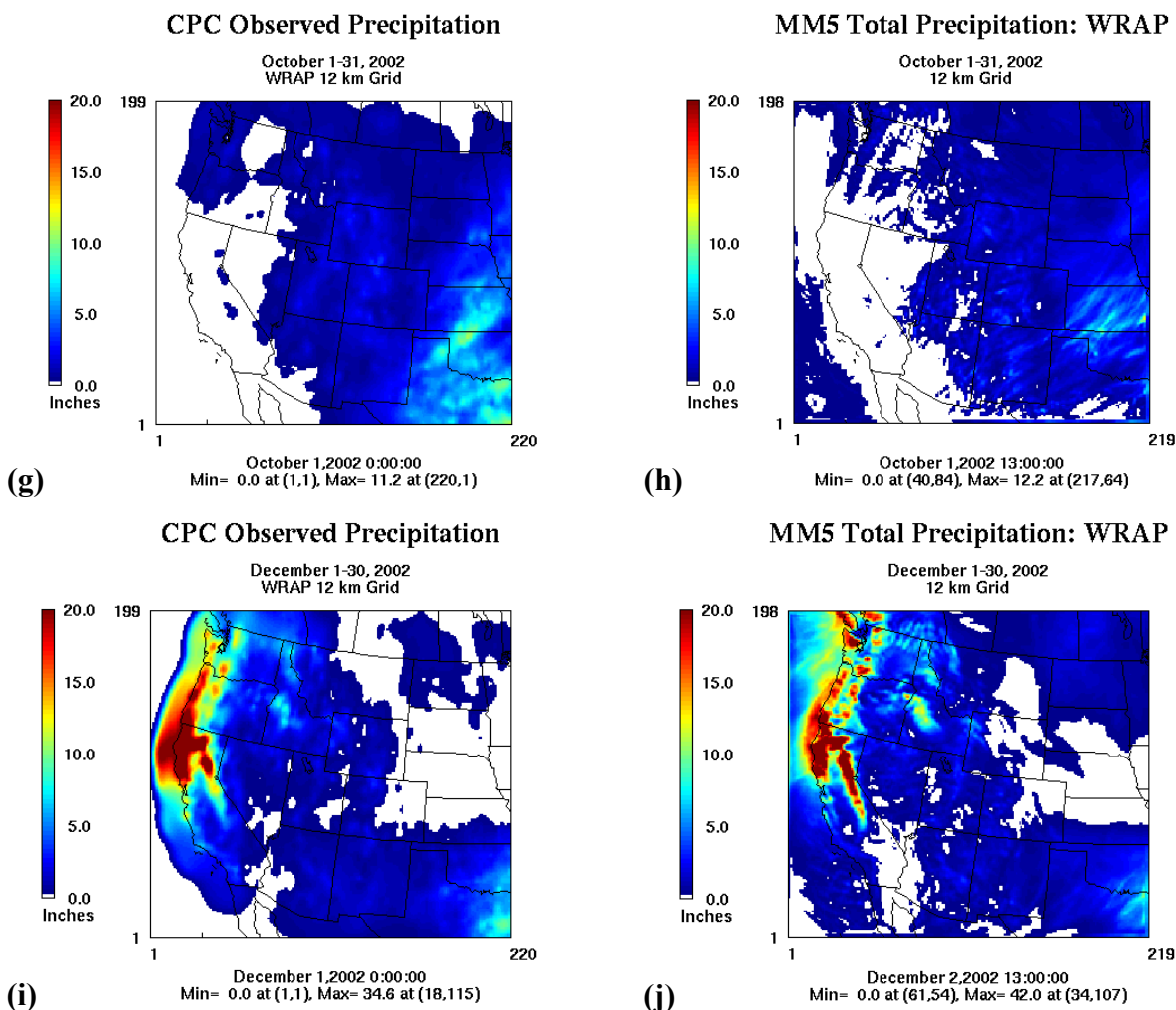


Figure 4-31 (cont'd.). Annual cycle in 12-km MM5 precipitation. (g) October CPC observed precipitation. (h) October MM5 predicted total precipitation. (i) December CPC observed precipitation. (j) December MM5 predicted total precipitation.

In summary, MM5 predicts the precipitation on the 12-km grid with reasonable skill over most of the annual cycle. The performance is better in winter than in summer. Throughout the year, the model tends to overpredict precipitation maxima, but does a good job of simulating the overall precipitation pattern. The new WRAP run exhibits better skill than the WRAP_0 run, particularly in July. The modeled rainfall is still excessive in July, but the severity of the over-prediction and the corresponding biases in July surface temperature and humidity have lessened.

4.8 Summary

In this task, we conducted a series of sensitivity tests and arrived at a revised 36-km MM5 configuration that resulted in significant improvements in the precipitation, temperature, humidity, and wind fields, all of which are likely to help produce more accurate CMAQ results. At both

12-km and 36-km resolutions, the new WRAP 2002 MM5 simulation produced results that are generally within the range of meteorological model results that have been used in the past for air quality applications. The new 36-km and 12-km runs represent a significant improvement in performance over the original WRAP_0 run. They show an improvement in the modeled precipitation fields, particularly in the summer in the Southwest. With a reduction in the overprediction of summer convective rainfall in both the 36- and 12-km runs, wet biases in the surface humidity and cold biases in the surface temperature have been reduced in the North and DesertSW subdomains in the summer months. Although the new WRAP run was optimized for summer performance over the WRAP region, the winter performance in the west did not deteriorate significantly. There was a loss of accuracy, particularly in temperature and humidity in the east, but this region is not the focus of WRAP. To summarize, the new WRAP 36/12-km run:

- Saw its surface wind performance improve significantly throughout the year relative to the WRAP_0 run due to observational nudging of surface winds.
- Showed significant improvement in summer rainfall and surface humidity performance relative to the WRAP_0 run in the WRAP region.
- Did worse than the original WRAP run for humidity performance in the east (at 36-km resolution). We can attribute both of these changes in performance to a reduction in the areal coverage in rainfall and an increase in convective rainfall in active cells (and therefore surface moisture) that occur when going from the KF scheme to the Betts-Miller scheme.
- Showed improved temperature performance in summer in the west, and slightly worse performance in winter relative to the WRAP_0 run.
- Showed a small overall degradation in performance in the east. Some of this was the result of eliminating the surface analysis nudging of temperature and moisture that was done in WRAP_0.

Our comparison of the two 36-km WRAP runs (WRAP_0 and new WRAP) to the CENRAP and VISTAS 36-km continental-scale annual runs showed:

- Overall, VISTAS performed best in the simulation of surface temperature and humidity. It had no outliers and no serious performance problems at any particular time or sub-domain. It is unclear whether this is due to the explicit moisture physics or convection schemes or to the interaction between them, or to effects of differences in FDDA.
- The new WRAP run performed best for surface winds throughout the year.
- For precipitation, the four runs were similar in terms of performance if the whole 36-km domain and the entire year were considered. Over the WRAP region, however, the new WRAP run performed best, with the smallest overprediction of convective rain of all runs. The overprediction of convective precipitation was most severe in the WRAP_0 run.
- For upper-air structure, CENRAP and VISTAS performed best and were similar to one another. We attribute this to the use of the Reisner 2 scheme, as the simulation of, for

example, the PBL inversion was relatively insensitive to the change of convection scheme in the WRAP runs.

- In all four 36-km runs, MM5 performed better in winter than in summer.
- Although WRAP_0 had the best surface statistics for temperature, its upper-air performance was worst of all four runs, which suggests that analysis nudging of surface temperature and humidity is counterproductive. The new WRAP run, which did not have analysis nudging of surface temperature and humidity, had larger errors in its temperature structure in the lowest levels of the atmosphere, but had a more realistic dew point profile and a smaller surface pressure bias than any of the four runs.

Based on the upper-air soundings, the most serious problem is the difficulty MM5 has in establishing the observed PBL structure. MM5 has trouble getting the PBL depth right, particularly in the stable nocturnal case. Also, the model's difficulty in simulating the observed fine structure of the dew point temperature profile and the overall level of saturation in the lower troposphere is cause for concern. It is important that the model produce cloud decks at the correct height. Errors in humidity and cloud prediction will have a negative impact on the accuracy of downwelling solar radiation, cause errors in the temperature profile and the surface fluxes, affecting chemistry, and making it difficult for the PM model to perform properly.

We conclude, based on the results of this study, that the 36-km and 12-km WRAP MM5 runs exhibit reasonably good performance and are certainly within the bounds of other meteorological databases used for prior air quality modeling efforts. It is therefore reasonable to proceed with their use as inputs for future CMAQ visibility modeling. Table 4-6 shows the final MM5 configuration that produced the results that will be used as input for the regional particulate matter and visibility modeling.

Table 4-6. Final MM5 configuration for 2002 annual run for 36-km and 12-km grids.

Run ID	LSM	PBL	Cumulus	Micro-physics	Analysis FDDA		Obs FDDA
					3-D	Surface	
36-km Grid	Pleim-Xiu	ACM	Betts-Miller	Reisner 2	W/T/H	W	W
12-km Grid	Pleim-Xiu	ACM	None	Reisner 2	W/T/H	W	W

4.9 Status of Task 2 Deliverables

Table 4-7 gives the status of each Task 2 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 4-7. Status of the Task 2 deliverables.

Deliverable	Status
2002 MM5 modeling protocol	Revised December 10, 2004; see http://pah.cert.ucr.edu/aqm/308/reports/mm5/WRAP_modeling_protocol_revsd.pdf
2002 preliminary MM5 modeling report	Completed March 2004; see http://pah.cert.ucr.edu/aqm/308/reports/2002_MM5_2003WRAP.pdf
2002 MM5 modeling sensitivity report	Revised December 10, 2004; see http://pah.cert.ucr.edu/aqm/308/reports/mm5/MM5SensitivityRevRep_Dec_10_2004.pdf
Response to peer-review comments on WRAP 2002 MM5 modeling	Completed December 17, 2004; see http://pah.cert.ucr.edu/aqm/308/reports/mm5/Response_to_Comments.pdf
2002 MM5 36/12-km distribution disks	Generated January 2005
2002 MM5 36/12-km CMAQ MCIP input files	Generated January 2005
2002 MM5 36/12-km CAMx input files	Generated January 2005
2002 MM5 36/12-km final evaluation report	Completed February 28, 2005; see http://pah.cert.ucr.edu/aqm/308/mm5_reports04.shtml

5. Task 3: 2002 Base Year Emissions Modeling, Processing, and Analysis

5.1 Introduction

From March 1, 2004, through February 28, 2005 (referred to in this report as project year 2004), the RMC emissions modeling efforts focused on (1) improving the emissions modeling infrastructure at the RMC; (2) developing a preliminary annual 2002 base case emissions simulation over the RPO Unified Continental 36-km Modeling Grid domain; (3) developing and evaluating emissions on the WRAP nested 12-km-resolution modeling domain; and (4) simulating various emissions perturbations for CMAQ sensitivity simulations. The RMC performed most of this emissions modeling with SMOKE version 2.0 (CEP, 2003). UCR and ENVIRON continued work begun in 2003 on the development of stand-alone emissions models for fugitive windblown dust (Mansell et al., 2004a) and agricultural ammonia emissions (Mansell, 2004a), respectively, providing emissions from these models to be merged with the emissions generated by SMOKE. UNC-CEP and UCR conducted all of the SMOKE modeling and quality assurance (QA), emissions modeling quality control (QC), and documentation.

During the first quarter of 2004, we finished implementing a comprehensive QA/QC protocol for emissions modeling to ensure that all RMC emissions modeling is well-documented, reproducible, and free of avoidable errors, such as double-counted or mistakenly dropped emissions data (Adelman, 2004). In January 2004, we completed a preliminary 36-km emissions simulation with SMOKE for January and July 2002 as a test of the emissions modeling protocol and new versions of the SMOKE scripts; this is referred to as preliminary 2002 simulation case A, or Pre02a_36 (Adelman and Omary, 2004). This simulation served as a prototype for emissions simulation Pre02b_36 (Holland and Adelman, 2004), the first annual CMAQ-ready emissions simulation for 2002 conducted by the RMC. With the delivery of 2002 WRAP fire emissions inventories by Air Sciences Inc. for prescribed fires and wildfires in April 2004, we created emissions simulation Pre02c_36 (Adelman and Holland, 2004) by merging these fire data with the typical-year agricultural fire emissions (version July 31, 2002) and emissions simulation Pre02b_36. In the fall of 2004, actual 2002 inventories for the WRAP, VISTAS, and Central Regional Air Planning Association (CENRAP) RPOs became available, along with revised prescribed and wildfire inventories for the WRAP states, a 2000 Canadian inventory, and results from the windblown dust and agricultural NH₃ emissions models mentioned above. The RMC combined these major data updates with other minor modifications to create the final preliminary 36-km 2002 simulation, Pre02d_36. After the annual 2002 meteorology data for the WRAP 12-km modeling domain became available in January 2005, we were able to complete the annual preliminary 12-km 2002 simulation, Pre02d_12, in February as the final simulation of project year 2004. Technical details, problems encountered and their resolutions, QA products, and qualitative summaries for emissions simulations Pre02a_36, Pre02b_36, and Pre02c_36 are available in the respective technical reports just cited. The same kinds of information for emissions simulations Pre02d_36 and Pre02d_12 are available later in this section.

Along with developing the above preliminary versions of the 2002 annual base case emissions simulation, we also created test emissions on the WRAP nested 12-km modeling domain (Pre02c_12), preliminary plume-in-grid (PinG) emissions for the top NO_x and SO₂ sources in the WRAP region (Pre02c_PinG), two one-month emission control scenarios for the nonroad diesel retrofit program (Pre02c_36s01), and two sensitivity simulations for testing the effects of natural versus anthropogenic fire emissions (Pre02e_36 and Pre02f_36). In addition, we integrated numerous data updates into the WRAP modeling from March 2004 through February 2005. Figure 5-1 is a timeline of all of the emissions simulations completed during project year 2004.

Simulation ID	11/03	12/03	1/04	2/04	3/04	4/04	5/04	6/04	7/04	8/04	9/04	10/04	11/04	12/04	1/05	2/05
Pre02a_36																
Pre02b_36																
Pre02c_36																
Pre02c_12																
Pre02c_PinG																
Pre02c_36s01																
Pre02e_36																
Pre02f_36																
Pre02d_36																
Pre02d_12																

Figure 5-1. Project year 2004 emissions processing schedule.

Table 5-1 lists the major emissions processing tasks we completed from March 2004 through February 2005 and indicates how they fit into the WRAP RMC 2004 work plan.

Table 5-1. Major emissions modeling tasks completed in project year 2004.

Simulation ID	Work Plan Task #	Completion Date	Description
Pre02a_36	3-1	01/2004	Winter/summer 2002 test 36-km simulation
Pre02b_36	3-2	05/2004	Preliminary annual 2002 36-km simulation
Pre02c_36	3-3	06/2004	Enhancement to simulation Pre02b_36 with the addition of WRAP prescribed, agricultural, and wildfires
Pre02c_12	3-4	07/2004*	Simulation to generate CMAQ emissions for the WRAP 12-km nested domain*

Simulation ID	Work Plan Task #	Completion Date	Description
Pre02c_PinG	3-5	07/2004	Simulation to generate plume-in-grid 36-km emissions for CMAQ; a one-month (January 2002) test dataset
Pre02c_36s01	3-3	9/2004	Nonroad mobile-source diesel retrofit sensitivity 36-km simulation
Pre02e_36	3-3	9/2004	Enhancement to simulation Pre02b_36 with the addition of natural fire events only
Pre02f_36	3-3	9/2004	Enhancement to simulation Pre02b_36 with the addition of agricultural fires and revised 2002 prescribed and wildfires
Pre02d_36	3-3	1/2005	Final preliminary annual 2002 36-km simulation
Pre02d_12	3-4	2/2005	Preliminary annual 2002 12-km simulation

*Meteorology data were not yet available at the time of the simulation; only non-meteorology-dependent emissions were completed.

The rest of Section 5 summarizes the results of each emissions case and how the data progressed from one simulation to the next. We first discuss all of the emissions inventories used in developing the preliminary 2002 modeling covered in this report (Section 5.2). Section 5.3 highlights the sources of and major updates to the SMOKE ancillary data (spatial surrogates, temporal profiles, etc.) used in these emissions simulations. Section 5.4 gives details on all of the emissions modeling simulations listed in Table 5-1. Section 5.5 describes the emissions quality control system that the RMC used to document and track the different modeling tasks. Next, we provide a summary of the 2004 deliverables from the RMC emissions modeling team, including the model-ready emissions files and QA products associated with each deliverable (Section 5.6). The progress of the WRAP 2002 annual base case emissions modeling is discussed in Section 5.7, which also includes summaries of the differences and qualitative comparisons among the various preliminary 2002 emissions cases. Section 5.8 presents technical details of the emissions sensitivities built from the preliminary base case 2002 simulations. A concise summary of the problems encountered in the 2002 emissions simulations and their corrections is then provided (Section 5.9), followed by a list of the outstanding issues to be addressed during the next round of modeling in 2005 (Section 5.10). Section 5.11 describes emissions data technology transfer activities that the RMC performed during this reporting period. We finish Section 5 with a discussion of the directions that we anticipate the RMC emissions modeling team will take through 2005 and into 2006 (Section 5.12).

5.2 WRAP 2002 Emissions Inventories

From December 2003 to December 2004, we built the 2002 WRAP emissions inventory database for the preliminary 2002 modeling with data from various inventory development contractors that are used by the WRAP Air Quality Modeling Forum and by other RPOs, the U.S. EPA, and Environment Canada. This section presents details about the inventories received, including the sources and formats of the files, how we applied them, and any problems we addressed or

modifications we made to integrate them into the preliminary 2002 modeling. While some of the information presented in this section is redundant of similar text in the final reports for simulations Pre02a_36, Pre02b_36, and Pre02c_36, we have included it because the purpose of this section is to present a unified summary of all of the emissions inventories we modeled from March 2004 through February 2005. Simulation Pre02c_36 was the last simulation we completed that used “placeholder” U.S. 2002 inventories; all of the non-WRAP U.S. inventories in simulation Pre02c_36 were either U.S. 1999 National Emissions Inventory (NEI99) or NEI96 inventories that the RMC grew to 2002 using U.S. EPA projection factors. For additional details about all of the emissions inventories used through simulation Pre02c_36, please refer to the final reports for the specific simulation. For simulation Pre02d_36, we transitioned to using actual 2002 inventories either developed explicitly for the RPOs or provided by the U.S. EPA as the preliminary NEI2002. The final inventory updates in project year 2004 occurred for simulation Pre02d_36. All subsequent simulations were either fire sensitivities based on simulation Pre02b_36 (Pre02e_36 and Pre02f_36) or a nested simulation (Pre02d_12) and did not integrate any new inventory data. In lieu of individual final reports for simulations Pre02d_36, Pre02e_36, Pre02f_36, and Pre02d_12, we are documenting these simulations collectively in this project report. The inventories used for Pre02d_36 represent the last set of inventory files received in 2004; the documentation for these data and the simulations that used them is included in this report.

Table A-1 in Appendix A gives details about the inventory files received after the completion of simulation Pre02c_36, which represent the final set of 2002 inventories used during project year 2004. The information in Table A-1 includes exact emissions inventory file names, the source agency of the files with the delivery date to the RMC, the number of records in the files, the spatial and temporal coverage of the files, and the pollutants contained in the files. The inventory files used in the Pre02d_36, Pre02e_36, Pre02f_36, and Pre02d_12 modeling are a combination of files created by WRAP inventory contractors, files created by contractors for other RPOs, the NEI2002 provided by the U.S. EPA, and inventories supplied by the U.S. EPA in cooperation with Environment Canada and the Mexican government. The files prepared for the WRAP, VISTAS, and CENRAP are actual 2002 inventories for each respective region, and the NEI2002 covers the areas of the U.S. domain not included in the RPO inventories. The Canadian data are a preliminary 2000 province-level inventory distributed by the U.S. EPA, and the Mexican data are the same 1999 dataset that the WRAP RMC used throughout all of the preliminary 2002 modeling. Additional details about these data are provided in Sections 5.2.1 through 5.2.11. First, we provide brief background information on the primary emissions categories used in SMOKE modeling.

Emissions inventories are typically divided into area, mobile, point, and biogenic source categories. These divisions stem from differing methods for preparing the inventories, different characteristics and attributes of the categories, and how the emissions are processed through models. Generally, emissions inventories are divided into the following source categories, which we refer to later in the section as “SMOKE processing categories.”

- *Stationary area:* Sources that are treated as being spread over a spatial extent (usually a county or air district) and that are not movable (as compared to nonroad mobile and on-road mobile sources). Because it is not possible to collect the emissions at each point of emission, they are estimated over larger regions. Examples of stationary area sources are

residential heating and architectural coatings. Numerous sources, such as dry cleaning facilities, may be treated either as stationary area sources or as point sources.

- *Mobile sources:* Vehicular sources that travel on roadways. These sources can be computed either as being spread over a spatial extent or as being assigned to a line location (called a link). Data in on-road inventories can be either emissions or activity data. Activity data consist of vehicle miles traveled (VMT) and, optionally, vehicle speed. Activity data are used when SMOKE will be computing emission factors via another model, such as MOBILE6. Examples of on-road mobile sources include light-duty gasoline vehicles and heavy-duty diesel vehicles.
- *Point sources:* These are sources that are identified by point locations, typically because they are regulated and their locations are available in regulatory reports. Point sources are often further subdivided into electric generating utilities (EGUs) and non-EGU sources, particularly in criteria inventories in which EGUs are a primary source of NO_x and SO₂. Examples of non-EGU point sources include chemical manufacturers and furniture refinishers. Point sources are included in both criteria and toxics inventories.
- *Biogenic land use data:* Biogenic land use data characterize the types of vegetation that exist in either county-total or grid cell values. The biogenic land use data in North America are available using two different sets of land use categories: the Biogenic Emissions Landcover Database (BELD) version 2 (BELD2), and the BELD version 3 (BELD3) (CEP, 2004b).

To initiate the preliminary 2002 modeling, we refined the emissions source categories from the standard definitions listed above to include more explicit emissions sectors. The advantage of using more detailed definitions of the source categories is that it leads to more flexibility in designing control strategies, substituting new inventory or profile data into the modeling, and managing the input and output data from SMOKE. The major drawback to defining more emissions source categories is the increased level of complexity that results from having a larger number of input datasets. Table 5-2 summarizes the entire group of source sectors that composed each of the major emissions simulations completed for the preliminary 2002 WRAP emissions modeling. The rest of Section 5.2 describes all of these various emissions sectors in detail. Each of the emissions sectors is described in terms of the SMOKE processing category, the year covered by the inventory, and the source(s) of the data. Additional details about the inventories are also provided, including any modifications that we made to prepare them for input into SMOKE.

Table 5-2. Emissions inventory categories included in the preliminary 2002 simulations.

Emissions Sector	Pre02a	Pre02b	Pre02c	Pre02d	Pre02e	Pre02f
Stationary Area	✓	✓	✓	✓	✓	✓
Road Dust	✓	✓	✓	✓	✓	✓
Windblown Dust				✓		
Fugitive Dust	✓	✓	✓	✓*	✓	✓
Agricultural and Natural NH ₃	✓	✓	✓	✓*	✓	✓

Emissions Sector	Pre02a	Pre02b	Pre02c	Pre02d	Pre02e	Pre02f
On-road Mobile	✓	✓	✓	✓	✓	✓
Nonroad Mobile	✓	✓	✓	✓	✓	✓
Offshore Mobile				✓		
Offshore Point	✓	✓	✓	✓	✓	✓
Stationary Point	✓	✓	✓	✓	✓	✓
WRAP Agricultural Fires	✓		✓	✓		✓
WRAP Prescribed (Rx) Fires			✓			
WRAP Anthropogenic Rx Fires				✓		✓
WRAP Natural Rx Fires				✓	✓	✓
WRAP Wildfires			✓	✓	✓	✓
VISTAS Fires				✓		
Biogenic	✓	✓	✓	✓	✓	✓

*These sources are represented explicitly as separate categories in simulation Pre02d.

5.2.1 Stationary area sources

We initialized the preliminary 2002 stationary-area-source emissions modeling up through simulation Pre02c_36 by combining an inventory developed by E.H. Pechan and Associates specifically for the WRAP modeling with the NEI96 (U.S. EPA, 2003a) “grown” to 2002 by the RMC. The annual WRAP inventory represented actual 2002 emissions and contained data for both the WRAP and CENRAP states (Pechan, 2003). To cover the rest of the U.S., we grew the NEI96 inventory to 2002 using Economic Growth Analysis System (EGAS) 4.0 growth factors (Pechan, 2001). We used the EPA 1995 Clear Skies inventory for Canada (U.S. EPA., 2003b) and the 1999 Big Bend Regional Aerosol and Visibility Observational Study (BRAVO) inventory for Mexico (Kuhns et al., 2003) to cover the non-U.S. inventories. In September and November 2004, we made the final round of inventory updates for the year, resulting in simulations Pre02d_36 and Pre02d_12. Starting in September, we created simulation Pre02d_36 by replacing the grown NEI96 data with updated inventories that Alpine Geophysics began distributing in May 2004: an actual 2002 area-source inventory for the VISTAS region (Alpine, 2004), the preliminary NEI2002 inventory for the rest of the U.S. (U.S. EPA, 2004b), and area-source fire data for the CENRAP and VISTAS states (Alpine, 2004). In November the U.S. EPA posted a preliminary 2000 area-source inventory for Canada through the Emissions Factors and Inventory Group (EFIG) web site (U.S. EPA, 2004c). We replaced the Canadian area-source inventories with these new data as the final area-source inventory update for simulation Pre02d. Table 5-3 summarizes the U.S. stationary-area-source inventories used for all simulations in the preliminary 2002 modeling. The highlighted cells in the table illustrate the major inventory update just described that occurred during the preliminary 2002 modeling for simulations Pre02d_36 and Pre02d_12.

Table 5-3. Preliminary 2002 stationary-area-source emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Stationary area Inventory Years: 2002 (U.S.), 1995 or 2000 (Canada), 1999 (Mexico) Temporal Coverage: Annual Pollutants: VOC, NO _x , CO, SO ₂ , PM ₁₀ , PM _{2.5} , NH ₃							
Simulation	WRAP	CENRAP	MRPO*	VISTAS	MANE-VU*	Mexico	Canada
Pre02a_36	Pechan, 2003	Pechan, 2003	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02b_36	Pechan, 2003	Pechan, 2003	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02c_36/12	Pechan, 2003	Pechan, 2003	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02c_PinG	Same as Pre02c but with top 100 NO _x and SO ₂ point sources treated with plume-in-grid						
Pre02c_36s01	Pechan, 2003	Pechan, 2003	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02d_36/12	Pechan, 2003	Pechan, 2003	U.S. EPA, 2004b	Alpine, 2004	U.S. EPA, 2004b	Kuhns et al., 2003	U.S. EPA, 2004c
Pre02e_36	Pechan, 2003	Pechan, 2003	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02f_36	Pechan, 2003	Pechan, 2003	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b

*MRPO = Midwest Regional Planning Organization; MANE-VU = Mid-Atlantic/Northeast Visibility Union

5.2.2 Road dust sources

To create the U.S. road dust emissions inventory for the preliminary 2002 modeling, we linearly interpolated between the 1996 and 2018 seasonal road dust inventories created by ENVIRON in late 2003 (Pollack et al., 2004). As a derivative of the 1996 and 2018 inventories, the 2002 road dust inventory uses the same methodology to account for the transportable fraction reductions as was used in developing the inventories for the WRAP §309 modeling performed in 2001-2003 (Pollack et al., 2004). The seasonal U.S. road dust inventory covers the entire country and includes PM_{2.5} and PM₁₀ emissions for both paved and unpaved roads. We extracted the source classification codes (SCCs) for paved and unpaved road dust emissions (2294000000 and 2296000000) from the Canada and Mexico area-source inventories to create separate road dust inventories for these sections of the modeling domain. Table 5-4 summarizes the road dust inventories used for the preliminary 2002 modeling. The road dust inventories did not change throughout all of the preliminary 2002 WRAP modeling.

Table 5-4. Preliminary 2002 road dust emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Stationary area Inventory Year: 2002 (US), 1995 (Canada), 1999 (Mexico) Temporal Coverage: Seasonal (U.S.), annual (Canada, Mexico) Pollutants: PM ₁₀ , PM _{2.5}							
Simulation	WRAP	CENRAP	MRPO	VISTAS	MANE-VU	Mexico	Canada
All Simulations	Pollack et al., 2004	Pollack et al., 2004	Pollack et al., 2004	Pollack et al., 2004	Pollack et al., 2004	Kuhns et al., 2003	U.S. EPA, 2003b

5.2.3 Windblown dust

Pre02d_36 was the first preliminary 2002 simulation completed by the RMC that contained emissions from the WRAP windblown dust model (Mansell, 2004a). Refer to Section 10 of this report for the technical details of the windblown dust emissions used in simulations Pre02d_36 and Pre02d_12.

5.2.4 Anthropogenic fugitive dust sources

For all of the preliminary 2002 simulations before Pre02d_36 and Pre02d_12, anthropogenic fugitive dust (referred to herein as just “fugitive dust”) emissions were included in the area-source inventory; they did not have transport fractions (which indicate the portion that is transported out of a source area) applied to them. To create the fugitive dust inventory for the Pre02d modeling, we removed the area sources represented by the SCCs in Table 5-5 and replaced them with data from the U.S. inventory prepared by Alpine Geophysics for VISTAS modeling (Alpine, 2004). The VISTAS inventory uses county-based transport fractions based on county land cover data. For Canada, we extracted the SCCs listed in Table 5-5 from the 2000 Canadian inventory (U.S. EPA, 2004c) for use in simulations Pre02d_36 and Pre02d_12. There are no fugitive dust emissions in the BRAVO 1999 inventory for Mexico. Table 5-6 summarizes the fugitive dust inventories used for the preliminary 2002 modeling. The highlighted cells in the table indicate the major inventory update that occurred during the preliminary 2002 modeling for simulations Pre02d_36 and Pre02d_12.

Table 5-5. SCCs removed from the area-source inventories and replaced with VISTAS or Canadian inventory data to represent explicit fugitive dust emissions.

SCC	Description	Canada*
2275085000	Aircraft;Unpaved Airstrips;Total	N
2311010000	Construction:General Building Construction;Total	Y
2311010070	Construction:General Building Construction;Vehicle Traffic	N
2311020000	Construction:Heavy Construction;Total	Y
2311030000	Construction: Road Construction;Total	Y
2325000000	Mining and Quarrying: All Processes;Total	Y

2801000003	Agriculture Production - Crops;Agriculture - Crops;Tilling	Y
2801000005	Agriculture Production - Crops;Agriculture - Crops;Harvesting	N
2801000008	Agriculture Production - Crops;Agriculture - Crops;Transport	Y
2805001000	Agriculture Production - Livestock;Beef Cattle Feedlots;Dust Kicked-up by Hooves	Y

* Y = SCC present in Canadian inventory, N = not present.

Table 5-6. Preliminary 2002 fugitive dust emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Stationary area Inventory Year: 2002 (US), 1995 (Canada), 1999 (Mexico) Temporal Coverage: Seasonal (U.S.), annual (Canada, Mexico) Pollutants: PM ₁₀ , PM _{2.5}							
Simulation	WRAP	CENRAP	MRPO	VISTAS	MANE-VU	Mexico	Canada
Pre02a_36	in area inventory	in area inventory	in area inventory	in area inventory	in area inventory	not available	in area inventory
Pre02b_36	in area inventory	in area inventory	in area inventory	in area inventory	in area inventory	not available	in area inventory
Pre02c_36/12	in area inventory	in area inventory	in area inventory	in area inventory	in area inventory	not available	in area inventory
Pre02c_PinG	Same as Pre02c but with top 100 NO _x and SO ₂ point sources treated with plume-in-grid						
Pre02c_36s01	in area inventory	in area inventory	in area inventory	in area inventory	in area inventory	not available	in area inventory
Pre02d_36/12	Alpine, 2004	Alpine, 2004	Alpine, 2004	Alpine, 2004	Alpine, 2004	not available	U.S. EPA, 2004c
Pre02e_36	in area inventory	in area inventory	in area inventory	in area inventory	in area inventory	not available	in area inventory
Pre02f_36	in area inventory	in area inventory	in area inventory	in area inventory	in area inventory	not available	in area inventory

5.2.5 Agricultural NH₃ sources

Pre02d_36 was the first preliminary 2002 simulation completed by the RMC that contained explicit emissions from the WRAP agricultural NH₃ emissions model (Mansell, 2004b). Refer to Section 2 of this report for the technical details of the model used to prepare NH₃ emissions for simulations Pre02d_36 and Pre02d_12. To limit redundancy in the emissions modeling, we removed several SCCs from the U.S. area-source inventory that were represented explicitly in the NH₃ emissions model. As only U.S. emissions are represented by the NH₃ model, we retained these SCCs in the area-source inventories for Mexico and Canada. Table B-1 in

Appendix B lists the SCCs and descriptions of the agricultural NH₃ emissions sources that we removed from the U.S. area-source inventory.

5.2.6 On-road mobile sources

To model the U.S. on-road mobile sources for all preliminary 2002 simulations except Pre02d_36 and Pre02d_12, we combined precomputed mobile-source emissions with mobile-source activity data from the NEI99 (U.S. EPA, 2004a). ENVIRON created SMOKE emissions inputs for the WRAP states by running stand-alone versions of MOBILE6 and PART5 (Pollack et al., 2004). These seasonal 2003 inventories treated California separately from the rest of the WRAP region because of state-specific controls and technologies for on-road mobile sources that apply only to California. For both the California and “Other-WRAP” inventories, these files contain prespecified PM_{2.5} inventories in addition to the gas-phase pollutants and PM₁₀ (particulate matter ≤10 µm in diameter). Because these inventories contain precomputed emissions (daily emissions by source by county), we modeled them as area sources. We modeled the rest of the U.S. as mobile sources with MOBILE6 in SMOKE using activity data from the annual NEI99. We used the EPA 1995 Clear Skies on-road mobile inventory for Canada (U.S. EPA., 2003b) and the BRAVO 1999 on-road mobile inventory for Mexico (Kuhns et al., 2003) to cover the non-U.S. inventories. For simulations Pre02d_36 and Pre02d_12 we replaced the non-WRAP U.S. activities with the preliminary NEI2002 (U.S. EPA, 2004b), and the Canadian inventory with the 2000 inventory that became available in November 2004 (U.S. EPA, 2004c). Table 5-7 summarizes the U.S. on-road mobile-source inventories that we used for all simulations in the preliminary 2002 modeling. The highlighted cells in the table illustrate the major inventory update that occurred for simulations Pre02d_36 and Pre02d_12.

Table 5-7. Preliminary 2002 on-road mobile-source emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Stationary area (WRAP, Canada, Mexico), mobile (rest of U.S.) Inventory Year: 2003 (WRAP), 2002 (rest of U.S.), 1995 or 2000 (Canada), 1999 (Mexico) Temporal Coverage: Seasonal (WRAP), annual (rest of U.S., Canada, Mexico) Pollutants: VOC, NO _x , CO, NH ₃ , SO ₂ , SO _{4 2.5} , PMC_PRE, EC _{2.5} , OC _{2.5} , OTHER _{2.5} , VMT, speed							
Simulation	WRAP	CENRAP	MRPO	VISTAS	MANE-VU	Mexico	Canada
Pre02a_36	Pollack et al., 2004	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02b_36	Pollack et al., 2004	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02c_36/12	Pollack et al., 2004	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02c_PinG	Same as Pre02c but with top 100 NO _x and SO ₂ point sources treated with plume-in-grid						
Pre02c_36s01	Pollack et al., 2004	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02d_36/12	Pollack et al., 2004	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	Kuhns et al., 2003	U.S. EPA, 2004c

SMOKE Processing Category: Stationary area (WRAP, Canada, Mexico), mobile (rest of U.S.) Inventory Year: 2003 (WRAP), 2002 (rest of U.S.), 1995 or 2000 (Canada), 1999 (Mexico) Temporal Coverage: Seasonal (WRAP), annual (rest of U.S., Canada, Mexico) Pollutants: VOC, NO _x , CO, NH ₃ , SO ₂ , SO _{4_2.5} , PMC_PRE, EC _{2.5} , OC _{2.5} , OTHER _{2.5} , VMT, speed							
Simulation	WRAP	CENRAP	MRPO	VISTAS	MANE-VU	Mexico	Canada
Pre02e_36	Pollack et al., 2004	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02f_36	Pollack et al., 2004	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	U.S. EPA, 2004a	Kuhns et al., 2003	U.S. EPA, 2003b

5.2.7 Nonroad mobile sources

To create the nonroad mobile-source inventory for all preliminary 2002 simulations, the RMC combined seasonal 2003 inventories for the WRAP states with the U.S. NEI, the Canadian National Pollutant Release Inventory, and data extracted from the Mexico area-source inventory. For modeling the WRAP region, we used an inventory developed by ENVIRON. Using NONROAD2003, ENVIRON created seasonal emissions inventories for the WRAP states only (Pollack et al., 2004). Like the on-road mobile-source emissions, the WRAP nonroad mobile-source inventories contain prespecified PM_{2.5} inventories in addition to the gas-phase pollutants and PM₁₀. For the simulations up through Pre02c_36, to model the rest of the U.S. we grew the NEI96 inventory (U.S. EPA., 2003a) to 2002 using EGAS 4.0 growth factors. We used the EPA 1995 Clear Skies on-road mobile-source data for Canada (U.S. EPA., 2003b) and the BRAVO 1999 on-road mobile inventory for Mexico (Kuhns et al., 2003) to cover the non-U.S. inventories. For simulations Pre02d_36 and Pre02d_12 we replaced the non-WRAP U.S. inventories with the preliminary NEI2002 (U.S. EPA, 2004b) and the Canadian inventory with the updated 2000 inventory that became available in November 2004 (U.S. EPA, 2004c). Table 5-8 summarizes the U.S. nonroad mobile-source inventories that we used for all simulations in the preliminary 2002 modeling. The highlighted cells in the table illustrate the major inventory update that we performed for simulations Pre02d_36 and Pre02d_12.

Table 5-8. Preliminary 2002 nonroad mobile-source emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Stationary area Inventory Year: 2003 (WRAP), 2002 (rest of U.S.), 1995 or 2000 (Canada), 1999 (Mexico) Temporal Coverage: Seasonal (WRAP), annual (rest of U.S., Canada, Mexico) Pollutants: VOC, NO _x , CO, NH ₃ , SO ₂ , SO _{4_2.5} , PMC_PRE, EC _{2.5} , OC _{2.5} , OTHER _{2.5}							
Simulation	WRAP	CENRAP	MRPO	VISTAS	MANE-VU	Mexico	Canada
Pre02a_36	Pollack et al., 2004	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02b_36	Pollack et al., 2004	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02c_36/12	Pollack et al., 2004	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b

SMOKE Processing Category: Stationary area Inventory Year: 2003 (WRAP), 2002 (rest of U.S.), 1995 or 2000 (Canada), 1999 (Mexico) Temporal Coverage: Seasonal (WRAP), annual (rest of U.S., Canada, Mexico) Pollutants: VOC, NO _x , CO, NH ₃ , SO ₂ , SO _{4_2.5} , PMC_PRE, EC _{2.5} , OC _{2.5} , OTHER _{2.5}							
Simulation	WRAP	CENRAP	MRPO	VISTAS	MANE-VU	Mexico	Canada
Pre02c_PinG	Same as Pre02c but with top 100 NO _x and SO ₂ point sources treated with plume-in-grid						
Pre02c_36s01	Pollack et al., 2004	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02d_36/12	Pollack et al., 2004	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	Kuhns et al., 2003	U.S. EPA, 2004c
Pre02e_36	Pollack et al., 2004	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02f_36	Pollack et al., 2004	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	U.S. EPA, 2003a	Kuhns et al., 2003	U.S. EPA, 2003b

5.2.8 Stationary point sources

We initialized the preliminary 2002 stationary-point-source emissions modeling by combining an actual 2002 inventory developed by E.H. Pechan and Associates specifically for the WRAP modeling with the NEI96 grown to 2002 by the RMC. For all simulations except Pre02d_36 and Pre02d_12, we used the entire annual WRAP inventory containing data for both the WRAP and CENRAP states (Pechan, 2003), and for the rest of the U.S. we grew the NEI96 inventory (U.S. EPA, 2003a) to 2002 using EGAS 4.0 growth factors (Pechan, 2001). We used version 1 of the EPA 1995 Clear Skies inventory for Canada (U.S. EPA, 2003b) and the BRAVO 1999 inventory for Mexico (Kuhns et al., 2003) to cover the non-U.S. inventories. The major update to the stationary-point-source inventory for simulations Pre02d_36 and Pre02d_12 was replacing all of the non-WRAP U.S. inventories with NEI2002 (U.S. EPA, 2004b) data. We removed the records for the CENRAP states from the 2002 WRAP inventory generated by Pechan and replaced these data with the preliminary NEI2002. Table 5-9 summarizes the stationary-point-source inventories that we used for all simulations in the preliminary 2002 modeling. The highlighted cells in the table illustrate the major inventory update that occurred for simulations Pre02d_36 and Pre02d_12.

Table 5-9. Preliminary 2002 stationary-point-source emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Point Inventory Year: 2002 (US), 1999 (Mexico) Temporal Coverage: Annual Pollutants: VOC, NO _x , CO, SO ₂ , PM ₁₀ , PM _{2.5} , NH ₃							
Simulation	WRAP	CENRAP	MRPO	VISTAS	MANE-VU	Mexico	Canada
Pre02a_36	Pechan, 2003	Pechan, 2003	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02b_36	Pechan, 2003	Pechan, 2003	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02c_36/12	Pechan, 2003	Pechan, 2003	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02c_PinG	Same as Pre02c but with top 100 NO _x and SO ₂ point sources treated with plume-in-grid						
Pre02c_36s01	Pechan, 2003	Pechan, 2003	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02d_36/12	Pechan, 2003	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02e_36	Pechan, 2003	Pechan, 2003	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	Kuhns et al., 2003	U.S. EPA, 2003b
Pre02f_36	Pechan, 2003	Pechan, 2003	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	(U.S. EPA., 2003a)	Kuhns et al., 2003	U.S. EPA, 2003b

5.2.9 Offshore sources

5.2.9.1 Offshore point sources

The RMC combined a 1996 emissions inventory for the Gulf of Mexico with 2002 data for California to create an offshore-point-source inventory for the preliminary 2002 modeling. We obtained the Gulf of Mexico data from the EPA Clear Skies database (U.S. EPA, 2003b). The California data we extracted from a spreadsheet provided by the California Air Resources Board (CARB) (Michael Benjamin, CARB, personal communication, February 11, 2004). Table 5-10 summarizes the U.S. offshore-point-source inventories we used. The offshore-point-source inventories did not change throughout all of the preliminary 2002 WRAP modeling.

Table 5-10. Preliminary 2002 offshore-point-source emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Point		
Inventory Year: 1996 (Gulf of Mexico), 2002 (CA)		
Temporal Coverage: Annual		
Pollutants: VOC, NO _x , CO, SO ₂ , PM ₁₀ , PM _{2.5} , NH ₃		
Simulation	Gulf of Mexico	California
All simulations	US. EPA, 2003b	Michael Benjamin, CARB, personal communication, February 11, 2004

5.2.9.2 Offshore mobile sources

During the QA of simulation Pre02c, we determined that a portion of the shipping emissions in the WRAP states was not being spatially allocated correctly. SCC 2280002000 in the nonroad inventory represents both in-port and ocean-going shipping emissions (Pollack et al., 2004). The ocean-going portion of this SCC accounts for shipping traffic outside of ports and within 25 miles of landfall. The “Marine Ports” spatial surrogate that we used to spatially allocate this source placed all of the emissions in ports and did not account for the ocean-going portion of the data. To reconcile this issue, UNC-CEP and ENVIRON split out the ocean-going emissions from SCC 2280002000 to a new source that we represented by SCC 2280002001.

After this correction, the original shipping SCC represented only in-port emissions and was spatially allocated using the “Marine Ports” surrogate. The new SCC represents the ocean-going emissions and is spatially allocated with a custom spatial surrogate created by UNC-CEP especially for the WRAP modeling. We created this new surrogate (“Ocean-going Shipping”) manually using information provided by ENVIRON about the locations of the ports with emissions represented in the WRAP nonroad mobile-source inventory. We allocated the emissions to cells within 25 miles of the ports in the WRAP nonroad mobile-source inventories that contained emissions. We used the data from the summer season nonroad mobile-source inventory to represent the annual ocean-going shipping emissions. For those counties that contained shipping emissions but did not have any ports, we allocated the emissions within 25 miles of land along the entire coast of the county. We introduced the offshore-mobile-source emissions into simulations Pre02d_36 and Pre02d_12. Table 5-11 summarizes the U.S. offshore-mobile-source inventory used for these two simulations. Figure 5-2 is an example of the ocean-going shipping emissions in the WRAP region of the 36-km modeling domain.

Table 5-11. Preliminary 2002 offshore-mobile-source emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Stationary area	
Inventory Year: 2002	
Temporal Coverage: Annual	
Pollutants: VOC, NO _x , CO, SO ₂ , PM ₁₀ , PM _{2.5} , NH ₃	
Simulation	U.S. Pacific Coast
Pre02d_36/12	Pollack et al., 2004

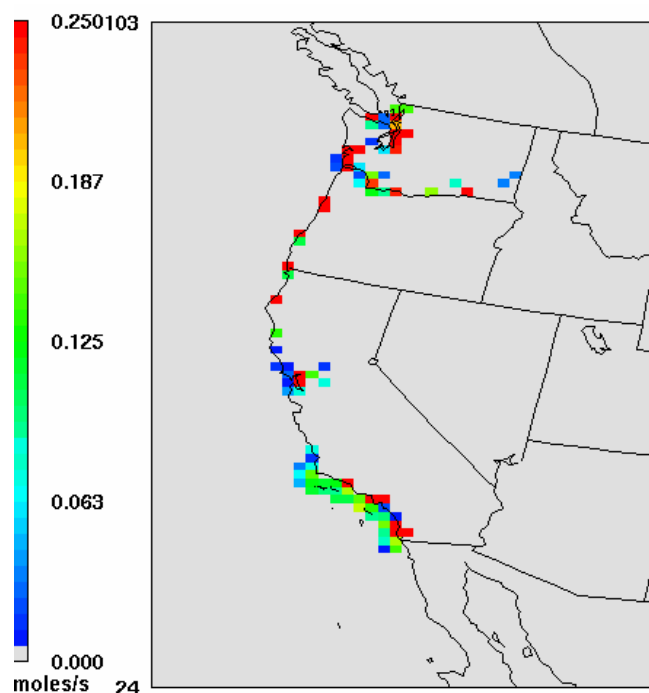


Figure 5-2. Example of WRAP ocean-going shipping CO emissions in the 36-km modeling domain.

5.2.10 Fire sources

The WRAP Fire Emissions Joint Forum (FEJF) contractors provided fire inventories as SMOKE point-source files for the 13-state WRAP region. Prior to the Pre02d_36 simulation, we modeled U.S. and Canadian fires outside of the WRAP domain in the area-source inventory; the Mexican inventories do not contain any fire data. One of the inventory updates for simulation Pre02d_36 included adding point-source fires for the VISTAS states (Alpine, 2004). The preliminary 2002 WRAP fire inventories included two separate fire categories: prescribed (“Rx”) burning, and wildfires. In September 2004 we received refined fire inventories from Air Sciences Inc. (the WRAP fire emissions inventory contractor) that split the prescribed fire inventory into natural and anthropogenic fires and included a new 2002 wildfire inventory (Randall, 2004a). All

WRAP fire inventories include daily emissions data and hourly, precomputed plume rise information. To represent agricultural burning in the preliminary 2002 modeling, we used the 2018 inventory that was originally developed during the RMC's §309 modeling and included base smoke management controls on the fire sources (Air Sciences, 2004). The 2002 prescribed and wildfire inventories were created specifically for the preliminary and final 2002 modeling (Randall, 2004a). The fire inventory contractor delivered the files as annual inventories with three files per fire category: (1) PTINV inventory files with latitude-longitude (lat-lon) locations for the fires; (2) PTDAY files with daily emissions totals for each fire; and (3) PTHOUR files with hourly plume rise characteristics that included for each fire the fraction of emissions allocated to model layer 1, the top of the plume in meters, and the bottom of the plume in meters. Additional details about each of the fire inventories used in the preliminary 2002 emissions modeling follow.

5.2.10.1 Agricultural fires

The RMC used the 2018 base smoke management agricultural burning inventory (version July 31, 2002) to represent agricultural fires in the WRAP region for the preliminary 2002 modeling. The agricultural fires are the one source that did not change throughout all of the preliminary 2002 modeling. Table 5-12 summarizes the agricultural fire inventory we used.

Table 5-12. Preliminary WRAP 2002 agricultural fire emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Point with precomputed plume rise	
Inventory Year: 2018	
Temporal Coverage: Daily emissions, hourly plume rise	
Pollutants: VOC, NO _x , CO, SO ₂ , PM ₁₀ , PM _{2.5} , NH ₃	
Simulation	Agricultural fires in the WRAP states
Pre02a_36	Air Sciences, 2004
Pre02b_36	not used
Pre02c_36/12	Air Sciences, 2004
Pre02c_PinG	Not applicable
Pre02c_36s01	Air Sciences, 2004
Pre02d_36/12	Air Sciences, 2004
Pre02e_36	not used
Pre02f_36	Air Sciences, 2004

5.2.10.2 Prescribed fires

In May 2003, Air Sciences Inc. provided actual 2002 prescribed-fire inventories for the WRAP region to include in the preliminary 2002 modeling (Randall, 2004a). After splitting the annual

inventory file into monthly files,* the RMC included these data in emissions simulation Pre02c_36. In September 2004 Air Sciences delivered to us a refined set of 2002 prescribed-fire inventories for the WRAP region that distinguished between natural prescribed fire events and anthropogenic ones (Randall, 2004b). Due to the large number of events in the natural-prescribed-fire inventory, we once again split the annual inventory into monthly files to avoid memory problems with SMOKE; the anthropogenic prescribed fires we were able to model as an annual inventory. The RMC included both of the refined prescribed-fire inventories in simulations Pre02d_36, Pre02d_12, and Pre02f_36, while in simulation Pre02e_36 we included only the natural-prescribed-fire inventory. Simulations Pre02e_36 and Pre02f_36, derived from the Pre02b_36 simulation, were designed for evaluating the effects of the new WRAP fire inventories and the effects of natural versus anthropogenic fire emissions on modeled haze in the WRAP region. To see the results of these emissions sensitivities on air quality model result, please refer to Section 12 of this report. Table 5-13 summarizes the prescribed-fire inventories that the RMC used in the different preliminary 2002 emissions simulations.

Table 5-13. Preliminary WRAP 2002 prescribed-fire emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Point with precomputed plume rise Inventory Year: 2002 Temporal Coverage: Daily emissions, hourly plume rise Pollutants: VOC, NO _x , CO, SO ₂ , PM ₁₀ , PM _{2.5} , NH ₃			
Simulation	Total Prescribed Fires in the WRAP States	Natural Prescribed Fires in the WRAP States	Anthropogenic Prescribed Fires in the WRAP States
Pre02a_36	not used	not used	not used
Pre02b_36	not used	not used	not used
Pre02c_36/12	Randall, 2004a	not uses	not used
Pre02c_PinG	Not applicable	Not applicable	Not applicable
Pre02c_36s01	Randal, 2004a	not used	not used
Pre02d_36/12	not used	Randall, 2004b	Randall, 2004b
Pre02e_36	not used	Randall, 2004b	not used
Pre02f_36	not used	Randall, 2004b	Randall, 2004b

5.2.10.3 Wildfires

In May 2004 Air Sciences Inc. provided actual 2002 wildfire inventories for the WRAP region to include in the preliminary 2002 modeling (Randall, 2004a). We included these wildfire emissions in the simulations based on the Pre02c inventories. Then in September, Air Sciences delivered a refined 2002 WRAP-region wildfire inventory to us (Randall, 2004b). We included this refined inventory in simulations Pre02d_36, Pre02d_12, Pre02e_36, and Pre02f_36. Table

* We split the files because the large number of sources in the annual inventory caused SMOKE to run out of memory.

5-14 summarizes the wildfire inventories that the RMC used in the various preliminary 2002 emissions simulations.

Table 5-14. Preliminary 2002 wildfire emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Point with precomputed plume rise	
Inventory Year: 2002	
Temporal Coverage: Daily emissions, hourly plume rise	
Pollutants: VOC, NO _x , CO, SO ₂ , PM ₁₀ , PM _{2.5} , NH ₃	
Simulation	Wildfires in the WRAP states
Pre02a_36	not used
Pre02b_36	not used
Pre02c_36/12	Randall, 2004a
Pre02c_PinG	Not applicable
Pre02c_36s01	Randall, 2004a
Pre02d_36/12	Randall, 2004b
Pre02e_36	Randall, 2004b
Pre02f_36	Randall, 2004b

5.2.10.4 Other fire sources

In the May 2004 release of VISTAS actual 2002 inventories, Alpine Geophysics provided point-source and area-source fires for the VISTAS and CENRAP regions. The RMC adopted these files for the WRAP, integrating them in the preliminary 2002 modeling starting with simulation Pre02d_36. The VISTAS fire inventories consist of both a point-source inventory for the large wildfires and an area-source inventory for the agricultural fires, solid waste burning, prescribed fires, and small wildfires. The VISTAS point-source fire inventory is structured like the WRAP point-source fire inventories, consisting of daily emissions and hourly precomputed plume rise information. The CENRAP fire inventory treats agricultural fires, prescribed fires, and wildfires, regardless of size, as stationary area sources. Other U.S. fire sources, such as municipal waste burning, yard waste burning, and structure fires, are contained in the area-source inventories for all regions of the country, including the WRAP states. Canadian fires are all contained in the area-source inventory and include agricultural fires, wildfires, municipal and residential waste burning, and structure fires. Mexican fires are also contained in the area-source inventory and include agricultural fires, municipal and residential waste burning, and structure fires. Table 5-15 summarizes the fire inventories that we used in the preliminary 2002 emissions simulations in addition to the WRAP agricultural, prescribed, and wildfire inventories discussed above.

Table 5-15. Preliminary 2002 other fire emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Point with precomputed plume rise (VISTAS); stationary area (entire domain) Inventory Year: 2002 (US), 1995/2000 (Canada), 1999 (Mexico) Temporal Coverage: Daily emissions (VISTAS), hourly plume rise (VISTAS), annual (entire domain) Pollutants: VOC, NO _x , CO, SO ₂ , PM ₁₀ , PM _{2.5} , NH ₃							
Simulation	WRAP	CENRAP	MRPO	VISTAS	MANE-VU	Mexico	Canada
Pre02a_36	Pechan, 2003	Pechan, 2003	U.S. EPA., 2003a	U.S. EPA., 2003a	U.S. EPA., 2003a	Kuhns et al., 2003	U.S. EPA., 2003b
Pre02b_36	Pechan, 2003	Pechan, 2003	U.S. EPA., 2003a	U.S. EPA., 2003a	U.S. EPA., 2003a	Kuhns et al., 2003	U.S. EPA., 2003b
Pre02c_36/12	Pechan, 2003	Pechan, 2003	U.S. EPA., 2003a	U.S. EPA., 2003a	U.S. EPA., 2003a	Kuhns et al., 2003	U.S. EPA., 2003b
Pre02c_PinG	Same as Pre02c but with top 100 NO _x and SO ₂ point sources treated with plume-in-grid						
Pre02c_36s01	Pechan, 2003	Pechan, 2003	U.S. EPA., 2003a	U.S. EPA., 2003a	U.S. EPA., 2003a	Kuhns et al., 2003	U.S. EPA., 2003b
Pre02d_36/12	Pechan, 2003	Alpine, 2004; U.S. EPA, 2003a	U.S. EPA, 2004b	Alpine, 2004	U.S. EPA, 2004b	Kuhns et al., 2003	U.S. EPA., 2004c
Pre02e_36	Pechan, 2003	Pechan, 2003	U.S. EPA., 2003a	U.S. EPA., 2003a	U.S. EPA., 2003a	Kuhns et al., 2003	U.S. EPA., 2003b
Pre02f_36	Pechan, 2003	Pechan, 2003	U.S. EPA., 2003a	U.S. EPA., 2003a	U.S. EPA., 2003a	Kuhns et al., 2003	U.S. EPA., 2003b

5.2.11 Biogenic sources

While most of the emissions inventory data came either directly from WRAP inventory contractors or from EPA, the RMC benefited from previous work done using the RPO Unified domain by acquiring gridded biogenic land use files developed by Alpine Geophysics for VISTAS modeling (Alpine, 2004). The VISTAS gridded land use data came to us in the form of binary input files for running the Biogenic Emissions Inventory System, version 3 (BEIS3) in SMOKE; they cover the entire RPO Unified domain, including Mexico and Canada. The first set of BEIS3 biogenic emission factors that we used through simulation Pre02c_36 was version 0.97 and came from EPA (2004d). Starting in simulation Pre02d_36 we used an updated set of emissions factors, version 0.98, also provided by EPA (2004d). The differences in these files relate to emissions factor changes for fir and spruce trees. Table 5-16 summarizes the biogenic emissions inputs that we used in the preliminary 2002 emissions simulations.

Table 5-16. Preliminary 2002 biogenic emissions inventory summary with references for inventories used in all simulations.

SMOKE Processing Category: Biogenic Inventory Year: 2002 Temporal Coverage: n/a Pollutants: n/a		
Simulation	Gridded Land Use	BELD Emissions Factors
Pre02a_36	Alpine, 2004	v0.97 (U.S. EPA, 2004d)
Pre02b_36	Alpine, 2004	v0.97 (U.S. EPA, 2004d)
Pre02c_36/12	Alpine, 2004	v0.97 (U.S. EPA, 2004d)
Pre02c_PinG	Not applicable	Not applicable
Pre02c_36s01	Alpine, 2004	v0.97 (U.S. EPA, 2004d)
Pre02d_36/12	Alpine, 2004	v0.98 (U.S. EPA, 2004d)
Pre02e_36	Alpine, 2004	v0.97 (U.S. EPA, 2004d)
Pre02f_36	Alpine, 2004	v0.97 (U.S. EPA, 2004d)

5.2.12 Inventories summary for the final preliminary 2002 simulations

Table 5-17 summarizes all of the inventories used in the final iterations of the preliminary 2002 WRAP modeling performed in 2004: simulations Pre02d_36 and Pre02d_12.* This table includes the inventory categories modeled, the inventories' spatial and temporal coverages, and the sources of the data. The cells in Table 5-17 provide references for the documentation for each inventory. The color codes correspond to the temporal coverages (see key at bottom of table). The spatial coverages of the inventories are provided in terms of the RPO or country represented in each inventory. The table includes inventory coverage for all five of the U.S. RPOs and for Mexico and Canada.

Table 5-17. Summary of final preliminary 2002 emissions inventories compiled during 2004 and used for simulations Pre02d_36 and Pre02d_12.

Inventory	WRAP	CENRAP	MRPO	VISTAS	MANE-VU	Mexico	Canada
Stationary area	Pechan, 2003	Pechan, 2003	U.S. EPA, 2004b	Alpine, 2004	U.S. EPA, 2004b	Kuhns et al., 2003	U.S. EPA, 2004c
Road dust	Pollack et al., 2004	Pollack et al., 2004	Pollack et al., 2004	Pollack et al., 2004	Pollack et al., 2004	Kuhns et al., 2003	U.S. EPA, 2003b
Windblown dust	Mansell, 2004a	Mansell, 2004a	Mansell, 2004a	Mansell, 2004a	Mansell, 2004a	Not available	U.S. EPA, 2004c
Fugitive dust	Alpine, 2004	Alpine, 2004	Alpine, 2004	Alpine, 2004	Alpine, 2004	Not available	U.S. EPA, 2004c

*The same kind of table for simulations Pre02a, Pre02b, and Pre02c was given in "2004 Interim Report for the Western Regional Air Partnership (WRAP) Regional Modeling Center (RMC)"; see Table 5-14 in that report.

Inventory	WRAP	CENRAP	MRPO	VISTAS	MANE-VU	Mexico	Canada
Agricultural NH ₃	Mansell, 2004b	Mansell, 2004b	Mansell, 2004b	Mansell, 2004b	Mansell, 2004b	Kuhns et al., 2003	U.S. EPA, 2004c
On-road mobile	Pollack et al., 2004	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	Kuhns et al., 2003	U.S. EPA, 2004c
On-road mobile (CA)	Pollack et al., 2004	Not applicable	Not applicable	Not applicable	Not applicable	Not applicable	Not applicable
Nonroad mobile	Pollack et al., 2004	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	Kuhns et al., 2003	U.S. EPA, 2004c
Stationary point	Pechan, 2003	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	U.S. EPA, 2004b	Kuhns et al., 2003	U.S. EPA, 2003b
Offshore point	CARB, 2004	U.S. EPA, 2003b	Not available	Not available	Not available	Not available	Not available
Offshore mobile	Pollack et al., 2004	Not available	Not available	Not available	Not available	Not available	Not available
WRAP agricultural fires	Randall, 2004b	Not applicable	Not applicable	Not applicable	Not applicable	Not applicable	Not applicable
WRAP anthropogenic Rx fires	Randall, 2004b,	Not applicable	Not applicable	Not applicable	Not applicable	Not applicable	Not applicable
WRAP natural Rx fires	Randall, 2004b	Not applicable	Not applicable	Not applicable	Not applicable	Not applicable	Not applicable
WRAP wildfires	Randall, 2004b	Not applicable	Not applicable	Not applicable	Not applicable	Not applicable	Not applicable
Other fire sources	Not applicable	Alpine, 2004; U.S. EPA, 2003a	U.S. EPA, 2004b	Alpine, 2004	U.S. EPA, 2004b	Kuhns et al., 2003	U.S. EPA, 2004c
Biogenic	Alpine, 2004	Alpine, 2004	Alpine, 2004	Alpine, 2004	Alpine, 2004	Alpine, 2004	Alpine, 2004
Annual inventory		Seasonal inventory		Daily meteorology-dependent emissions			

5.3 WRAP 2002 Ancillary Emissions Inputs

In addition to emissions inventories, SMOKE requires various kinds of supporting information, such as data that describe how to distribute the emissions in space and time, data that enable the partitioning of emitted pollutants to different chemical parameterizations, and meteorology data for modeling certain source categories. We refer to these supporting data as SMOKE ancillary inputs. Examples of other ancillary information include tables of default stationary-point-source stack parameters; numeric codes for indexing countries, states, and counties; and detailed descriptions of the modeled sources by SCC. For all ancillary information other than the meteorology data, the SMOKE directory structure stores these data in a general data directory aliased by the environment variable GE_DAT.

Except for the temporal profile/cross-reference files and the spatial surrogates/cross-reference files, all of the nonmeteorology ancillary emissions input files that we used for the preliminary 2002 modeling originated from the SMOKE version 2 distribution (sources for the temporal and spatial ancillary files are discussed below). We initiated the preliminary 2002 modeling with nonmeteorology ancillary SMOKE inputs from the §309 modeling that the RMC performed in 2002-2003. Throughout the preliminary 2002 modeling we made minor updates to these data and added new inventory-specific information as they were delivered with the new inventories. We also generated an initial set of 2002 36-km and 12-km meteorology data that we used in all of the preliminary 2002 emissions modeling to model plume rise from stationary point sources and fires, biogenic emissions, and on-road mobile activities; these data are described in detail in Section 4 of this report. The rest of Section 1.3 highlights the sources of and major updates to the SMOKE ancillary data used in the preliminary 2002 modeling and is organized by each major class of ancillary data. Tables A-2 and A-3 in Appendix A summarize the ASCII and binary ancillary input files used in the Pre02d_36 modeling. For detailed listings of the ancillary inputs used in Pre02a_36, Pre02b_36, and Pre02c_36, please refer to the final reports for those simulations.

5.3.1 Temporal allocation data

SMOKE uses temporal profiles and SCC cross-reference files to apply monthly, weekly, and daily temporal variability to annual and daily emissions inventories. Temporal profiles are a group of scalars that describe the fraction of emissions allocated to each specific temporal unit (i.e., month of the year, day of the week, or hour of the day). An accompanying temporal cross-reference file associates monthly, weekly, and diurnal profiles (indexed with a numeric code) to SCCs. Temporal profile and cross-reference files combine to form the SMOKE temporal allocation data and contain profiles for most inventory sources; for sources that do not have entries in these files, default profiles are applied. The default temporal profiles are flat—in other words, they do not vary across months, days, or hours. We initiated the preliminary 2002 emissions modeling with temporal data developed during the WRAP §309 modeling (Houyoux et al., 2003).

Throughout the preliminary 2002 modeling, the RMC integrated new inventories into the WRAP modeling that required the addition of new profiles and cross-references to the base temporal data. Adelman and Omary (2004) document the addition of temporal profiles to model the new SCCs contained in the WRAP on-road mobile-source inventory. Adelman and Holland (2004) describe the addition of diurnal profiles for the new WRAP fire sources. For the Pre02d modeling, we added month-specific stationary-point-source profiles provided by Alpine Geophysics (2004) for VISTAS modeling that are based on continuous emissions monitoring (CEM) data. We also added cross-references for the new 2002 fire SCCs that apply the fire profiles developed for modeling simulation Pre02c (Adelman and Holland, 2004). The temporal allocation data files used in the final round of preliminary 2002 36-km emissions modeling (simulation Pre02d_36) are documented in Table A-2.

5.3.2 Spatial allocation data

SMOKE uses spatial surrogates and SCC cross-reference files to allocate county-level emissions inventories to model grid cells. GIS-calculated fractional land use values define the percentage of a grid cell that is covered by standard sets of land use categories. For example, spatial surrogates can define a grid cell as being 50% urban, 10% forest, and 40% agricultural. In addition to land use categories, spatial surrogates can also be defined by demographic or industrial units, such as population or commercial area. Similar to the temporal allocation data, an accompanying spatial cross-reference file associates the spatial surrogates (indexed with a numeric code) to SCCs. The U.S. EPA distributes GIS Shapefiles, unified spatial surrogates, and spatial cross-referencing data for modeling the U.S., Canada, and Mexico. We used the unified surrogates and cross-references files to build the spatial allocation dataset used to model the preliminary 2002 emissions.

The RMC initiated the preliminary 2002 emissions modeling with spatial surrogates distributed by the U.S. EPA. Adelman and Omary (2004) describe the integration of the “old” EPA surrogates into simulation Pre02a_36, and Holland and Adelman (2004) describe the application of the same surrogates for simulation Pre02b_36. With the delivery of the VISTAS inventory and ancillary data from Alpine Geophysics in May 2004, we obtained a copy of the “new” EPA surrogates for the RPO Unified 36-km modeling domain. We transitioned to using these data in simulation Pre02c_36 (Adelman and Holland, 2004). The “new” EPA surrogates (U.S. EPA, 2004) use 65 surrogate categories as opposed to the 15 categories contained in the “old” surrogate dataset. UNC-CEP developed spatial surrogates for Canada on the RPO Unified 36-km domain and mapped the standard ESRI Shapefile codes to those contained in the EPA “new” surrogates. For modeling Mexico, we used Shapefiles developed for the BRAVO modeling to create surrogates for Mexico on the RPO Unified 36-km domain (U.S. EPA, 2004e). The Mexico surrogates use the 15 land use categories contained in the EPA “old” surrogates. For the 12-km modeling, we applied the EPA Shapefiles in the “new” surrogate database to create spatial surrogates for the WRAP 12-km modeling domain. We used the same Shapefiles for Canada and Mexico that we had applied in the 36-km modeling. A minor difference between the 36-km and 12-km modeling is that we mapped the ESRI/CIESIN Shapefile codes for Mexico to the U.S. EPA “new” surrogate codes (EPA99); Table 5-18 documents the mapping of spatial surrogate codes used by the RMC for the 12-km preliminary 2002 simulations (Pre02c_12 and Pre02d_12). The spatial allocation data files used in the final round of preliminary 2002 36-km emissions modeling (simulation Pre02d_36) are documented in Table A-2.

Table 5-18. Mapping of ESRI/CIESIN to EPA99 codes for 12-km Mexican spatial surrogates.

ESRI Code	Description	Maps to...	EPA99 Code	Description
1	Agriculture	→	310	Total agriculture
2	Airports	→	700	Airport area
3	Land area	→	340	Land
4	Housing	→	110	Housing

ESRI Code	Description	Maps to...	EPA99 Code	Description
7	Major highways	→	240	Total road miles
8	Population	→	100	Population
9	Ports	→	800	Marine ports
10	Railroads	→	260	Total railroad miles

5.3.3 Chemical speciation data

SMOKE uses chemical profiles and SCC cross-reference files to map inventory pollutants to the various chemical parameterizations required by air quality models. For the preliminary 2002 modeling, we used Carbon Bond IV gas-phase chemistry and the third-generation CMAQ aerosol model chemistry parameterizations (aero3). We modeled the emissions inventories specifically for these chemistry mechanisms, adding SCCs to the base chemical cross-reference file for new sources in the WRAP inventories. Adelman and Holland (2004) describe the addition of new VOC and PM_{2.5} profiles and cross-reference information to model the WRAP fire sources. Adelman and Omary (2004) describe the addition of chemical cross-reference codes to accommodate the new on-road mobile-source SCCs contained in the 2002 WRAP inventories. The changes that we made to the base chemical speciation data used for the preliminary 2002 modeling, which originated from the SMOKE version 2.0 distribution, were relatively minor. The chemical allocation data files used in simulation Pre02d_36 are documented in Table A-2.

5.3.4 Meteorology data

SMOKE uses meteorology data to model specific processes for stationary point sources and fires, biogenic emissions, and on-road mobile activities. The SMOKE/BEIS3.12 integration uses temperature and radiation data to calculate biogenic emissions. SMOKE uses temperature and atmospheric stability variables to calculate plume rise from point sources and the vertical layer structure of the meteorology to allocate the fire inventories with pre-computed plume rise to the appropriate model layers. The SMOKE/MOBILE6 integration uses temperatures and humidity data to adjust mobile-source emissions factors. For additional details on how hourly meteorology data are used by SMOKE, please refer to CEP (2004b). The RMC generated the meteorology data used for the 36-km and 12-km emissions modeling runs. For documentation about these data, refer to Section 4 of this report. The binary meteorology input data files used in simulation Pre02d_36 are documented in Table A-3.

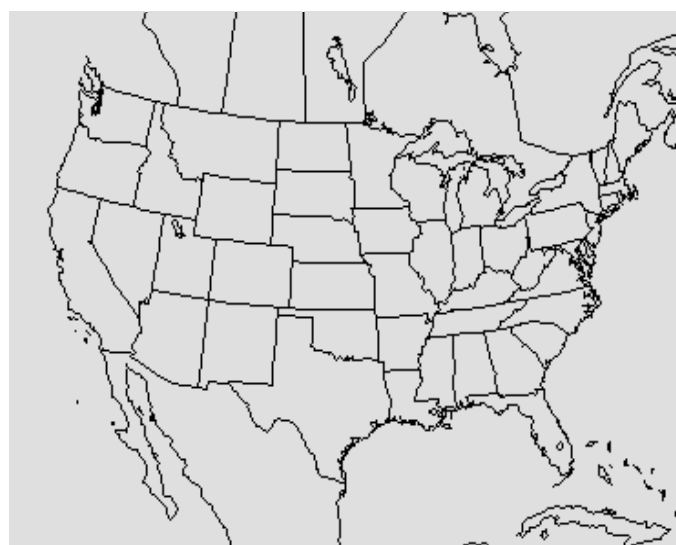
5.3.5 Other emissions input data

Table A-2 lists all of the other nonmeteorology ancillary input data used in simulation Pre02d_36. For the most part, these additional support files did not change from their original forms in the SMOKE version 2.0 distribution. We made minor modifications to these supporting

emissions input files as the preliminary 2002 emissions modeling progressed, such as adding SCC descriptions for new sources in the inventory and adding descriptions of the spatial surrogates used for the three countries in the modeling domain.

5.4 Description of FY 2004 Emissions Modeling Simulations

As discussed earlier, emissions modeling performed by the RMC in project year 2004 focused primarily on developing the WRAP 2002 base case emissions simulation. From March 2004 to February 2005, we completed four preliminary 2002 (Pre02) emissions simulations on the RPO Unified 36-km domain (Figure 5-3): Pre02a_36, Pre02b_36, Pre02c_36, and Pre02d_36. We also finished one full simulation on the WRAP 12-km domain (Figure 5-4), Pre02d_12; two fire sensitivity simulations on the 36-km domain, Pre02e_36 and Pre02f_36; and several test simulations for assessing the RMC's capabilities for performing plume-in-grid modeling (Pre02_PinG), emissions reduction sensitivities (Pre02c_36s01), and nested modeling (Pre02c_12).



Grid Specification	Value
Columns	148
Rows	112
Layers	19
X-origin	-2,736,000 m
Y-origin	-2,088,000 m
X-center	-97 degrees
Y-center	40 degrees
X-cell	36,000 m
Y-cell	36,000 m
Vertical Top	10,000 m
Vertical Layers (σ)	1.0, 0.995, 0.99, 0.985, 0.98, 0.97, 0.96, 0.95, 0.94, 0.92, 0.9, 0.88, 0.86, 0.82, 0.77, 0.7, 0.6, 0.45, 0.25, 0.0

Figure 5-3. RPO Unified Continental 36-km Modeling Grid domain.

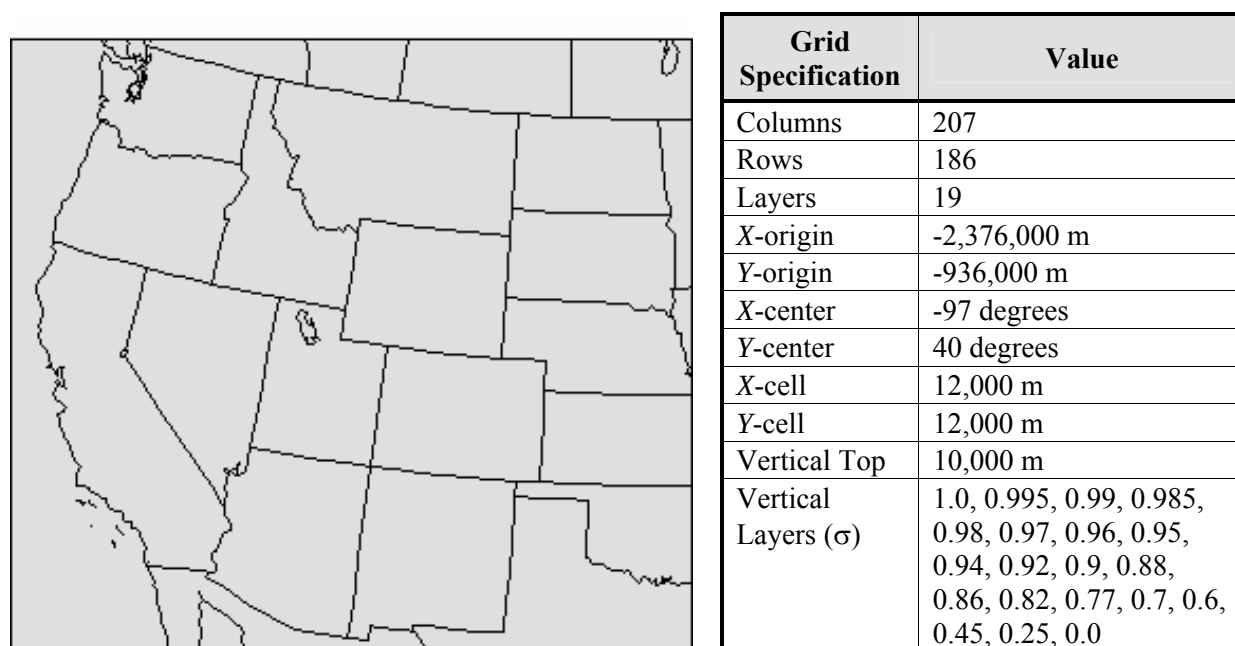


Figure 5-4. WRAP nested 12-km modeling domain.

We used these Pre02 simulations to test the SMOKE scripts, quality assure the preliminary 2002 emissions inventories generated by the WRAP Air Quality Modeling Forum inventory contractors, refine the definition of the emissions sectors, and provide preliminary results for conducting emissions sensitivity simulations with CMAQ. Table 5-1 in Section 5.1 and Table 5-2 in the introductory paragraphs of Section 5.2 summarize key information on all of the preliminary emissions simulations covered in this section.

5.4.1 Emissions simulation Pre02a_36

The RMC initiated the 2004 emissions modeling tasks by completing preliminary 2002 simulation case A (Pre02a_36). A six-month simulation of the winter (December, January, February) and summer (June, July, August) months of 2002, Pre02a_36 carried over from the 2003 WRAP RMC work plan (Tonnesen et al., 2004) and served to resolve any major problems with the emissions modeling system and with the preliminary 2002 emissions and meteorology datasets. It also acted as a test bed for the WRAP emissions modeling QA protocol (Adelman, 2004). Table 5-2 lists the emissions source categories included in simulation Pre02a_36.

With the completion of simulation Pre02a_36, we established a version control system for emissions datasets, modeling inputs, SMOKE scripts and executables, and important pieces of documentation for the 2002 emissions modeling. Details about the emissions inventories used in simulation Pre02a_36 are included in the 2003 emissions modeling final report (Adelman and Omary, 2004). The quality assurance web site for simulation Pre02a_36 is http://pah.cert.ucr.edu/aqm/308/Pre02a_36.shtml. After successfully evaluating the emissions

modeling results for Pre02a_36, we moved on to the first annual emissions simulation using the 2002 meteorology and emissions inventories for the RMC in 2004: preliminary 2002 simulation case B (Pre02b_36).

5.4.2 Emissions simulation Pre02b_36

Compared with Pre02a_36, simulation Pre02b_36 integrated a few minor changes to the input data as well as revisions to the emissions modeling QA protocol. We modified the SMOKE scripts following the Pre02a_36 simulation in order to modularize the system further, add error-checking loops, and break up the input and output directories by source category. We also added more in-line documentation to the scripts and cleaned up extraneous lines of source code to make the SMOKE user interface at the RMC more transparent. In addition to correcting some inventory-related issues discovered during the QA of Pre02a_36, we added offshore-point-source emissions in the Gulf of Mexico and off the coast of California, and removed the WRAP agricultural fires from the simulation in order to have an emissions simulation with no fires in the WRAP region to use in fire emissions sensitivities. Table 5-2 lists the emissions source categories included in simulation Pre02b_36. On the ancillary input side of the modeling, we upgraded the spatial surrogates used in Pre02a_36 with new EPA spatial surrogates for the U.S. and Canada. We continued to use the surrogates from Pre02a_36 to spatially allocate the Mexican emissions. Details about all of the changes made between simulations Pre02a_36 and Pre02b_36 are included in the emissions simulation Pre02b_36 final report (Holland and Adelman, 2004). The QA web site for simulation Pre02b_36 is http://pah.cert.ucr.edu/aqm/308/Pre02b_36.shtml.

During the final phase of the Pre02b_36 modeling, we received the 2002 WRAP fire inventories from the FEJF inventory contractor. The next major update to the RMC emissions inventory included the 2002 fires in simulation Pre02b_36, which resulted in the creation of the next preliminary 2002 annual simulation: Pre02c_36.

5.4.3 Emissions simulation Pre02c_36

After receiving the 2002 WRAP fire inventories from the FEJF inventory contractor in April 2004, we preprocessed the files and modeled them through SMOKE for inclusion in emissions simulation Pre02c_36. This simulation differed from Pre02b_36 only in the addition of the 2002 prescribed fire and wildfire and 2018 agricultural fire (version 07/31/02) inventories. Table 5-2 lists the emissions source categories included in simulation Pre02c_36. Details about all of the changes made between simulations Pre02b_36 and Pre02c_36 are included in the emissions simulation Pre02c_36 final report (Adelman and Holland, 2004). The QA web site for simulation Pre02c_36 is http://pah.cert.ucr.edu/aqm/308/Pre02c_36.shtml.

Before conducting the next annual preliminary simulation in the series (Pre02d_36), we completed several other, short-term simulations based on simulation Pre02c_36: (1) a simulation for testing nested grid modeling, (2) a simulation for testing PinG treatment of point sources, and (3) an emissions sensitivity study targeting a specific source category (nonroad mobile diesel engines). These are discussed in Sections 5.4.4 through 5.4.6.

5.4.4 Emissions simulation Pre02c_12

We began work on the emissions for the WRAP nested 12-km modeling domain (Figure 5-4 above) in July 2004. UNC-CEP prepared spatial surrogates using the EPA unified 12-km surrogates (EPA99) for the U.S. and Canada (U.S. EPA, 2004) and ESRI/CIESIN Shapefiles for Mexico (ESRI, 2002; CIESIN, 2004). To facilitate the cross-referencing of the spatial surrogate codes to specific SCCs, we mapped the ESRI/CIESIN codes to the EPA99 codes being used for the U.S. and Canada, as explained in Section 5.3.2 (see Table 5-18 above). With the WRAP 12-km meteorology data not available until late 2004, we modeled only those source categories that did not require meteorology information to derive emissions estimates (area, nonroad mobile, on-road mobile for the WRAP states, and road dust). Once we completed the processing and QA of the non-meteorology-dependent emissions sectors, we archived the SMOKE scripts and executables in the RMC version control system and deleted the output files to conserve disk resources. We never used the results from emissions simulation Pre02c_12 for air quality modeling; we developed this simulation to test the 12-km spatial surrogates and prepare the scripts for the annual 12-km simulation. When the 12-km meteorology data became available, we modeled the entire emissions simulation, including non meteorology-dependent data, using the best available inventories at that time. A description of the full annual preliminary 2002 12-km simulation (Pre02d_12) is described below in Section 5.4.10. The QA web site for the Pre02c_12 12-km-resolution emissions modeling is http://pah.cert.ucr.edu/aqm/308/qa_pre02b12.shtml.

5.4.5 Emissions simulation Pre02c_PinG

A parallel activity to the Pre02c_36 12-km-resolution emissions modeling was the creation of a one-month plume-in-grid (PinG) emissions simulation for testing SMOKE emissions with the CMAQ Plume Dynamics Model (PDM). We used SMOKE to select the top 100 NO_x and top 100 SO₂ stationary point sources in the WRAP states from emissions simulation Pre02c to receive the PinG treatment. Due to a shortcoming in the way SMOKE selects sources for the PinG treatment, we had to split the stationary-point-source inventories into two components: the WRAP states and the non-WRAP portion of the domain. After dividing the inventory, we applied the PinG selection criteria to the WRAP inventory and prepared CMAQ-ready PinG emissions. SMOKE selected 144 unique sources to receive the PinG treatment in the WRAP region. The reason SMOKE selected 144 sources and not 200 (top 100 NO_x and top 100 SO₂) was that many of these sources are redundant (i.e., the same source exists in both lists). The annual PinG emissions simulation was never completed as the status of the CMAQ PinG test simulation. We were waiting on the results of this test simulation before proceeding with the rest of the modeling.

5.4.6 Emissions simulation Pre02c_36s01

In September 2004 we completed a two-and-a-half-month emissions sensitivity with simulation Pre02c that targeted nonroad mobile diesel engines in three WRAP states. Working with the WRAP Economic Analysis Forum, we developed a preliminary set of control factors for simulating the effects of a diesel retrofit emission control program on agricultural, mining, and construction nonroad mobile sources in Arizona, North Dakota, and Montana. If the Economic

Analysis Forum determines that air quality modeling results using Pre02c_36s01 emissions lend compelling evidence to the effectiveness of these types of controls, then we would revisit the simulation, targeting with greater precision the sources and pollutants that the actual controls would affect. Additional information on simulation Pre02c_36s01 is provided in Section 5.8.

5.4.7 Emissions simulation Pre02d_36

Simulation Pre02d_36 was the final preliminary annual 36-km 2002 simulation of the 2004 project year. To prepare for it, we made several improvements to the Pre02c emissions, such as substituting new inventories for the non-WRAP states and Canada, and updating the temporal and chemical allocation profiles used in SMOKE. Details about all of the changes made between simulations Pre02c_36 and Pre02d_36 are given in this subsection.

As we were completing emissions simulation Pre02c_36, we also began collecting updated 2002 inventory data to include in simulation Pre02d_36. We ultimately compiled new inventory data for each sector for every region of the 36-km modeling domain, except for Mexico, to create Pre02d_36. In addition to integrating newly available inventory data into the WRAP emissions modeling, we also corrected a few errors that we discovered during the modeling and QA of simulation Pre02c_36. The data collection effort for Pre02d_36 began in May 2004 with the release of the VISTAS 2002 emissions inventory by Alpine Geophysics, and finished in November 2004 with the release of a preliminary 2000 national Canadian inventory by the U.S. EPA. The only source categories that did not need reprocessing for simulation Pre02d_36 were the offshore point sources and the agricultural fire emissions. Due to inventory updates, refinements, or additions, the RMC reprocessed every other source category beginning in November 2004 and finishing the modeling and QA of simulation Pre02c_36 in January 2005.

The emissions modeling tasks we performed for the Pre02d_36 simulation consisted of the following components:

- Receive and preprocess the 2002 VISTAS and preliminary 2002 U.S. NEI inventories from Alpine Geophysics.
 - Split the area-source inventories by emissions source sector and spatial region to conform with the WRAP RMC emissions inventory configuration (Section 5.2). We split these inventories into the following components: stationary area, fugitive dust, and road dust for the VISTAS, CENRAP, and “other U.S.” regions of the modeling domain.
 - Remove the fugitive dust sources that are contained in the dust inventory prepared by Alpine (which uses county-based transport fractions) from the U.S. area-source inventories. Table 5-5 lists the dust sources that we removed from these inventories.
 - Remove the agricultural and natural NH₃ emissions sources from the U.S. area-source inventories that are represented in the WRAP process-based NH₃ emissions model. Table B-1 lists the NH₃ emissions sources that we removed from these inventories.
- Receive and preprocess the revised 2002 wildfire and prescribed fire emissions inventories from Air Sciences Inc. that distinguish between natural and anthropogenic

fires. This involved splitting the annual natural prescribed fire inventory into monthly files.

- Integrate the 2018 base smoke management agricultural burning area-source inventory received in July 2002 during the §309 modeling.
- Integrate the gridded output from the WRAP windblown dust model.
- Integrate the gridded output from the ENVIRON NH₃ emissions model.
- Ensure correct temporal and spatial coverage of the inventories.
- Run SMOKE for the annual simulation.
- Perform QA on the annual period results.
- Deliver the emissions for use in CMAQ modeling.

More information on these components of the Pre02d_36 simulation is given in various sections of this report. In Sections 5.2 and 5.3, respectively, we described the SMOKE inventory files and SMOKE ancillary files used. In Sections 5.5 and 5.6, we provide summaries and descriptions that illustrate the application of the WRAP QA protocol to the emissions modeling for this task; the documentation and QA web site for simulation Pre02d_36 are accessible at http://pah.cert.ucr.edu/aqm/308/Pre02d_36.shtml. Section 5.7 discusses the differences between simulation Pre02d_36 and the two previously completed annual simulations, Pre02b_36 and Pre02c_36. In Section 5.9 we describe the problems and issues that arose during the modeling of this simulation, and make recommendations about what can be done in the next round of 2002 emissions modeling to improve the data collection, modeling, and QA efforts. Appendix A summarizes the input and output data (Tables A-1 through A-3) and the SMOKE configuration options (Table A-4) for simulation Pre02d_36. Appendix C contains emissions density maps for the significant pollutants from all the major emissions source categories modeled in this simulation. Appendix D contains bar charts that qualitatively compare simulations Pre02c_36 and Pre02d_36, illustrating how the inventory updates that occurred between these two simulations affect the emissions totals in each region of the modeling domain.

5.4.8 Emissions simulation Pre02e_36

The RMC designed the annual emissions simulation Pre02e_36 to study the effects of natural versus anthropogenic fire emissions. With the delivery of the revised 2002 fire inventories by Air Sciences in September 2004, we designed this simulation to evaluate the effects of the new natural prescribed and wildfire inventories on the modeling. We created simulation Pre02e_36 by adding the natural prescribed and wildfire inventories to simulation Pre02b_36, the base simulation that contained no fires at all; a comparison between Pre02b_36 and Pre02e_36 therefore illustrates how the natural fire inventories affect the modeling. As simulation Pre02b_36 was extensively quality assured and documented in Holland and Adelman (2004) and we changed it to create Pre02e_36 only by adding the revised fire inventories, we did not have to perform much additional QA on simulation Pre02e_36. The fire inventories that distinguish Pre02e_36 from Pre02b_36 are documented and quality assured in Section 5.2.10. Section 5.7 discusses the differences between simulation Pre02e_36 and the other annual simulations

completed in 2004. Section 5.8 also summarizes the emissions sensitivities completed during this calendar year, including simulations Pre02e_36 and Pre02f_36.

5.4.9 Emissions simulation Pre02f_36

We designed the annual emissions simulation Pre02f_36 to study the effects of the revised 2002 fire emissions inventories and to study the effects of natural fire emissions versus all fire emissions. When we received the revised 2002 fire inventories in September 2004, we designed this simulation for comparison with simulations Pre02b_36, Pre02c_36, and Pre02e_36. We created simulation Pre02f_36 by adding the base smoke management agricultural fires, natural and anthropogenic prescribed fires, and revised wildfire inventories to simulation Pre02b_36, the base simulation that contained no fires at all. A comparison between Pre02b_36 and Pre02f_36 therefore illustrates how adding all of the 2002 fire inventories affects the air quality modeling results. Comparing simulations Pre02c_36 and Pre02f_36 shows the effects of the old versus new fire inventories. Finally, comparing simulations Pre02e_36 and Pre02f_36 illustrates the effects of natural fire inventories only versus all fire inventories. As simulation Pre02b_36 was extensively quality assured and documented in Holland and Adelman (2004) and we changed it to create Pre02f_36 only by adding the above revised fire inventories, we did not have to perform much additional QA on simulation Pre02f_36. The fire inventories that distinguish Pre02f_36 from Pre02b_36 are documented and quality assured in Section 5.2.10. Section 5.7 discusses the differences between simulation Pre02f_36 and the other annual simulations completed in 2004. Section 5.8 also summarizes the emissions sensitivities completed during this calendar year, including simulations Pre02e_36 and Pre02f_36.

5.4.10 Emissions simulation Pre02d_12

The RMC completed the entire 12-km annual meteorology data set in January 2005, allowing us to begin the modeling and QA of all the 12-km emissions. We initiated the 12-km emissions modeling with simulation Pre02c_12 in July 2004, debugging the SMOKE scripts and checking the initial results of the fine-grid simulation (see Section 5.4.4). We completed the full 12-km emissions simulation, Pre02d_12, by the end of February 2005. To create spatial surrogates for this simulation, we used the EPA 65-category “new” 12-km surrogates (U.S. EPA, 2004e) (see Section 5.3.2). We applied the same ESRI/CIESIN Shapefiles that we used for the Pre02d_36 simulation, simply applying them to the finer-scale 12-km grid. The inventory QA that we applied to simulation Pre02d_36 also applied to the 12-km nested grid; basic QA of the 12-km emissions involved confirming that we had allocated the data to the correct model grid cells. The same input and output data and SMOKE configuration options for simulation Pre02d_36 summarized in Appendix A also applied to simulation Pre02d_12. We prepared the 12km Pre02d emissions for use in a nested simulation that is based off the 36km Pre02d simulation. Appendix C contains emissions density maps by county for the significant pollutants from all of the major emissions source categories modeled in Simulation Pre02d_12. These maps are not based on a model grid resolution but merely show county level emissions normalized by the county land area. Appendix D contains bar charts comparing the inventories from simulations Pre02c and Pre02d, illustrating the effects of the inventory updates that occurred between these two simulations. Similar to the density maps, these results are model grid-independent as they are based on state totals only and are applicable to all model grid resolutions.

5.5 RMC Emissions Modeling Deliverables and QA/QC Products

Quality assurance in the context of emissions modeling refers to ensuring that the results of the simulations are of the highest quality possible with respect to the data. Quality control, on the other hand, refers to ensuring that the model simulations completed successfully and without errors. QA focuses on the quality of the data; QC focuses on the process of modeling, archiving, and documenting the data. Some of RMC products, like the emissions spatial plots and the simulation web sites, are used for both QA and QC. Other products, such as the SMOKE settings document are used for QC only. This section describes both the QA and QC products that the RMC used during this project year to ensure high quality model results and that the modeling software performed as we expected.

Table 5-19 lists the RMC web site locations and the Bugzilla ticket numbers associated with all of the emissions simulations processed from March 2004 through February 2005 (see Section 5.4). Bugzilla is an on-line bug tracking system that we use as an alternative to conventional e-mail for tracking and archiving correspondence among the emissions modeling team members. To access the database containing the Bugzilla tickets, visit <http://bugz.unc.edu> and use the “Enter a bug #” box to search for the ticket numbers listed in Table 5-19. The web sites listed in that table contain links to documentation and QA/QC graphics for each of the simulations. Those reports and QA/QC graphics, plus the CMAQ-ready emissions they document, constitute the deliverables for Task 3 in the WRAP RMC 2004 work plan. Section 5.6 summarizes the deliverables and QA/QC products generated by the RMC during this reporting period.

Table 5-19. Web sites and Bugzilla ticket numbers for preliminary 2002 emissions simulations.

Simulation ID	Web Site for Links to Documentation and QA Graphics	Bugzilla Ticket #
Pre02a_36	http://pah.cert.ucr.edu/aqm/308/Pre02a_36.shtml	805, 858, 859
Pre02b_36	http://pah.cert.ucr.edu/aqm/308/Pre02b_36.shtml	905, 924, 925, 929, 930, 933, 939, 941-944, 949, 952-958, 960, 967, 968, 973-977, 979, 981, 982, 985, 989, 991, 994
Pre02c_36	http://pah.cert.ucr.edu/aqm/308/Pre02c_36.shtml	992, 999, 1007, 1010
Pre02b_12	http://pah.cert.ucr.edu/aqm/308/Pre02b_12.shtml	1067
Pre02c_PinG	None	1068
Pre02c_36s01	None	1356
Pre02d_36	http://pah.cert.ucr.edu/aqm/308/Pre02d_36.shtml	1104, 1146, 1179, 1184, 1185, 1259, 1260, 1340, 1364, 1411, 1412, 1431, 1454, 1482

Simulation ID	Web Site for Links to Documentation and QA Graphics	Bugzilla Ticket #
Pre02e_36	None	None
Pre02f_36	None	None
Pre02d_12	http://pah.cert.ucr.edu/aqm/308/Pre02d_12.shtml	1512

The following subsections summarize the deliverables and QA products we generated during project year 2004. It also includes a summary of the SMOKE time and disk requirements for annual simulations on the RMC compute servers (using simulation Pre02c_36 as an example), and documents the location of the data on the servers and the version control system we used.

We generated all of the SMOKE modeling results for these simulations on the RMC computing cluster. The input files, SMOKE executables, SMOKE scripts, and model output are all available through the RMC. We documented simulations Pre02a through Pre02c with comprehensive final reports (Adelman and Omary, 2004; Holland and Adelman, 2004; Adelman and Holland, 2004); these include descriptions of the work performed to complete the simulations, comparisons to the previous simulation, and QA products documenting the input files and model configurations used for each simulation. We have documented the final preliminary 2002 simulation, Pre02d, in this report. The web sites documenting the QA procedures performed on these simulations are listed in Table 5-19 above.

5.5.1 SMOKE time requirements and disk use

Managing the disk use and time requirements of the SMOKE simulations is as large a component of the emissions quality control as is the assurance of quality results. With large-spatial-scale, annual simulations like those described above, the length of time required for completing the simulations and the amount of disk space required to store all of the input, intermediate, and final output files are both massive. Table 5-20 summarizes the run times and disk use requirements for each emissions component of simulation Pre02c_36. The statistics in Table 5-20 are approximations. The disk use estimates account for the intermediate and output files only; the actual disk requirements for the 36-km Pre02c simulation are slightly larger than those shown. The totals show that simulation Pre02c_36 required over 1.6 terabytes of disk storage and took almost 400 total hours to complete. Figures 5-5 and 5-6 are graphical summaries of the time requirements and disk use by source category and SMOKE program. Only the SMOKE programs that required the greatest amount of disk space and took the longest to run are displayed in these figures.

Table 5-20. SMOKE time and disk use statistics for simulation Pre02c_36 km.

Source Category	Disk Use (MB)	Disk Use (%)	Run Time (Hours)	Run Time (%)
Stationary area	25,540	1.6	8.54	2.1
Road dust	3,776	0.2	1.33	0.3
Nonroad mobile	20,675	1.3	5.12	1.3
On-road mobile	29,150	1.8	80.55	20.1
Point	431,028	26.4	82.75	20.7
Offshore	181,743	11.1	9.07	2.3
Ag fire	219,489	13.4	55.03	13.8
Rx fire	243,713	14.9	71.48	17.9
Wildfire	251,263	15.4	20.97	5.2
Biogenic	29,503	1.8	4.08	1.0
Merge	199,655	12.2	60.83	15.2
Total	1,635,535	100.0	399.75	100.0

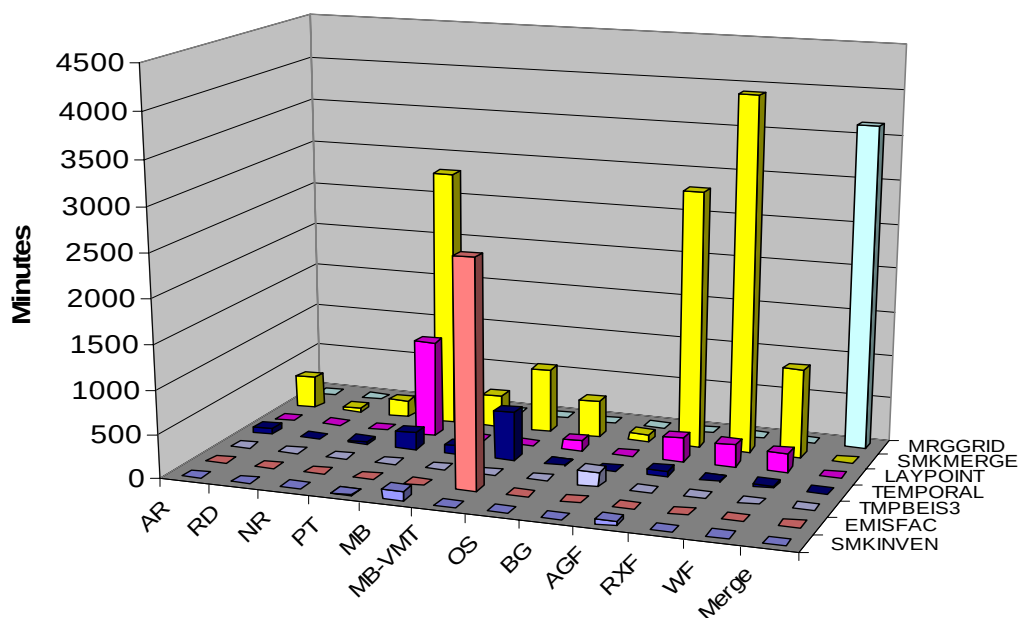


Figure 5-5. Simulation Pre02c_36 timing statistics by source and SMOKE program for the programs that took the longest to run. (AR: stationary area, RD: road dust, NR: nonroad mobile, PT: point, MB: WRAP on-road mobile, MB-VMT: non-WRAP on-road mobile, OS: offshore point, BG: biogenic, AGF: agricultural fires, RXF: prescribed fires, WF: wildfires)

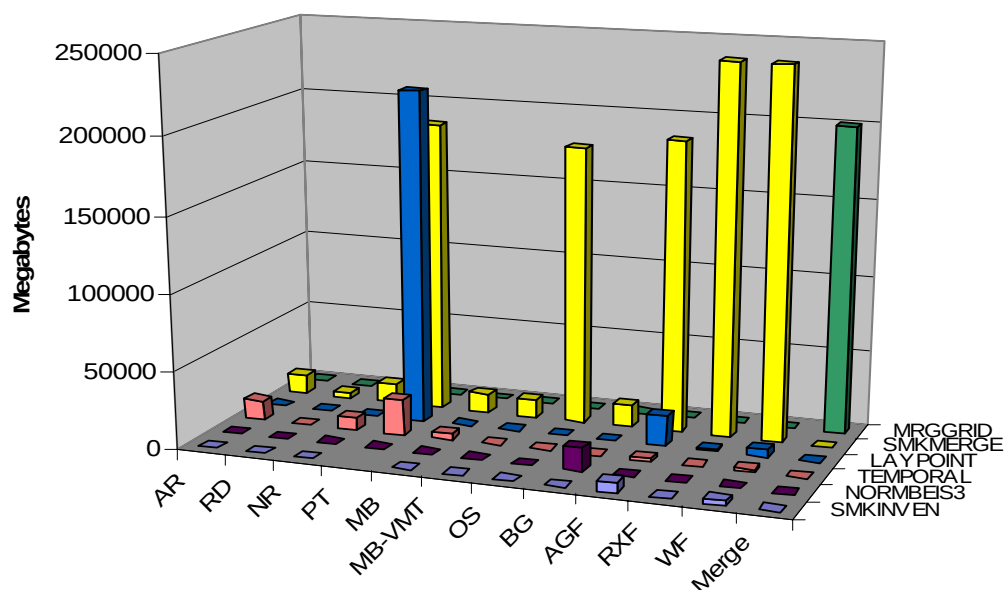


Figure 5-6. Simulation Pre02c_36 disk usage by source and SMOKE program for the programs that required the greatest amount of disk space. (AR: stationary area, RD: road dust, NR: nonroad mobile, PT: point, MB: WRAP on-road mobile, MB-VMT: non-WRAP on-road mobile, OS: offshore point, BG: biogenic, AGF: agricultural fires, RXF: prescribed fires, WF: wildfires)

5.5.2 RMC version control

To facilitate reproducibility of the RMC emissions modeling results and to provide enhanced QC of the modeling, we first implemented the WRAP emissions modeling QA protocol (Adelman, 2004) during simulation Pre02a_36. The protocol defines strict procedures for data and simulation management, administering the SMOKE modeling system and input/output data, and documenting all modeling procedures. As specified in the QA protocol, we used the Concurrent Versions System (CVS) to provide version control for the simulations completed in 2004. Version control is a system for archiving the scripts, configuration files, and input files so that a simulation can be reproduced in the future. CVS uses a system of revision tags, or text identifiers, to label both ASCII and binary files. As the RMC adds new files or updates existing files to the modeling system, a CVS command is invoked to tag the files and associate them with the applicable simulation. As the simulation is completed and the QA finalized, a final CVS tag is added to the files that can be used to recall all of the scripts, executables, and inputs that generated the emissions simulation. Table 5-21 lists the CVS revision tags used for version control during the preliminary 2002 modeling.

Table 5-21. CVS revision tags for preliminary 2002 modeling.

Simulation ID	CVS Revision Tag
Pre02a_36	Pre02a_36_Final
Pre02b_36	Pre02b_36_Final
Pre02c_36	Pre02c_36_Final
Pre02b_12	Pre02c_12_Final
Pre02c_PinG	Pre02c_36_Ping_Final
Pre02c_36s01	Pre02c_36s01_Final
Pre02d_36	Pre02d_36_Final
Pre02e_36	Pre02e_36_Final*
Pre02f_36	Pre02f_36_Final*
Pre02d_12	Pre02d_12_Final

*Assigns directory only.

To invoke the CVS revision tags on the RMC compute servers, the CVSROOT environment variable must be set to point to the location of the preliminary 2002 modeling archives. The CVSROOT location on the RMC machines is /home/aqm3/edss2/archive. Once CVSROOT is defined, the installation for any of the simulations listed in Table 5-21, including the run scripts, executables, and all input files, can be recalled from the archive by issuing the command “cvs checkout -r ‘CVS Revision Tag’”. For example, to check out the files needed to reproduce the Pre02b_36 simulation, you would invoke the command “cvs checkout -r Pre02b_36_Final” from the command line anywhere on the RMC servers.

5.5.3 Quality assurance products

In addition to version control, the RMC emissions modeling QA protocol also defines a series of QA products that must be created to document every simulation that produces emissions input for CMAQ. Before delivering the results of an emissions simulation to the RMC air quality modeling team, the RMC emissions modelers generate and scrutinize tabular and graphical summaries that summarize the simulation and provide insight into its quality. The emissions QA protocol contains a checklist of QA procedures that must be completed before the simulation results are ready to be given to the air quality modelers. The checklist provides guidance for ensuring that each step of the SMOKE modeling process is checked and documented. The final reports for simulations Pre02a through Pre02c contain completed QA checklists documenting that each simulation was thoroughly reviewed. The QA checklist for simulation Pre02d is contained in Appendix E. For the many QA procedures in the checklist that do not produce tangible products such as emissions plots or tabulated information, the checklist itself is the documentation substantiating completion of the QA procedures. Other, more tangible QA products that we generate include spatial plots of the daily maximum emissions for each source sector and pollutant, daily and annual time-series plots of the emissions, linear regressions comparing annual inventory summaries against reports from each SMOKE process (e.g., inventory import, speciation, spatial allocation), and daily vertical emissions profiles of the point-source simulations. Refer to the links in Table 5-19 to see these QA products for each preliminary 2002 simulation.

5.6 WRAP Preliminary 2002 Emissions Progress

As noted in Section 5.3, the preliminary 2002 emissions modeling performed by the RMC in project year 2004 was an iterative process whereby each simulation was built from the previous one. We used the six-month simulation Pre02a to test the emissions QA protocol, the SMOKE run scripts, and the preliminary 2002 emissions inventories and meteorology. After making adjustments to both the modeling protocol and the input data, we moved on to the first annual simulation of the year, Pre02b. With the delivery of the 2002 WRAP fire inventories, we then created simulation Pre02c by adding these new data on top of simulation Pre02b. Adding updated 2002 fire data to the emissions from simulation Pre02b_36 resulted in simulations Pre02e_36 and Pre02f_36. To create simulations Pre02d_36 and Pre02d_12, we combined entirely new inventories for the non-WRAP states, revised Canadian inventory data, gridded emissions data from the WRAP windblown dust model and the ENVIRON NH₃ emissions model, and the revised 2002 fire inventories. While the final reports on the first three simulations mentioned above detail the modeling and QA performed for each, they do not include comparisons between the simulations to demonstrate how the preliminary 2002 base emissions simulation progressed through project year 2004. This section contains comparisons of simulations Pre02b, Pre02c, and Pre02d to illustrate how the inventory changes that we made affected the overall distribution of emissions among the major source categories and across the various regions of the modeling domain. For details about the exact inventory changes that occurred between these three simulations, refer to Section 5.4.

As we used Pre02a simply as a short-time-period test for the annual simulation Pre02b, the changes to the inventory inputs between these two simulations were minor, so a comparison between the inventories used for these two cases is unnecessary. The changes to the Pre02b inventory that resulted in simulation Pre02c included the addition of 2002 wildfire and prescribed fire inventories and the 2018 base smoke management agricultural fire inventory. The Pre02d inventory represented several updates to all regions of the modeling domain. Table 5-22 summarizes the updates by source category that occurred between the Pre02c and Pre02d inventories.

Table 5-22. Summary of emissions updates between the Pre02c and Pre02d inventories.

Source Category	Pre02d Update
Stationary Area	- Upgraded the NEI96 grown to 2002 with the preliminary NEI2002 for the non-WRAP states - Removed the NH₃ SCCs represented by the ENVIRON NH₃ model from all U.S. inventories - Removed the fugitive dust SCCs represented from all U.S. inventories - Added the VISTAS and CENRAP area-source fire inventories; removed these fire sources from the non-WRAP stationary-area-source inventory

Source Category	Pre02d Update
Nonroad Mobile	- Upgraded the NEI96 grown to 2002 with the preliminary NEI2002 for the non-WRAP states - Removed the refueling SCCs represented by MOBILE6 from the WRAP inventory - Split the shipping SCC into in-port and ocean-going sources; allocated the ocean-going sources to marine grid cells within 25 miles of the coast
On-road Mobile	Upgraded NEI99 to NEI2002 for non-WRAP states
Stationary Point	- Replaced CENRAP records in the WRAP inventory with NEI2002 records - Added the VISTAS hourly CEM inventory and temporal profiles for modeling sources in the VISTAS region
Fugitive Dust	Added an explicit fugitive dust category that uses an inventory with county-based transport fractions
Road Dust	No change
Windblown Dust	Added gridded emissions from the WRAP windblown dust model for U.S. sources
Agricultural and Natural NH ₃	Added gridded emissions from the ENVIRON NH₃ model for U.S. sources; these replaced emissions for SCCs in the stationary area inventory
Prescribed Fire	Replaced the WRAP 2002 prescribed fire inventory with revised inventories that differentiate between natural and anthropogenic events
Agricultural Fire	No change
Wildfire	- Upgraded to the revised 2002 inventory for the WRAP states - Added the 2002 VISTAS fire inventory
Offshore Point	No change
Offshore Mobile	Add an explicit offshore-mobile-source category derived from nonroad mobile shipping SCCs
Biogenic	Upgraded the white spruce and fir emissions factors based on revised U.S. EPA data
Canada	Upgraded all of the nonpoint inventory to the preliminary 2000 National Canadian Inventory
Mexico	No change

Tables 5-23 and 5-24 are cursory summaries of the annual total emissions by pollutant between the Pre02b, Pre02c, and Pre02d inventories for the entire U.S. and the WRAP states, respectively, for all modeled source categories combined. Figures 5-7 and 5-8 illustrate the U.S. domainwide trends indicated in these tables: (1) the total non-NH₃ and non-PM₁₀ emissions slightly increased between the Pre02b and Pre02c inventories and then decreased with the Pre02d inventory; and (2) the total NH₃ and PM₁₀ emissions increased with each new inventory. Tables 5-25 through 5-27 expand upon Table 5-23 by showing the total annual U.S. emissions

for the Pre02b, Pre02c, and Pre02d inventory pollutants by source category. Tables 5-28 through 5-30 expand upon Table 5-24 in the same way for the total annual WRAP-region emissions.

Figures 5-9 through 5-16 illustrate the differences among the Pre02b, Pre02c, and Pre02d inventories. Figures 5-9 through 5-11 show the total emissions differences among the three inventories in each of the major regions of the 36-km modeling domain. These figures illustrate the interregional differences in magnitude of the total emissions among the five RPOs, Canada, and Mexico. A comparison between Figures 5-9 and 5-10 demonstrates that only the WRAP emissions changed between these two simulations, the result of adding fire emissions in the WRAP region. Comparing Figures 5-10 and 5-11 shows the overall reduction in emissions for most pollutants in the U.S. and Canada. This comparison also illustrates the effect of the windblown dust emissions in the increase in PM₁₀ emissions between the Pre02c and Pre02d inventories. Figures 5-12 through 5-14 are pie chart summaries of the total U.S. emissions for the Pre02b, Pre02c, and Pre02d inventories. Figures 5-15 and 5-16 are pie chart summaries of the total WRAP-domain emissions for the Pre02c and Pre02d inventories. These emissions pie charts show how the contribution of each of the major emissions components to the total emissions changed among the various inventories. The effects of adding the first set of 2002 fire emissions are most evident in comparing the CO and PM pie charts in Figures 5-12 and 5-13. A comparison of Figures 5-13 and 5-14 shows the effects of the NH₃ model's emissions in the NH₃ pie chart, and the effects of adding the windblown dust and other explicit dust categories in the three PM pie charts. Figures 5-15 and 5-16 illustrate the source category contributions to the total emissions for the WRAP states only for the Pre02c and Pre02d inventories. These figures magnify the effects of the WRAP fire inventories relative to the total U.S. pie charts.

Figures 5-17 through 5-24 expand on the WRAP-region pie charts in Figure 5-16 by showing the contribution of each of the emissions source categories to the total annual emissions in each of the WRAP states in simulation Pre02d for the major inventory pollutants (CO, VOC, NO_x, SO₂, NH₃, PM_{2.5}, PM₁₀, and coarse particulate matter [PMc]). For the pollutants that are related to land area or population—such as VOC emissions, which are dominated by the biogenic sources, and NO_x emissions, which are dominated by the mobile- and area-source sectors—California tends to be the largest emissions source state in the WRAP region. Oregon is the largest emitter of CO, PM₁₀, and PM_{2.5} in the WRAP region, due to an active wildfire year in 2002. North Dakota is the largest SO₂ emitter in the WRAP states because of large contributions from the area- and point-source sectors. California, Montana, and South Dakota are the largest emitters of NH₃ in the WRAP region, attributable to the high amount of agricultural activity in these states captured in the new agricultural and natural NH₃ inventory. Although Oregon was the largest emitter of PM₁₀ and PM_{2.5} in the WRAP region during 2002, when the wildfire signal from PM_{2.5} is removed by looking at PMc, Oregon drops to the fifth-largest emitter of PMc behind California, North Dakota, South Dakota, and Colorado. Outside of Oregon, the PMc emissions levels are affected primarily by the fugitive dust and road dust sectors.

The inventory comparisons presented here also apply to the 12-km (Pre02c_12 and Pre02d_12), PinG (Pre02c_PinG), and fire sensitivity (Pre02e_36 and Pre02f_36) simulations. All of the inventories used in the preliminary 2002 emissions modeling are included in these analyses.

Table 5-23. Comparison among the three Pre02 simulations of annual U.S. pollutant totals in tons/year for all source categories combined.

Pollutant	Pre02b	Pre02c	Pre02d
CO	115,323,289	128,369,633	69,281,420
NO _x	26,155,742	26,444,753	16,546,150
VOC	74,773,640	75,399,946	68,584,807
NH ₃	5,094,587	5,156,807	5,487,759
SO ₂	19,512,966	19,590,788	15,250,166
PM ₁₀	12,271,953	13,542,065	17,099,895
PM _{2.5}	4,206,658	5,298,888	5,225,398
PMc	8,065,560	8,243,442	6,645,623

Table 5-24. Comparison among the three Pre02 simulations of annual WRAP-region pollutant totals in tons/year for all source categories combined*

Pollutant	Pre02b	Pre02c	Pre02d
CO	21,468,363	34,514,706	34,488,024
NO _x	4,248,803	4,537,814	4,532,715
VOC	24,134,792	24,761,099	24,686,023
NH ₃	1,038,013	1,100,233	1,823,284
SO ₂	1,247,963	1,325,785	1,324,388
PM ₁₀	2,903,972	4,174,085	4,922,535
PM _{2.5}	942,716	2,034,946	1,924,883
PMc	1,961,521	2,139,403	1,688,846

*Does not include offshore point sources.

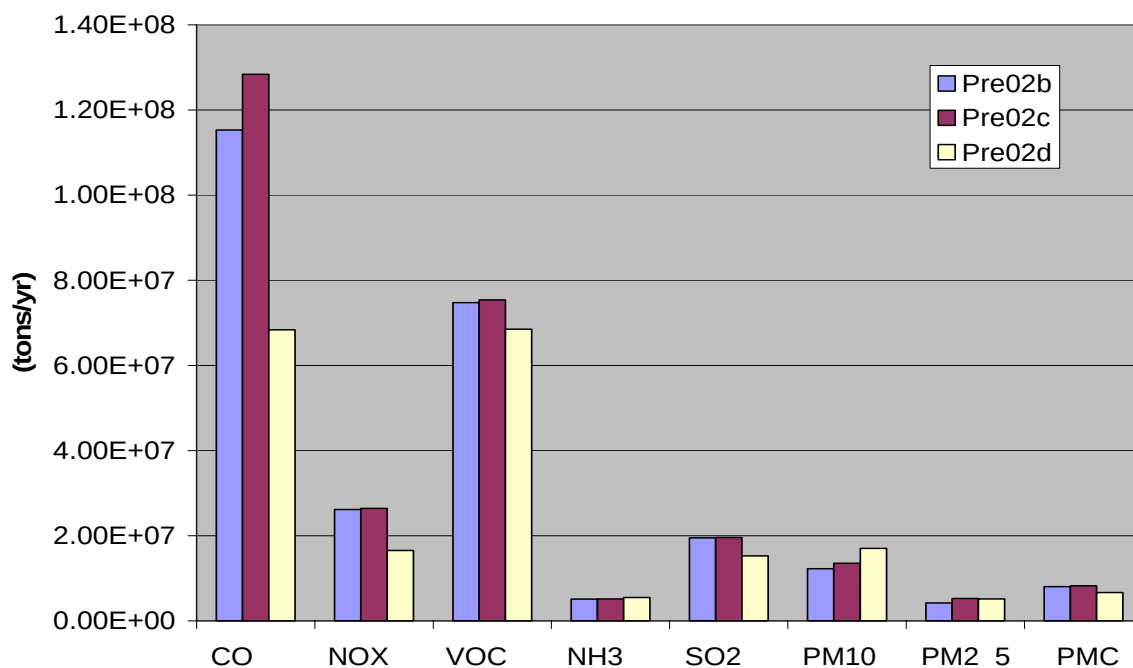


Figure 5-7. U.S. total emissions comparison of three annual Pre02 simulations.

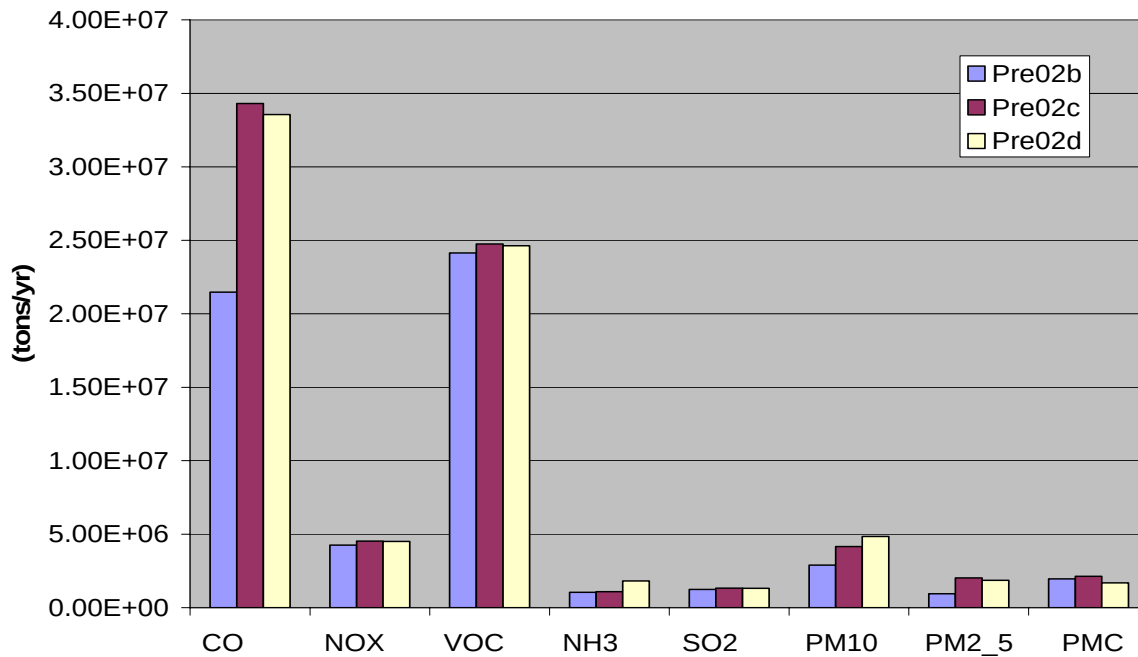


Figure 5-8. WRAP-region total emissions comparison of three annual Pre02 simulations.

Table 5-25. Pre02b U.S. pollutant totals by source category

Category	CO	NO _x	VOC	NH ₃	SO ₂	PM ₁₀	PM _{2.5}	PMc
Area	8788585	2133791	8743374	4547733	1328943	7381849	2351239	5030603
Biogenic	6335679	968676	54484314	0	0	0	0	0
On-road	69371953	8078587	5868161	251904	273748	225877	170672	55205
Nonroad	25336215	5320217	3166860	12032	942749	471442	423330	48382
Road Dust	0	0	0	0	0	2917582	507809	2409776
Point	5458565	9515094	2462456	282919	16967419	1275162	753570	521592
Offshore	32293	139377	48474	0	107	40	39	2
Total	115323289	26155742	74773640	5094587	19512966	12271953	4206658	8065560

Table 5-26. Pre02c U.S. pollutant totals by source category

Category	CO	NO _x	VOC	NH ₃	SO ₂	PM ₁₀	PM _{2.5}	PMc
Area	8788585	2133791	8743374	4547733	1328943	7381849	2351239	5030603
Biogenic	6335679	968676	54484314	0	0	0	0	0
On-road	69371953	8078587	5868161	251904	273748	225877	170672	55205
Nonroad	25336215	5320217	3166860	12032	942749	471442	423330	48382
Road Dust	0	0	0	0	0	2917582	507809	2409776
Point	5458565	9515094	2462456	282919	16967419	1275162	753570	521592
Rx Fire	753945	19826	37702	3523	5436	73922	64302	9620
Ag Fire	217083	10129	20353	4379	1353	22083	20954	1129
Wildfire	12075316	259056	568251	54318	71032	1174106	1006973	167133
Offshore	32293	139377	48474	0	107	40	39	2
Total	128369633	26444753	75399946	5156807	19590788	13542065	5298888	8243442

Table 5-27. Pre02d U.S. pollutant totals by source category

Category	CO	NO _x	VOC	NH ₃	SO ₂	PM ₁₀	PM _{2.5}	PMc
Area	8997365	1588240	8053704	155713	1228561	1434640	1280075	154557
Biogenic	6335679	968676	54484314	0	0	0	0	0
On-road	14077418	1565522	1205058	51452	39573	57953	45619	12334
Nonroad	22400629	4316894	2508503	6562	509894	410306	358358	51949
Road Dust	0	0	0	0	0	3011884	526178	2485710
Windblown Dust	0	0	0	0	0	5228817	0	0
Ammonia	0	0	0	5114196	0	0	0	0
Fugitive Dust	0	0	0	0	0	4243739	841450	3402280
Point	4418380	7683523	1666043	98185	13395672	1455641	1093396	362237
Anthro Rx Fire	363499	7799	17106	1636	2139	35344	30313	5032
Natural Rx Fire	363759	6935	13001	1212	1902	25343	22080	3263
Ag Fire	217083	10129	20353	4379	1353	22084	20955	1129
Wildfire	12075316	259056	568251	54318	71032	1174106	1006973	167133
Offshore	32293	139377	48474	107	40	39	2	0
Total	69281420	16546150	68584807	5487759	15250166	17099895	5225398	6645623

Table 5-28. Pre02b WRAP-region pollutant totals by source category

Category	CO	NO _x	VOC	NH ₃	SO ₂	PM ₁₀	PM _{2.5}	PMc
Area	1448071	453881	1741918	961371	153465	2117539	640254	1477275
Biogenic	2662325	288738	20640180	0	0	0	0	0
On-road	12630468	1399267	1097751	45603	32312	53796	42621	11175
Nonroad	4059991	1101916	422651	4537	155124	75230	69735	5767
Road Dust	0	0	0	0	0	470112	82714	387403
Point	667508	1005001	232292	26501	907063	187296	107393	79901
Total	21468363	4248803	24134792	1038013	1247963	2903972	942716	1961521

Table 5-29. Pre02c WRAP-region pollutant totals by source category

Category	CO	NO _x	VOC	NH ₃	SO ₂	PM ₁₀	PM _{2.5}	PMc
Area	1448071	453881	1741918	961371	153465	2117539	640254	1477275
Biogenic	2662325	288738	20640180	0	0	0	0	0
On-road	12630468	1399267	1097751	45603	32312	53796	42621	11175
Nonroad	4059991	1101916	422651	4537	155124	75230	69735	5767
Road Dust	0	0	0	0	0	470112	82714	387403
Point	667508	1005001	232292	26501	907063	187296	107393	79901
Rx Fire	753945	19826	37702	3523	5436	73922	64302	9620
Ag Fire	217083	10129	20353	4379	1353	22084	20955	1129
Wildfire	12075316	259056	568251	54318	71032	1174106	1006973	167133
Total	34514706	4537814	24761099	1100233	1325785	4174085	2034946	2139403

Table 5-30. Pre02d WRAP-region pollutant totals by source category

Category	CO	NO _x	VOC	NH ₃	SO ₂	PM ₁₀	PM _{2.5}	PMc
Area	1448071	453881	1674437	12479	153465	320940	289328	31607
Biogenic	2662325	288738	20640180	0	0	0	0	0
On-road	12630468	1399267	1097751	45603	32312	53796	42621	11175
Nonroad	4059996	1101910	422651	4537	155123	85159	79089	6070
Road Dust	0	0	0	0	0	490176	87032	403144
Windblown Dust	0	0	0	0	0	1308787	287933	1020854
Ammonia	0	0	0	1672618	0	0	0	0
Fugitive Dust	0	0	0	0	0	1219504	239098	980394
Point	667508	1005001	232292	26501	907063	187296	107393	79901
Anthro Rx Fire	363499	7799	17106	1636	2139	35344	30313	5032
Natural Rx Fire	363759	6935	13001	1212	1902	25343	22080	3263
Ag Fire	217083	10129	20353	4379	1353	22084	20955	1129
Wildfire	12075316	259056	568251	54318	71032	1174106	1006973	167133
Total	34488024	4532715	24686023	1823284	1324388	4922535	2212816	2709700

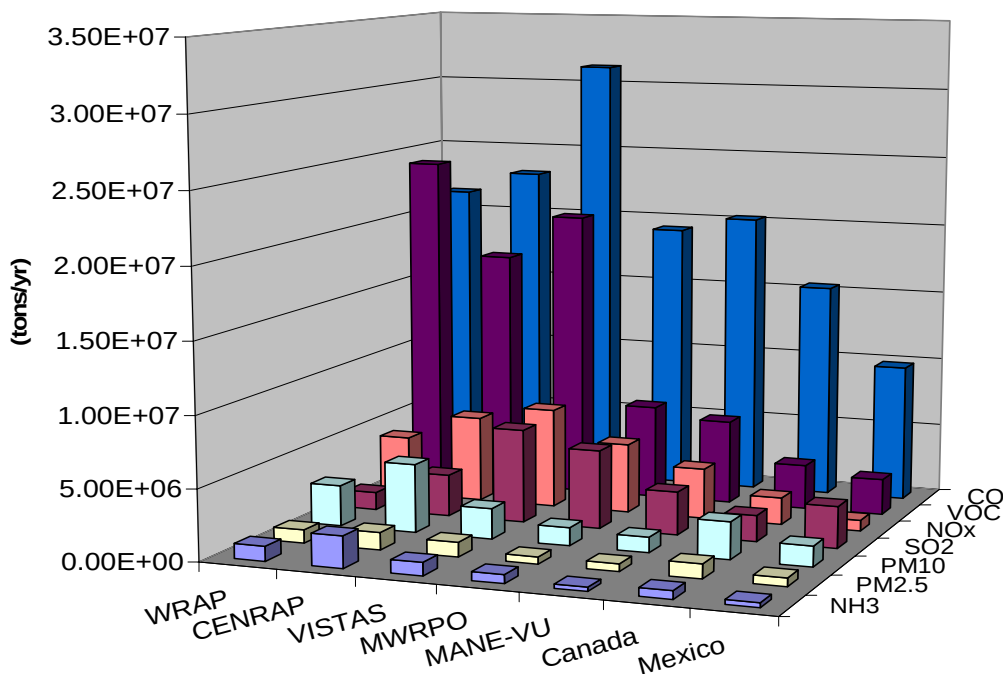


Figure 5-9. Pre02b_36 total domain annual emissions summary.

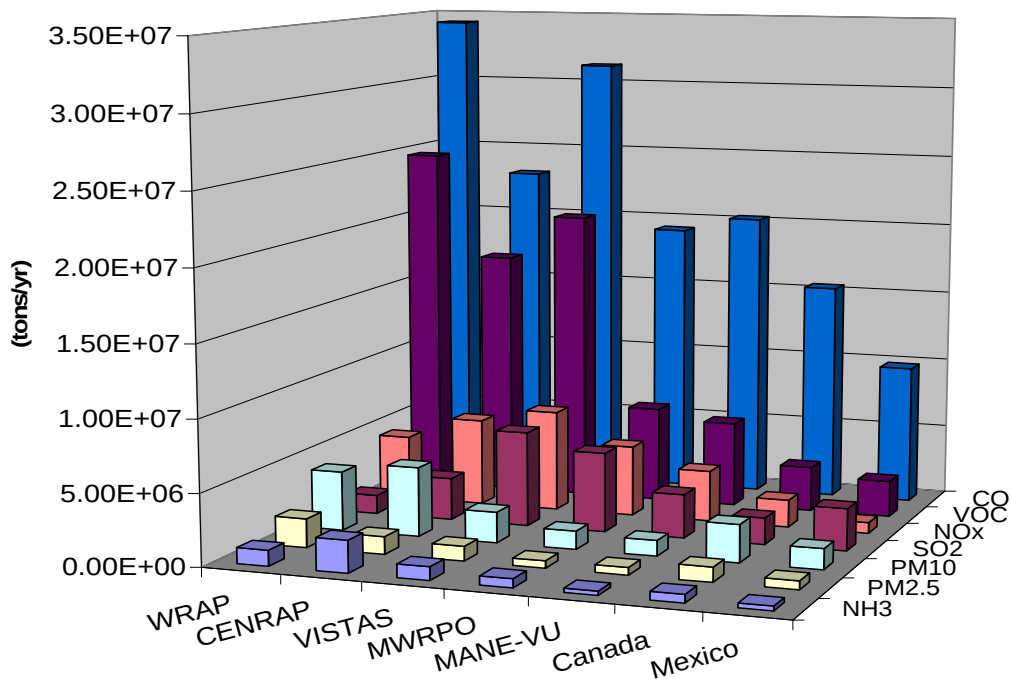


Figure 5-10. Pre02c_36 total domain annual emissions summary.

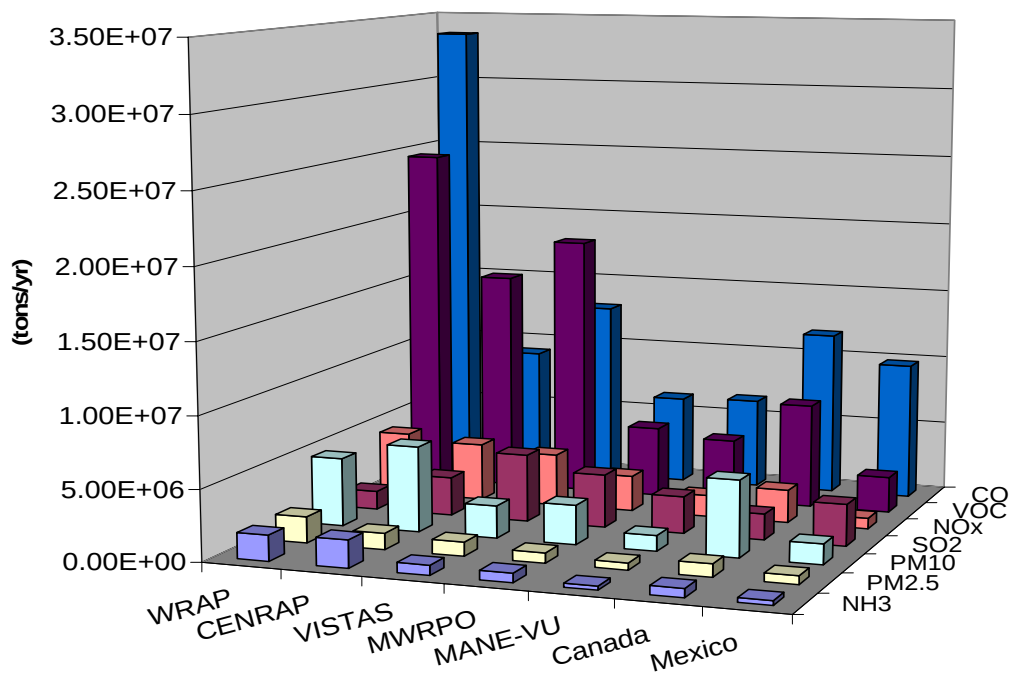


Figure 5-11. Pre02d_36 total domain annual emissions summary.

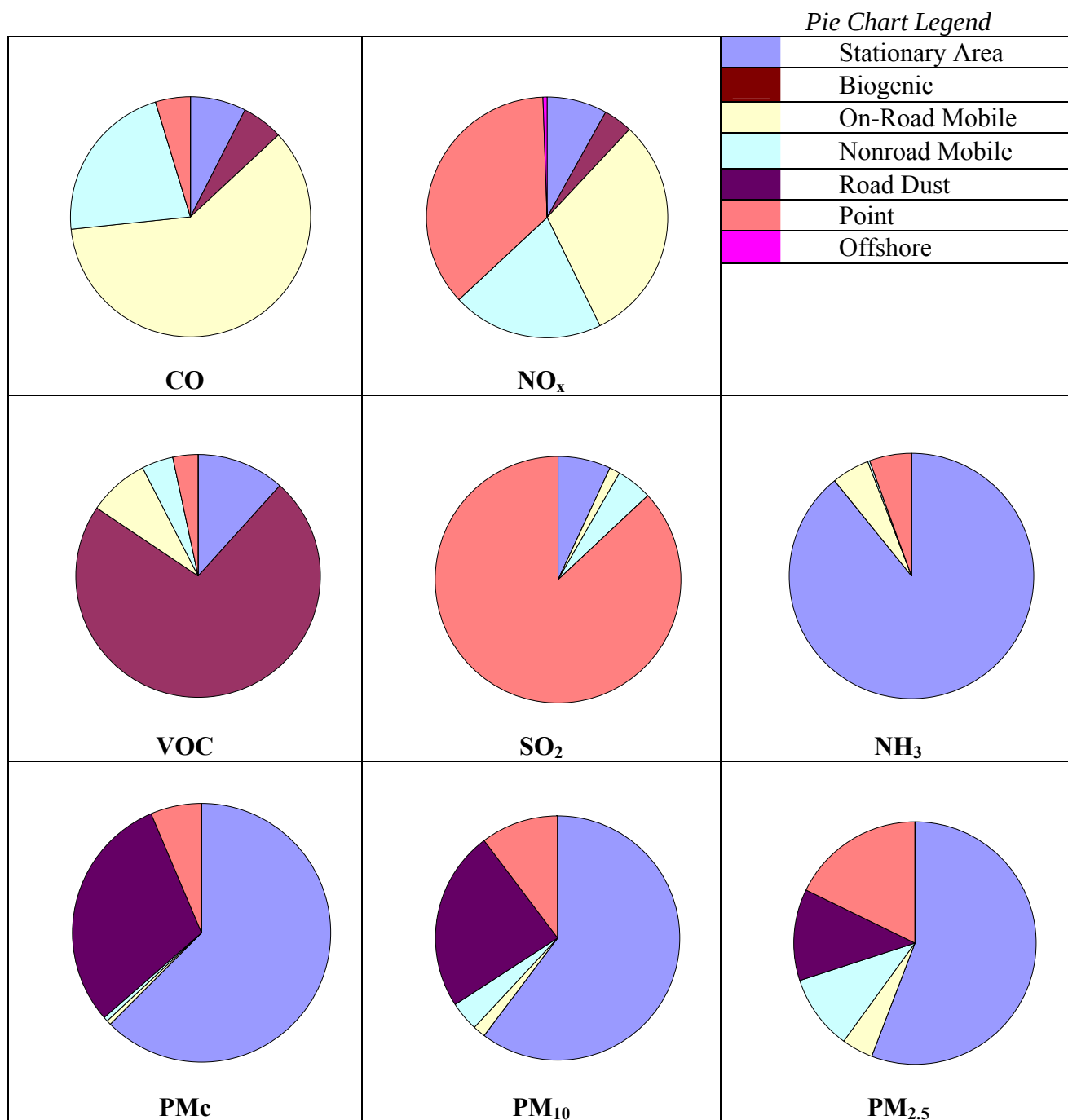


Figure 5-12. Pre02b total U.S. annual emissions pie charts.

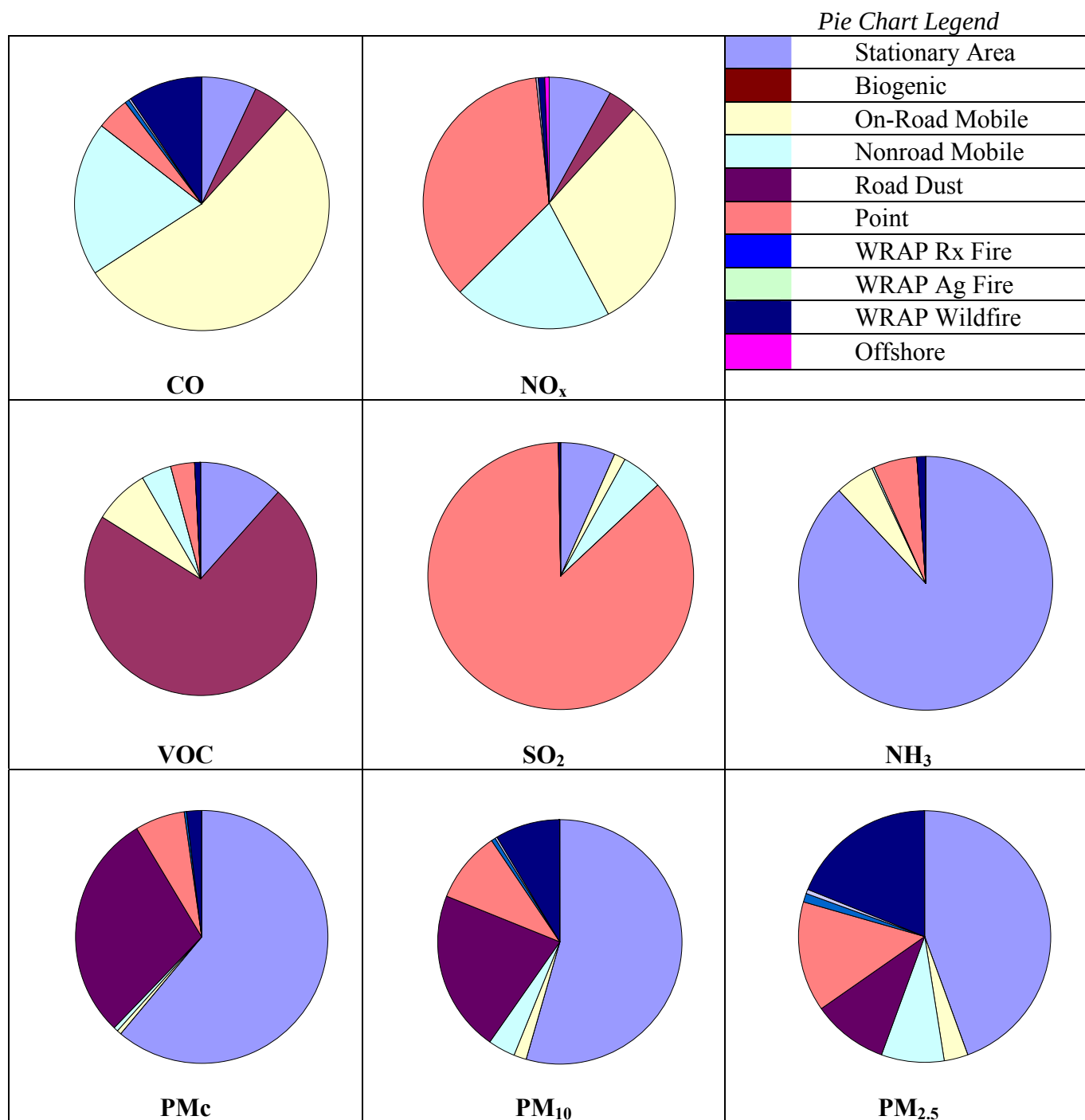


Figure 5-13. Pre02c total U.S. annual emissions pie charts.

Pie Chart Legend

	Stationary Area
	NH ₃ Model
	Biogenic
	On-Road Mobile
	Nonroad Mobile
	Road Dust
	Fugitive Dust
	Windblown Dust
	Point
	Offshore
	WRAP Nat Rx Fire
	WRAP Anthro Rx Fire
	WRAP Ag Fire
	WRAP Wildfire

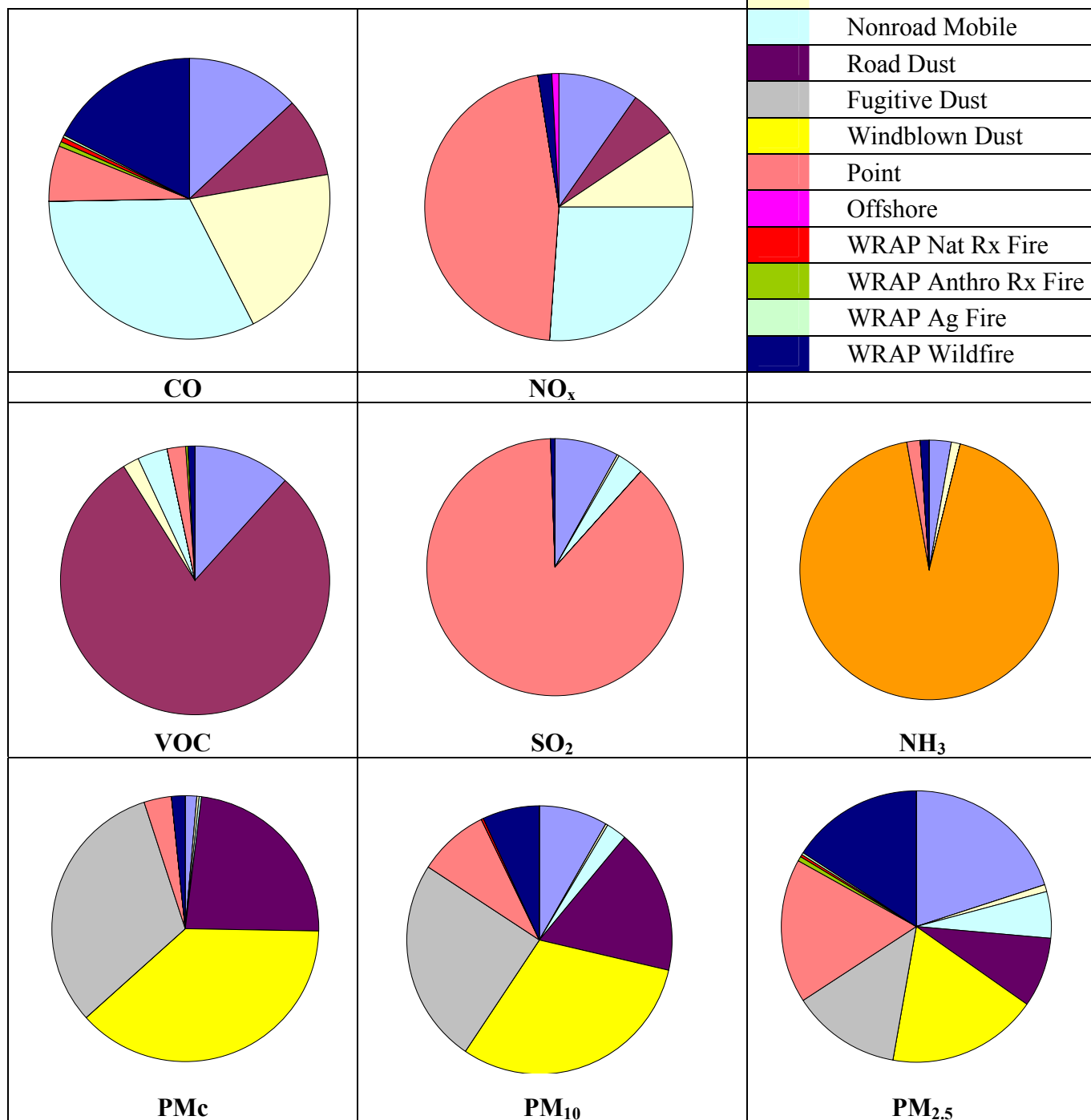


Figure 5-14. Pre02d total U.S. annual emissions pie charts.

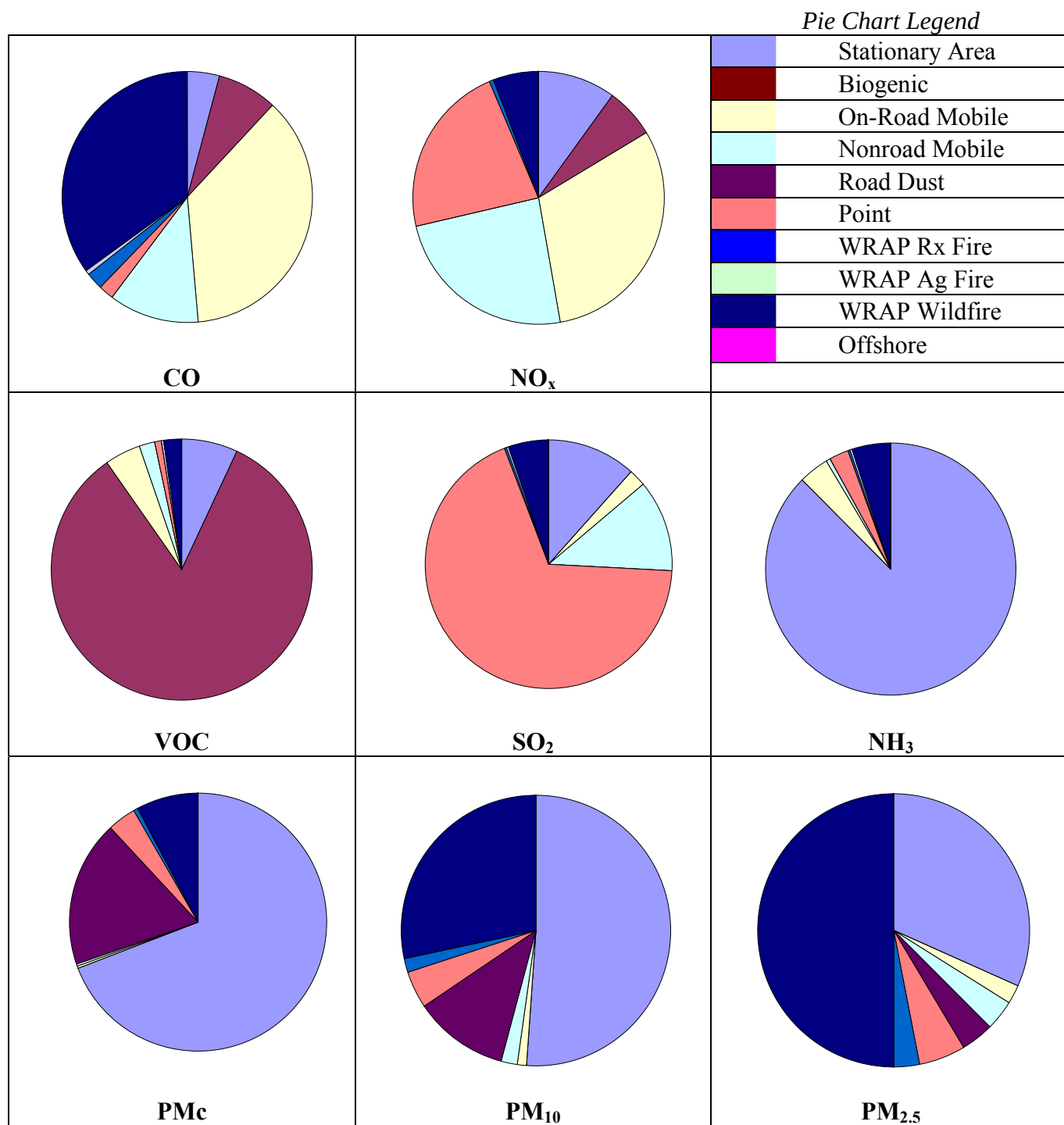


Figure 5-15. Pre02c WRAP annual emissions pie charts.

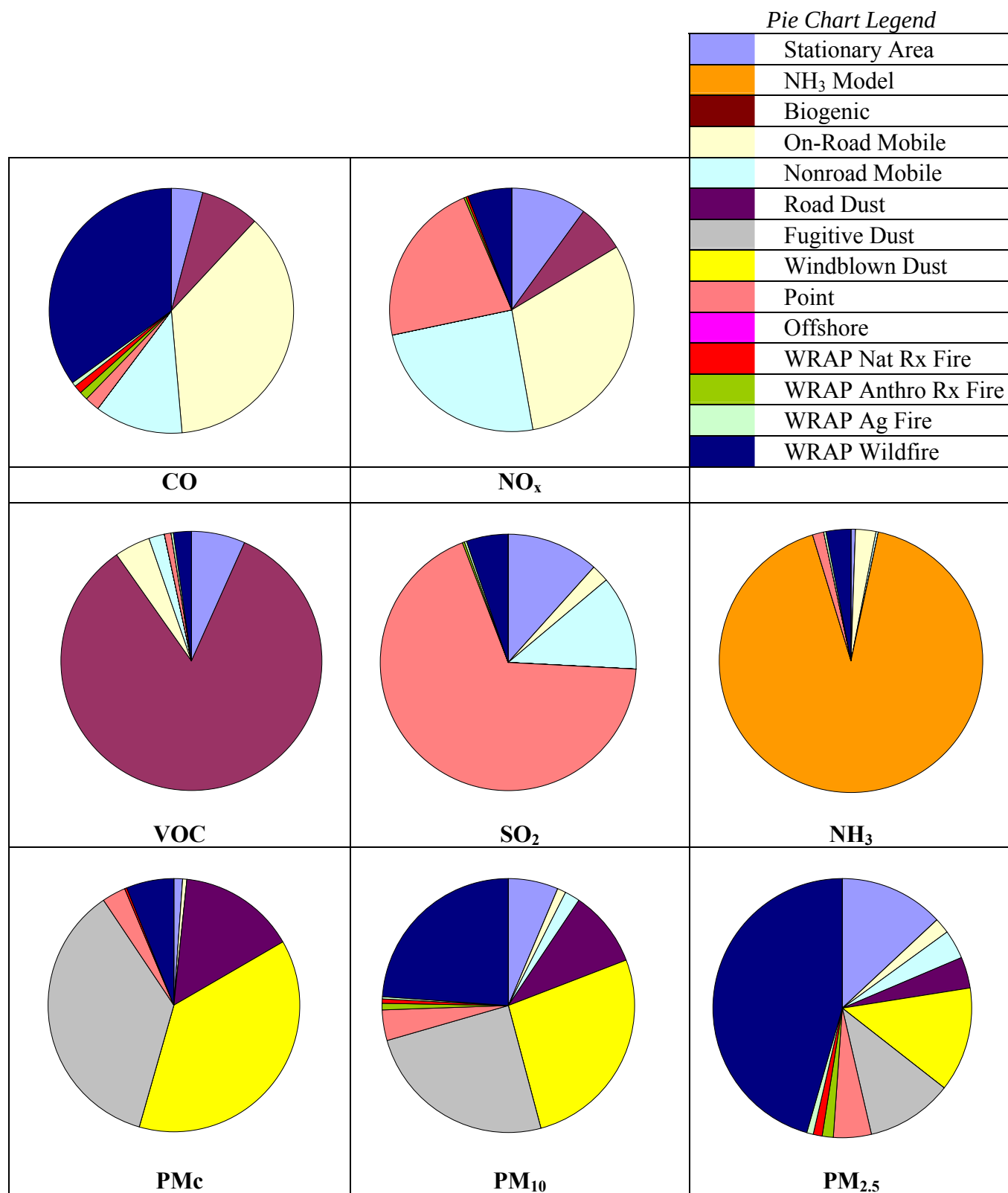


Figure 5-16. Pre02d WRAP annual emissions pie charts.

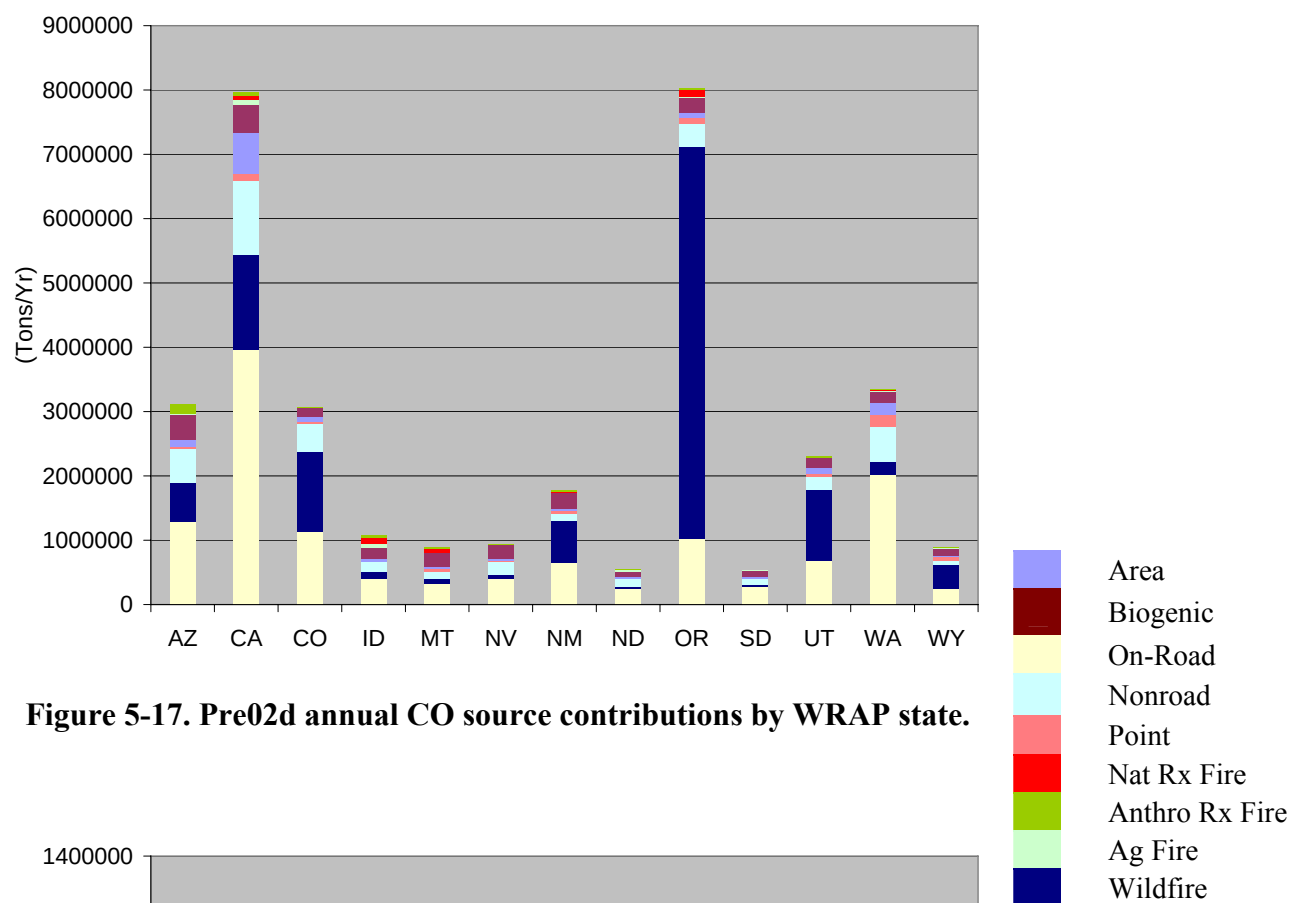


Figure 5-17. Pre02d annual CO source contributions by WRAP state.

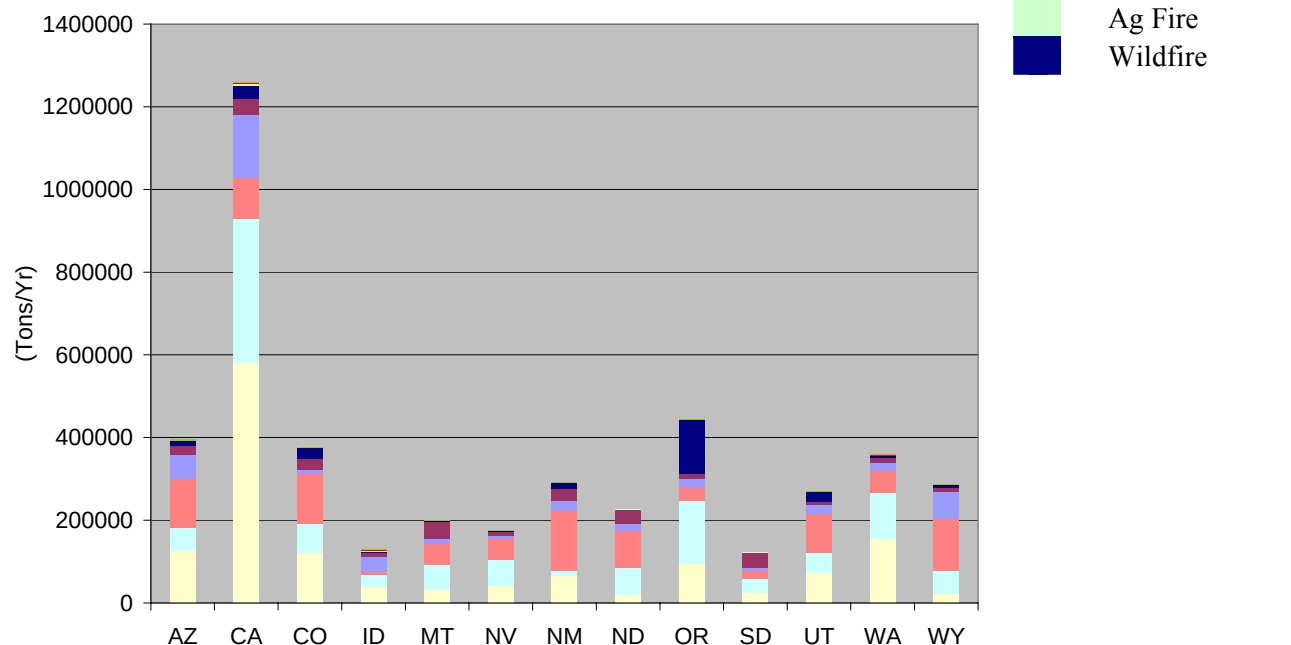


Figure 5-18. Pre02d annual NO_x source contributions by WRAP state.

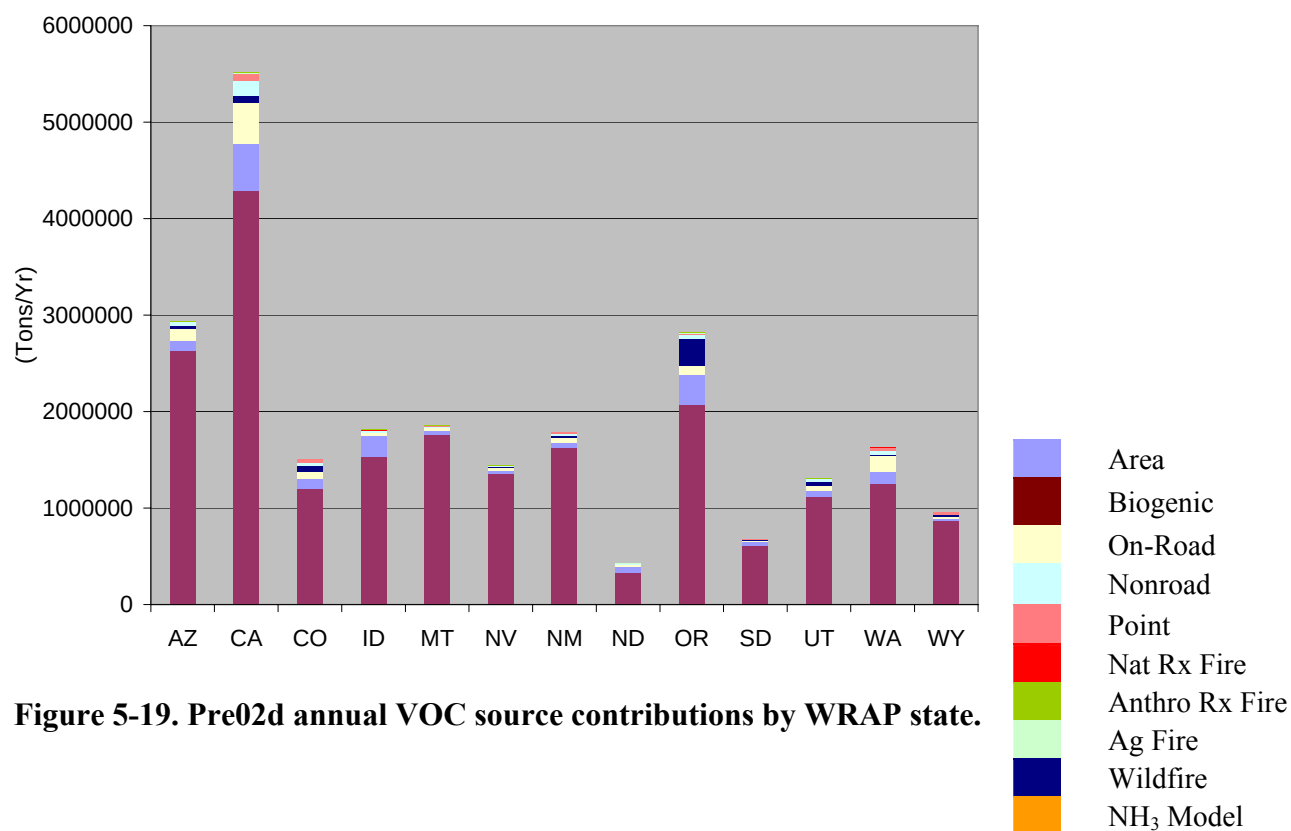


Figure 5-19. Pre02d annual VOC source contributions by WRAP state.

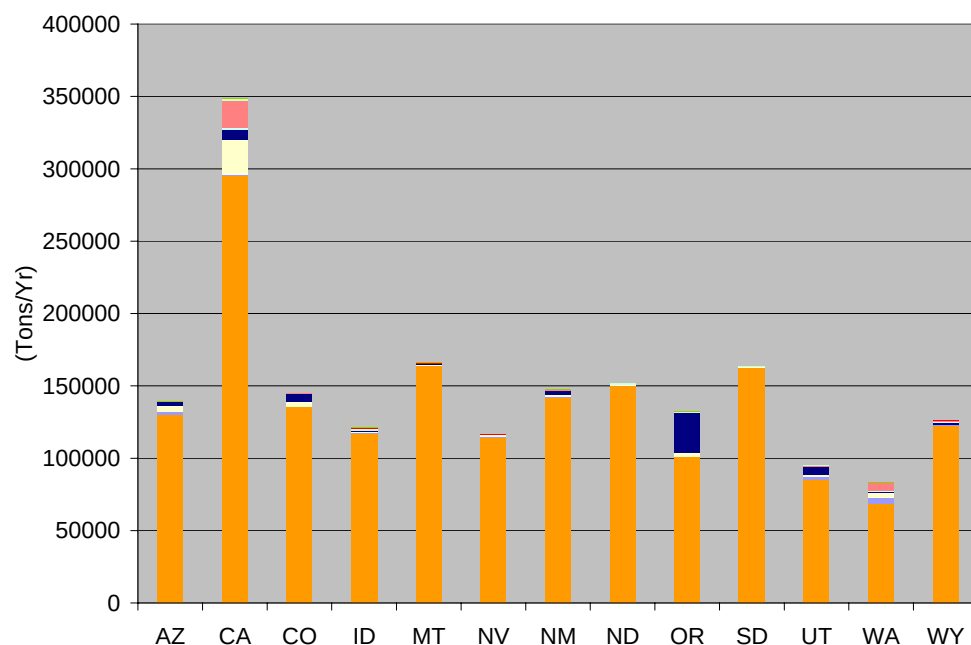


Figure 5-20. Pre02d annual NH₃ source contributions by WRAP state.

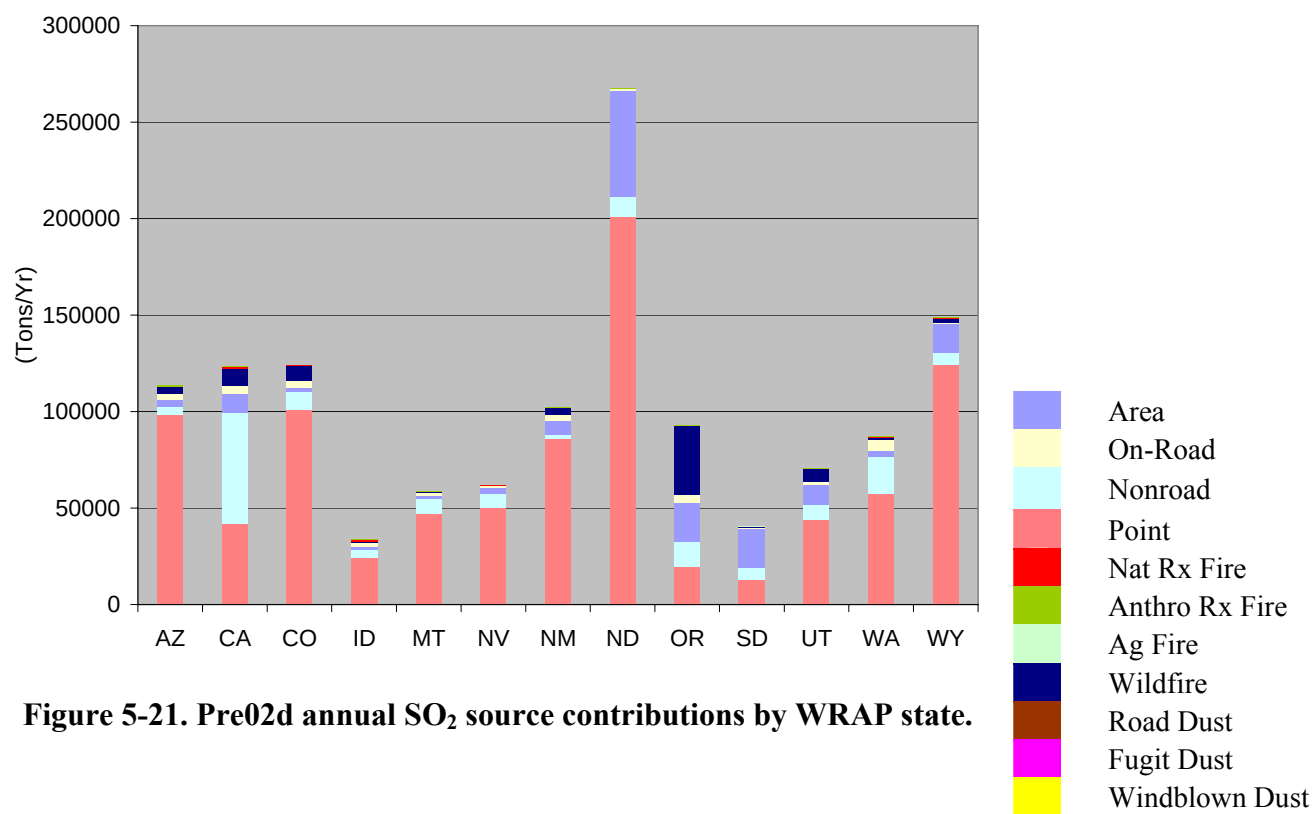


Figure 5-21. Pre02d annual SO₂ source contributions by WRAP state.

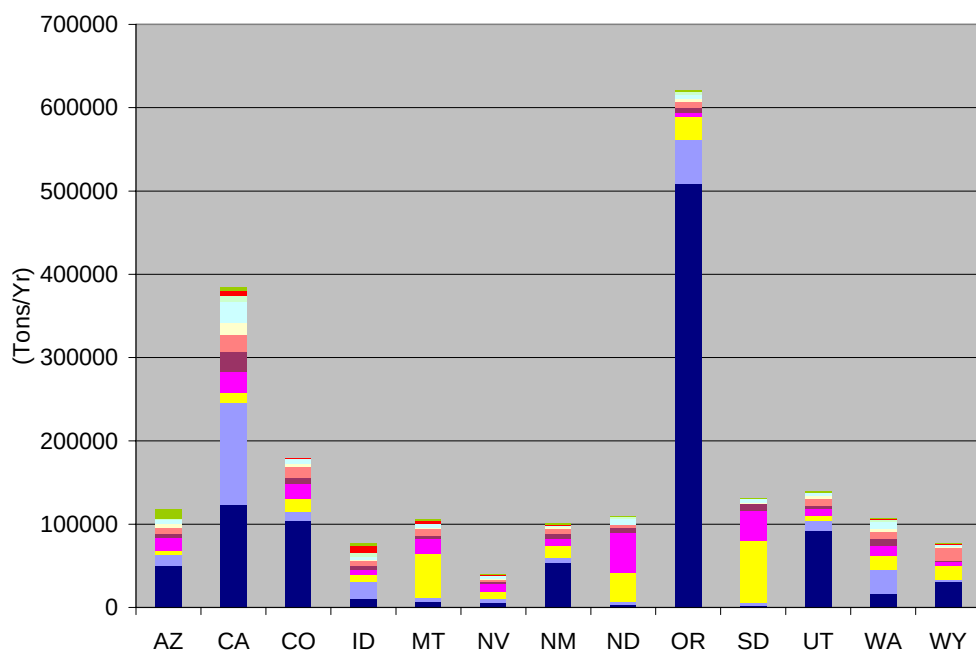


Figure 5-22. Pre02d annual PM_{2.5} source contributions by WRAP state.

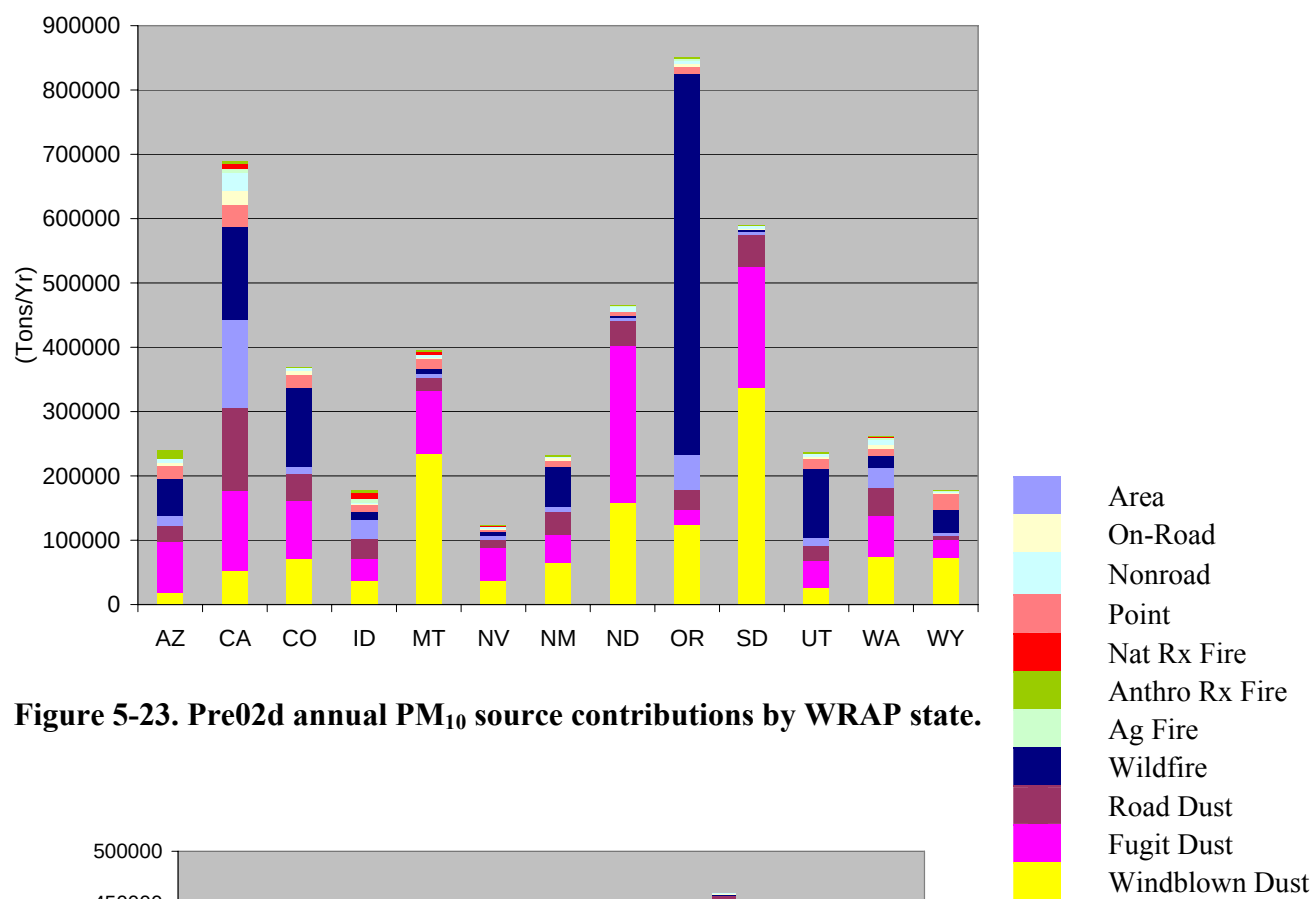


Figure 5-23. Pre02d annual PM₁₀ source contributions by WRAP state.

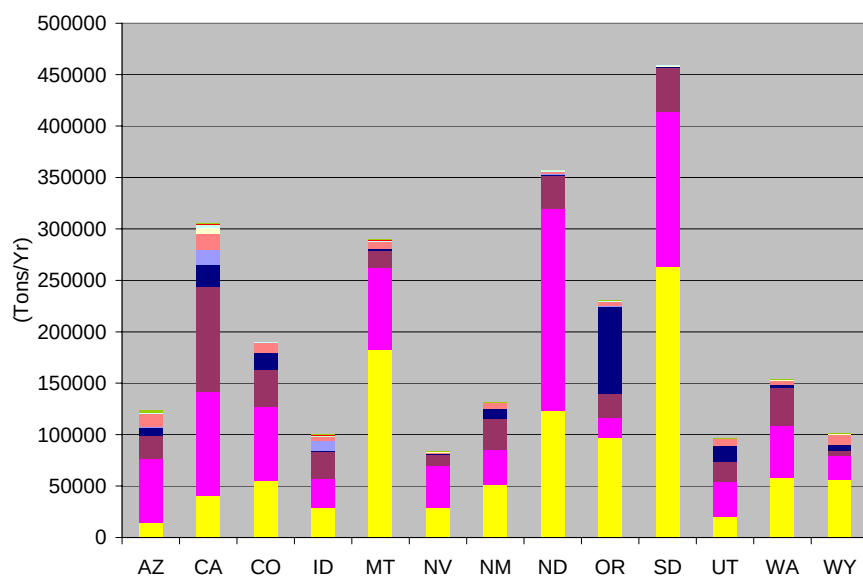


Figure 5-24. Pre02d annual PM_c source contributions by WRAP state.

5.7 Emissions Sensitivities

As most of the RMC's efforts during project year 2004 were focused on developing and refining the 2002 emissions base case, the number of emissions sensitivities performed during the reporting period was limited.

- A group of sensitivities for testing the effects of different configurations of the fire inventories (Task 11) was carried over from the 2003 work plan and is covered in detail in Section 12 of this report.
- Although simulation Pre02c is considered an extension of the preliminary 2002 base case modeling rather than an emissions sensitivity, Pre02c could be evaluated as an emissions sensitivity of the WRAP fire inventories by comparing it with Pre02b. Comparisons between the two simulations are provided in Section 5.7.
- Using the revised 2002 WRAP fire emissions inventories, we designed two sensitivities to test the effects of these new fire inventories on the air quality modeling. We designed simulation Pre02e_36 to evaluate the effects of natural versus anthropogenic fires and simulation Pre02f_36 to study the overall effects of the new fire inventories on the modeling. Additional details about simulations Pre02e_36 and Pre02f_36 are found in Sections 5.4.8 and 5.4.9, respectively.
- Although several emissions sensitivities were outlined in the 2004 RMC work plan (for evaluating different configurations of the agricultural NH₃ emissions and windblown dust models, plus a series of other unspecified sensitivities), we were able to complete only one emission control sensitivity that was derived from the Pre02c_36 simulation: Pre02c_36s01, which was introduced in Section 5.4.6 and is discussed in more detail below.

Simulation Pre02c_36s01 addressed nonroad mobile diesel controls. Working with the WRAP Economic Analysis Forum, we implemented a control scenario to evaluate the effects of the diesel retrofit program on nonroad diesel emissions in Arizona, North Dakota, and Montana. The Economic Analysis Forum provided us with control factors by Federal Implementation Standards (FIPS) code and SCC. We used this information to generate a SMOKE input file to apply the diesel retrofit program controls to VOC, CO, and PM emissions in the applicable counties in those three states. As the WRAP nonroad mobile-source inventory is not detailed enough for us to apply the controls to the exact sources that were targeted, we decided to use a more conservative approach that would control more simulated emissions than the actual controls would impact. This conservative approach overstates the effects of the control program by affecting more emissions sources and pollutants than is realistic. The Economic Analysis Forum contractor that provided the control factors agreed that the conservative approach was reasonable because of the relatively limited amount of emissions that the controls target in the model (Tom Timbario, Emissions Advantage, personal communication, October 13, 2004). Emissions Advantage and the RMC agreed that if the conservative approach showed significant results when used in an air quality modeling simulation, we would then revisit the Pre02c_36s01 sensitivity simulation and refine the controls to be more realistic. Analysis of the modeling results are available in the Economic Analysis Framework Test Application report (BBC, 2004)

5.8 Problems Encountered and Corrections

This section summarizes the emissions modeling problems we encountered during the preliminary 2002 modeling and the corrections we made. Subsections on the various emissions components present details about each major issue, including an explanation of the issue, how it was discovered, and (if necessary) the corrective actions implemented. If the issue did require corrective action, we also explain how we confirmed the fix.

5.8.1 Stationary area sources

- **Area Issue #1**

- ◆ **Question:** Why did we observe large differences between winter and summer area-source CO emissions in the eastern U.S. and Canada? Spatial plots of the emissions showed large differences in magnitude ($>100\%$) across vast spatial extents in some areas of the modeling domain.
- ◆ **Answer:** The differences in CO emissions are due to (1) seasonal activity trends and (2) different approaches for spatially allocating residential wood smoke and prescribed-fire emissions.
 - As those wood combustion sources are the largest sources of CO in the stationary-area-source inventory, the highly seasonal temporal profiles applied to them result in large differences in the emissions throughout the year.
 - The reason behind the spatial patterns of the emissions differences is related to how the emissions from those combustion sources are spatially allocated.
Canada: Due to the lack of high-resolution spatial surrogates for Canada, the area-source emissions are spatially allocated at the province level, as opposed to the county level in the U.S. The large-magnitude wood smoke emissions are spread over a wide spatial extent and appear to impact major areas of Canada in the modeling domain when spatial plots of the emissions are viewed.
United States: In the eastern U.S., the prescribed-fire emissions exhibit wide spatial impacts as opposed to the western U.S. because in the 2002 WRAP inventory, fires are treated as point sources and are concentrated to single grid cells in the WRAP states. Treated as area sources in the inventory for the eastern U.S., the fire emissions appear to have larger spatial impacts because they are being fractionally allocated to the area of entire counties.

- **Area Issue # 2**

- ◆ **Question:** Why were there no NH_3 emissions from area sources in the eastern U.S.? Spatial plots of the emissions showed NH_3 emissions everywhere in the domain except the eastern U.S.
- ◆ **Answer:** The NH_3 column in the NEI96 inventory that we used for the preliminary 2002 modeling was corrupted, resulting in the loss of some data. After reinstalling the inventory on the RMC machines, we regenerated the simulation with SMOKE. The

spatial plots created from this new simulation showed complete coverage for all area-source pollutants.

- **Area Issue # 3**

- ◆ *Question:* After integrating the NH₃ model emissions into simulations Pre02d_36, why were there still NH₃ emissions from the modeled sources in the VISTAS area-source inventory?
- ◆ *Answer:* To keep from double-counting emissions, we removed the SCCs covered by the NH₃ emissions model from the U.S. area-source inventories. The first round of the removal missed the sources in the VISTAS inventory. We discovered during QA of simulation Pre02d_36 that the sources we were supposed to have removed were still in the VISTAS inventory. We removed the sources and reran the area-source simulation.

5.8.2 Nonroad mobile sources

- **Nonroad Issue # 1**

- ◆ *Question:* Why did the spatial plots of CO, NO_x, and SO₂ show emissions in water cells off the coasts of Canada?
- ◆ *Answer:* The Canadian nonroad mobile-source inventory contains shipping emissions that are spatially allocated in shipping lanes off the coasts of Canada.

- **Nonroad Issue #2**

- ◆ *Question:* Why do time-series plots of the domain-total area-source emissions show that the emissions for the month of January are lower than in December and February?
- ◆ *Answer:* We expect all three winter months to have the same emissions magnitude. In this case, however, December and February are the same but January is lower. For some reason the WRAP area-source emissions did not get imported correctly for the January simulation and we lost these emissions from the results. A simple rerun of SMOKE for the month of January resolved the issue. The final time-series plot shows that the emissions magnitudes for December, January, and February are the same.

- **Nonroad issue #3**

- ◆ *Question:* Why did the WRAP nonroad mobile-source emissions exhibit less diurnal variability than the rest of the domain?
- ◆ *Answer:* Animations of the emissions data showed strong diurnal variability in the nonroad mobile-source emissions everywhere but in the WRAP states. Diagnostic analysis revealed that because of a new lumped SCC contained in the WRAP inventory, we were assigning the default uniform temporal profiles to the WRAP

nonroad emissions. These default profiles are flat, meaning that they assign the emissions uniformly across all months, days, and hours. These flat profiles caused the WRAP nonroad mobile-source emissions to exhibit less diurnal variability relative to the rest of the domain. Since the WRAP inventory contractor created these SCCs specifically for the 2002 WRAP modeling, we did not have cross-references for them in the default SMOKE ancillary input files. To correct this problem, we added cross-references for these new SCCs to the temporal, speciation, and spatial cross-reference files. We also added descriptions of these new WRAP nonroad SCCs to the SMOKE SCC description file. Table 5-31 lists the descriptions and the temporal, speciation, and spatial cross-reference codes applied to these new SCCs. After rerunning SMOKE with the corrected cross-reference codes, animations of the nonroad mobile-source emissions showed that the diurnal variability in these emissions in the WRAP states was more similar to that in the rest of the domain.

Table 5-31. Description and profile assignments for new WRAP 2002 nonroad mobile SCCs.*

SCC	Description	TREF code [†]	SREF code [†]	GRF code [†]
2200001000	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Recreational Equipment; Total	26	VOC: 1186 PM2.5: 35700	1
2200002000	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Construction and Mining Equipment; Total	26	VOC: 1186 PM2.5: 35700	1
2200003000	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Industrial Equipment; Total General Industrial	26	VOC: 1186 PM2.5: 35700	1
2200004000	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Lawn and Garden Equipment; Total	26	VOC: 1186 PM2.5: 35700	2
2200005000	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Agricultural Equipment; Total	26	VOC: 1186 PM2.5: 35700	6
2200006000	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Commercial Equipment; Total	26	VOC: 1186 PM2.5: 35700	1
2200007000	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Logging Equipment; Total	26	VOC: 1186 PM2.5: 35700	14
2200008000	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Aircraft; Total	26	VOC: 1186 PM2.5: 35700	10
2200008005	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Airport Ground Support Equipment; Airport Ground Support Equipment	26	VOC: 1186 PM2.5: 35700	10
2200009000	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Underground Mining Equipment; Total	26	VOC: 1186 PM2.5: 35700	1
2200010000	Mobile Sources; Off-highway Vehicles; Gasoline+CNG+LPG; Industrial Equipment; Total Oil Field Equipment	26	VOC: 1186 PM2.5: 35700	1

*New abbreviations used in this table: CNG = compressed natural gas; LPG = liquefied petroleum gas.

[†] TREF, SREF, and GRF are SMOKE cross-reference input files for temporal allocation, chemical speciation, and spatial allocation, respectively.

- **Nonroad Issue #4**

- ◆ *Question:* Why do the time-series plots of the nonroad mobile-source emissions show monthly as opposed to the expected seasonal variability?
- ◆ *Answer:* Similar to the area-source emissions, the nonroad emissions data exhibit strong seasonal temporal patterns. The time-series plots of the nonroad emissions showed more monthly variation than we expected. Diagnostic analyses revealed that because the time-series plots are derived from domainwide emissions totals (U.S. + Canada + Mexico), conflicting definitions of the seasons between the U.S. and Canada affect the temporal patterns in the aggregate emissions totals. In the U.S., the winter temporal profiles encompass the months January, February, and March; spring includes April, May, and June; etc. In Canada, the winter temporal profiles encompass the months December, January, February; spring comprises March, April, May; etc. Buried in the time-series plots are two different patterns of seasonal variability, one for the U.S. and one for Canada. Because these definitions are out of phase, they give the aggregate time-series plots the appearance of monthly variation. We did not do anything to correct this issue. Two schools of thought exist on what months constitute each season. These two schools of thought are captured in the U.S. versus Canadian temporal profiles.

- **Nonroad Issue #5**

- ◆ *Question:* Shipping emissions in the WRAP nonroad inventory are all allocated to ports, but the inventory represents both in-port and ocean-going emissions.
- ◆ *Answer:* UNC-CEP and ENVIRON split the shipping SCC in the nonroad inventory into in-port and ocean-going sources. We used the original SCC to represent the in-port component of the data and modeled them as emissions occurring at the ports. ENVIRON provided guidance on how to split the inventory to obtain the ocean-going component of the data. We allocated these emissions to cells within 25 miles of the ports or landfall. The Pacific coast of the WRAP domain now correctly represents the shipping emissions in the nonroad mobile-source inventory.

- **Nonroad Issue #6**

- ◆ *Question:* Why were on-road mobile-source refueling emissions counted in both the nonroad and MOBILE6-derived inventories?
- ◆ *Answer:* The developer of the WRAP on-road mobile-source emissions inventory alerted us to the fact that refueling emissions are contained in the on-road mobile-source inventory that they derived with MOBILE6. Investigation of the nonroad inventory revealed that we are counting refueling emissions in that inventory as well. Looking at the processes that the RMC is modeling with MOBILE6 for the non-WRAP states also reveals that we are modeling the refueling emissions in the on-road inventory there. To correct this double-counting issue, we removed the refueling SCCs from the WRAP nonroad inventory and turned off the refueling emissions

process in the non-WRAP on-road mobile simulations. Because of the form in which we received the mobile-source inventory data from the WRAP inventory developers, we are forced to be inconsistent in the way we model refueling emissions in the WRAP and non-WRAP states. For the WRAP states, we are using precomputed MOBILE6 emissions that include refueling emissions and a nonroad inventory that does not include refueling emissions. For the non-WRAP states we are running MOBILE6 to calculate on-road mobile emissions without computing refueling emissions, and using a nonroad mobile inventory that does contain refueling emissions. A more consistent approach would be either to run MOBILE6 for the entire domain and represent refueling emissions in the on-road mobile inventory or to use the precomputed refueling emissions in the nonroad mobile inventory for the entire domain.

5.8.3 Road dust sources

The RMC encountered no major QA issues during the road dust emissions modeling.

5.8.4 On-road mobile sources

- **On-road Issue #1**
 - ◆ *Question:* What was causing MOBILE6 to crash on the RMC computers?
 - ◆ *Answer:* We discovered that we can run MOBILE6 only on a dedicated node because of memory limitations. MOBILE6 requires too much system memory to run on both processors of a node. We now run MOBILE6 on dedicated RMC machines.
- **On-road Issue #2**
 - ◆ *Question:* Why do the MOBILE6 emissions files sporadically contain bad values and infinities?
 - ◆ *Answer:* We are speculating that networking traffic corrupts the write functions of some SMOKE programs. We think that the system is the culprit and not SMOKE. Rerunning the modeling period where the bad values occurred corrects the problem, thus identifying the state of the system as the variable affecting the model results. When we find files containing bad values, we rerun SMOKE to correct the problem.
- **On-road Issue #3**
 - ◆ *Question:* Why do the on-road mobile-source time-series plots show weekly and monthly variability? There does not appear to be any uniformity in the temporal patterns.
 - ◆ *Answer:* Unlike the stationary-area- or nonroad mobile-source emissions, on-road mobile-source emissions are derived using hourly temperatures. The influence of the hourly meteorology causes emissions differences on an hourly basis.

- **On-road Issue #4**

- ◆ *Question:* Why were PM emissions double-counted in the states outside of the WRAP domain?
- ◆ *Answer:* Analyses of the spatial plots of the on-road mobile-source emissions revealed that PM emissions existed in both the VMT simulations and the precomputed emissions simulations in the non-WRAP states. The redundancy indicated that the emissions were being double-counted during the final merge of the files. We removed the PM contribution from the precomputed emissions and reran the simulations. Now PM is being calculated only by MOBILE6 for the non-WRAP states.

- **On-road Issue #5**

- ◆ *Question:* Why do the spatial plots of the on-road mobile-source emissions show that there is no SO₂ from mobile sources in Canada, nor NH₃ from mobile sources in Mexico?
- ◆ *Answer:* The Canadian and Mexican emissions inventories do not contain on-road mobile-source emissions for SO₂ or NH₃, respectively.

5.8.5 Point sources

5.8.5.1 Stationary point sources

- **Point Issue #1**

- ◆ *Question:* Why did the first PinG simulation drop all of the emissions in the WRAP states?
- ◆ *Answer:* Spatial plots of vertically summed emissions showed that there were no stationary-point-source emissions in the WRAP states following the PinG SMOKE simulation. Because we wanted to select only PinG sources in the WRAP states, we attempted to define the WRAP region as a subdomain of the entire modeling region. SMOKE was not able to handle the definition of the subdomain and ended up dropping all emissions in the WRAP states. The solution to the problem was to split the point-source inventory between the WRAP and non-WRAP states. We then applied the PinG selection criteria to the WRAP inventory and merged it with the non-WRAP point-source inventory later. The vertically summed spatial plots derived from this new simulation revealed that only a select subset of cells in the WRAP states are affected by the PinG simulation.

- **Point Issue #2**

- ◆ *Question:* Why were there stationary point NH₃ sources in the CENRAP states that are 50% larger than similar sources in other parts of the modeling domain?

- ◆ *Answer:* An error in the NEI96 propagated through to the WRAP 2002 stationary-point-source inventory, which was based on the NEI96. The NEI2002 released by the EPA in 2004 corrected these errors. We removed the CENRAP point sources from the WRAP inventory and replaced these data with the NEI2002.

5.8.5.2 Fire sources

- **Fire Issue #1**

- ◆ *Question:* Why was SMOKE having a memory fault when we tried to import the prescribed-fire inventory?
- ◆ *Answer:* The prescribed-fire emissions inventory is too large (too many sources) to process as an annual inventory. We broke the inventory into monthly segments and it processed through SMOKE with no problems.

- **Fire Issue #2**

- ◆ *Question:* What do the vertical profile plots for the prescribed and wildfire emissions show large emissions spikes in layer 15 on some days?
- ◆ *Answer:* Some prescribed and wildfire emissions reach to the top of the model (layer 19). When the emissions layers are capped at layer 15, all of the emissions that are allocated above layer 15 are collapsed into the top emissions layer by SMOKE. We reconfigured SMOKE to extend the emissions layers for prescribed and wildfires to layer 19. Regenerated vertical profile plots then showed a smooth falloff of the emissions with height.

- **Fire Issue #3**

- ◆ *Question:* Why was SMOKE unable to recognize the time zone “AKT” in the 2002 fire inventories?
- ◆ *Answer:* The 2002 fire inventories contained data for Alaska that are tagged with the time zone code “AKT”. SMOKE is not configured to run using the AKT time zone, so it crashed when it read this field in the inventory files. As Alaska is outside of the WRAP 36-km modeling domain, we changed the time zone of the Alaska emissions to “PST” to allow SMOKE to run through to completion. The Alaska emissions are not being used in this application of the preliminary 2002 modeling, so this modification to the time zone for these sources is irrelevant.

- **Fire Issue #4**

- ◆ *Question:* Why did the new prescribed fire and wildfire sources have default temporal and speciation profiles applied, when we created profiles specifically for these sources during the §309 modeling in 2002?

- ◆ *Answer:* The new 2002 fire inventories contained SCCs that we had never modeled. We needed to add these SCCs to the temporal and speciation cross-reference files to apply the correct temporal and chemical profiles to these new sources. After adding the correct cross-references to these sources to the SMOKE input files, we reran the natural and anthropogenic fire emissions and the revised wildfire emissions through SMOKE. QA on the new simulation revealed that the correct profiles are now being applied to these sources.

5.8.5.3 Offshore sources

- **Offshore Issue #1**

- ◆ *Question:* Why did the first version of the off-shore emissions inventory for California contain sources on-shore?
- ◆ *Answer:* Spatial plots of the off-shore emissions revealed several sources on-shore in California. We adjusted the lat-lon coordinates for these sources to place them in their intended locations off the coast.

5.8.6 Biogenic sources

The RMC encountered no major QA issues during the biogenic emissions modeling.

5.8.7 SMOKE ancillary input files

5.8.7.1 Spatial surrogates

- **Surrogate Issue #1**

- ◆ *Question:* When we implemented the new spatial cross-reference file from EPA, why did SMOKE indicate that it could not find surrogates for Dade County, FL?
- ◆ *Answer:* The EPA spatial cross-reference files use an updated FIPS code for Miami-Dade County, FL. We updated all of the inventory files for Florida to be consistent with the new coding scheme. By changing the FIPS code for Dade County from 12025 to 12086 in the appropriate inventory files, we made the inventories compatible with the new cross-reference files.

- **Surrogate Issue #2**

- ◆ *Question:* Why were there a large number of SCCs from the WRAP inventory missing from the new EPA spatial cross-reference file?
- ◆ *Answer:* The WRAP inventory contained more recent information than the EPA surrogates file. Switching to the new EPA surrogates in April 2004 and obtaining the new cross-reference file for these surrogates corrected most of these missing SCC assignments.

5.8.7.2 Temporal profiles

The RMC encountered no major QA issues with the temporal profiles.

5.8.7.3 Speciation profiles

The RMC encountered no major QA issues with the speciation profiles.

5.9 Outstanding Emissions Issues

This section outlines two sets of issues with the preliminary 2002 modeling. The first set below are those that needed to be resolved after simulation Pre02c. These were listed in the WRAP 2004 interim report, but had not yet been resolved at that time. As discussed below, we corrected many of the issues from the Pre02c simulation in simulation Pre02d. The second set are issues that came to light during the Pre02d modeling and that are yet to be resolved. They will need to be corrected in the next round of 2002 modeling.

- **Pre02c emissions issues (now corrected):**
 - ◆ We did not include windblown dust emissions in simulation Pre02c.
 - Emissions from the WRAP windblown dust model were added in simulation Pre02d.
 - ◆ No transport fractions were applied to the fugitive dust emissions sources within the stationary-area-source inventory.
 - Fugitive dust sources were treated explicitly in simulation Pre02d using an inventory that contains transport fraction corrections based county land-cover data.
 - ◆ Placeholder 2002 emissions inventories were used for the non-WRAP U.S. states. (We were waiting for actual 2002 emissions inventories from the other RPOs.)
 - In simulation Pre02d we replaced the placeholder inventories with the VISTAS 2002 inventories and the NEI2002.
 - ◆ We did not include output from the ENVIRON NH₃ emissions model in simulation Pre02c.
 - We added emissions from the NH₃ model in simulation Pre02d.
 - ◆ We used an outdated Canadian emissions inventory.
 - In simulation Pre02d we replaced all of the nonpoint Canadian inventories with the 2000 National Canadian Inventory.
 - ◆ There were no 12-km meteorology data to use for finishing the emissions simulations on the nested WRAP domain.
 - Annual meteorology data for the 12-km WRAP modeling domain became available in February 2005, allowing us to complete the 12-km emissions simulation.

- ◆ We did not include offshore-mobile-source (shipping) emissions in simulation Pre02c.
 - For simulation Pre02d, we split the shipping emissions in the nonroad inventory into in-port and ocean-going sources. The ocean-going emissions only are a fraction of the shipping emissions, but there is still work required to add emissions from the commercial shipping lanes and in international waters.
- ***Pre02d emissions issues (still to be corrected):***
 - ◆ We need to replace the placeholder NEI2002 inventories with actual 2002 inventories from the other RPOs as they become available. The MANE-VU, CENRAP, and Midwest RPOs all have 2002 inventories that we will include in the next iteration of the 2002 emissions base case simulation.
 - ◆ No in-flight aircraft emissions were included.
 - ◆ We treated Mexican and Canadian emissions with U.S. rather than local holidays.
 - ◆ We need to replace the 1999 Mexican emissions inventory with the 2000 inventory that will be available in Spring 2005.
 - ◆ We need to replace the Gulf of Mexico offshore-point-source emissions inventory with the 2002 Minerals Management area- and point-source inventories.
 - ◆ Emissions from many natural sources are missing, such as geogenic, volcanic, and sea salt emissions.
 - ◆ We need to replace the preliminary Canadian 2000 inventories with the final version of these data.
 - ◆ We need to upgrade the RMC systems to SMOKE version 2.1.

5.10 Emissions Data Technology Transfer

As part of an outreach program, the RMC prepared a number of SMOKE reports and gridded emissions data in ASCII format and sent them to Cassie Archuleta of Air Resource Specialists, Inc. These reports included annual totals by state for area, mobile, nonroad mobile, point, road dust, and offshore sources from scenario Pre02b, and daily reports for the fire and biogenic sources from scenario Pre02c.

Also for Cassie Archuleta, we summed and extracted yearly totals for PMFINE and PMC from netCDF files, and prepared ASCII gridded emissions files for area, point, road dust, and windblown dust sources and total emissions. We also sent her files of NH₃ data from the ammonia emissions model developed by ENVIRON, as gridded data and “by county” data for total NH₃ and by NH₃ category.

Annual averages for EXT, DECV, OC, and EC were calculated and sent to Air Resource Specialists, Inc., as ASCII gridded values for scenarios Pre02b, Pre02c, Pre02e, and Pre02f.

We sent SMOKE programs and scripts to the Park Services in Colorado and helped them install and run these scripts for scenario Pre02d. The Pre02 inventory and meteorology data along with some SMOKE outputs were also sent to them. Other SMOKE reports were sent to the Utah Division of Air Quality.

5.11 Next Steps

As stated at the beginning of Section 5, the primary goal of the RMC emissions modeling team in project year 2004 was to develop a comprehensive 2002 base case emissions inventory for the WRAP. Through the modeling of the various preliminary base case simulations discussed above, we refined and quality-assured the WRAP 2002 emissions inventories. The next step in the emissions simulation task is to conduct the final (as opposed to preliminary) 2002 base case simulation. We anticipate starting on this simulation after the RMC finishes preparing the final 36-km and 12-km meteorology data in early 2005. The first step in simulating the final 2002 base case will be to upgrade the RMC modeling system to SMOKE version 2.1 (CEP, 2004a). Then, as the data become available, we will reprocess the meteorology-dependent emissions categories, integrate any new inventory data that become available, and address any issues/problems discovered during the QA process for simulation Pre02d. In addition to the new meteorology, we expect new Mexican inventories, additional U.S. RPO 2002 inventories, and updates to the WRAP windblown dust emissions to become available before the final 2002 base case simulation is completed. The final 2002 emissions modeling will be completed for both the continental 36-km domain and the nested WRAP 12-km domain. Depending on the results of the PinG emissions sensitivity that is pending with the RMC, the final 2002 emissions may also include some PinG emissions for the largest WRAP point sources.

After completing the final 2002 base case simulation, we will work on creating a future-year, 2018 base case emissions simulation. After finalizing the 2018 emissions, we will begin conducting emissions sensitivities to evaluate natural sources of haze in the WRAP region. Throughout all of the modeling that the RMC emissions modeling team will complete in 2005, we will continue to refine the WRAP emissions modeling QA protocol and streamline the process of running annual emissions simulations, completing the quality assurance, and transmitting the data to the air quality modeling team for input to CMAQ or CAMx.

5.12 Status of Task 3 Deliverables

Table 5-32 gives the status of each Task 3 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 5-32. Status of the Task 3 deliverables.

Deliverable	Status
2002 36-km winter/summer emissions simulation	Completed in January 2004: simulation Pre02a_36
2002 36-km annual emissions simulation	Completed in May 2004: simulation Pre02b_36
Periodic major updates to the annual 2002 simulation	Completed in June 2004: simulation Pre02c_36 Completed in December 2004: simulation Pre02d_36 Completed in September 2004: simulation Pre02e_36 Completed in September 2004: simulation Pre02f_36
2002 12-km emissions simulation	Completed meteorology-independent emissions in August 2004: simulation Pre02c_12 Completed in February 2005: simulation Pre02d_12
Emissions for PinG case	Completed one-month preliminary PinG emissions simulation in August 2004: simulation Pre02c_36_PinG

6. Task 4: Air Quality Model Evaluation for 2002 Annual Simulation

In this section we present the operational model performance evaluation of the preliminary 2002 Base D (pre02d) CMAQ base case annual simulation. The pre02d scenario is the fourth and final preliminary 2002 base case emissions scenario generated as part of the WRAP 2002 modeling using preliminary and projected estimates of 2002 emissions (see Section 5).^{*} We applied CMAQ for the 2002 calendar year on the 36-km continental RPO Unified domain and the 12-km WRAP modeling domain. For meteorological input, the pre02d CMAQ base case simulation used results from the final WRAP 2002 MM5 simulation discussed in Section 4. The CMAQ pre02d model performance evaluation presented in this section focuses on the performance for PM components within the WRAP subregion, although model performance across the entire continental U.S. is also presented. The CMAQ 2002 pre02d 36- and 12-km simulations were evaluated using gas-phase and particulate matter species and wet deposition from the Interagency Monitoring of Protected Visual Environments (IMPROVE) network, the Clean Air Status and Trends Network (CASTNet), the Speciated Trends Network (STN), and the National Atmospheric Deposition Program (NADP) network, as well as the Southeastern Aerosol Research and Characterization 24-hour (SEARCH) and hourly (SEARCH_H) observations networks in the southeastern United States. Many displays of CMAQ model performance have been generated for the pre02d base case simulation and are contained on the project web site:

<http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#pre02d>

Section 6 summarizes the operational evaluation of the CMAQ pre02d base case simulation for PM species only in the WRAP subregion. The reader is invited to peruse the project web site for additional model performance information.

6.1 Operational Evaluation Approach

As the 2002 CMAQ pre02d simulation is an interim simulation using preliminary emissions inputs, the model performance evaluation is neither comprehensive nor exhaustive. Rather, it is designed to test the 2002 modeling approach and to identify any obvious flaws in the modeling system and model inputs so that any corrections needed can be applied to the subsequent revised 2002 CMAQ base case simulation to be conducted in 2005. The WRAP 2002 CMAQ modeling database is intended be used to develop the visibility SIPs and TIPs due in December 2007 (see Section 1.1.1). Accordingly, our operational evaluation focuses on the six components of PM that are used to generated visibility estimates using the IMPROVE aerosol extinction equation (these include four of the major components of PM_{2.5}):

^{*}Future 2002 emissions modeling performed in the next project year will be based on final 2002 emissions inventories.

- Sulfate (SO₄)
- Particulate nitrate (NO₃)
- Organic carbon (OC)
- Elemental carbon (EC) or light-absorbing carbon (LAC)
- Other inorganic fine PM (soil)
- Coarse mass (CM)

The IMPROVE aerosol extinction equation (Malm et al., 2000) assumes that SO₄ and NO₃ are completely neutralized by ammonium (NH₄). This is partly because the standard IMPROVE measurements do not include NH₄. Thus, the evaluation below only briefly discusses NH₄ model performance using derived NH₄ “observations” for the IMPROVE network by assuming NH₄ completely neutralizes the SO₄ and NO₃ measurements.

6.1.1 Performance evaluation tools

One of the challenges in evaluating an annual PM-ozone model simulation is the synthesis and interpretation of many graphical and tabular displays of model performance into a few concise and descriptive displays that identify the most salient features of model performance. As part of the WRAP evaluation of the 2002 36- and 12-km CMAQ pre02d base case simulations, we used several analysis tools that automatically generated numerous graphical and statistical summaries used to gauge model performance, taking advantage of their various descriptive and complementary characteristics:

- *UCR Analysis Tools*: The UCR analysis tools were used extensively in the WRAP §309 modeling for 1996, and are run on a Linux platform separately for each monitoring network. Graphics are automatically generated using gnuplot, and the software generates the following:
 - ◆ Tabular statistical measures
 - ◆ Time-series plots
 - ◆ Scatterplots for three stratifications: (1) all sites in the selected subregion and selected time period (allsite_allday); (2) all days in the selected time period for each site (allday_onesite); and (3) all sites within the selected subregion for each day (allsite_oneday).
- *ENVIRON Analysis Tools*: ENVIRON also has model evaluation analysis tools similar to the UCR tools. Because they were redundant, they were not used in the WRAP study. However, as part of the WRAP §309 SIP analysis, ENVIRON developed specialized evaluation tools that interface with the UCR tools to analyze visibility model performance for the best-20% and worst-20% visibility days that are used in visibility projections.
- *Bugle Plots*: Dr. James Boylan of the Georgia Department of Natural Resources has developed a technique for displaying model bias and error with model performance goals

and criteria as a function of observed concentration that allows the performance goals to expand as the concentrations decrease.

The analysis tools generated thousands of statistical measures and graphical displays of model performance that cannot all be displayed in this report. We went through the plots and measures using slide shows, looking for indications of potentially faulty inputs or model formulation problems that should be corrected for the revised 2002 CMAQ simulations and pulling out key descriptive displays for this report.

Note that model performance statistics are calculated separately for each of the monitoring networks. Different PM measurement technology can produce different measurement values even when measuring the same air parcel. Thus, we did not mix measurements from different networks when calculating model performance metrics.

6.1.2 Subdomains analyzed

Using the monitoring networks listed in the first paragraph of Section 6, we analyzed PM model performance for the preliminary 2002 CMAQ 36-km and 12-km pre02d base case simulations for just the WRAP subregion. Note that because the SEARCH network monitors reside only in the southeastern U.S., the model performance for the SEARCH and SEARCH_H networks is not included in this report.

6.1.3 Model performance goals and criteria

The issue of model performance goals for PM species is an area of ongoing research and debate. For ozone modeling, EPA has established performance goals for 1-h ozone normalized mean bias and gross error of $\leq \pm 15\%$ and $\leq 35\%$, respectively (U.S. EPA, 1991). EPA's draft fine PM modeling guidance notes that performance goals for ozone should be viewed as upper bounds of model performance that PM models may not be able to always achieve, and that we should demand better model performance for PM components that make up a larger fraction of the PM mass than those that are minor contributors (U.S. EPA, 2001). Measuring PM species is not as precise as monitoring ozone. In fact, the differences in measurement techniques for some species likely exceed the more stringent performance goals, such as those for ozone. For example, recent comparisons of the PM species measurements using the IMPROVE and STN measurement technologies found differences from approximately $\pm 20\%$ (SO_4) to $\pm 50\%$ (EC) (Solomon et al., 2004).

For the preliminary 2002 CMAQ pre02d base case modeling, we adopted three levels of model performance goals or criteria for bias and gross error (Table 6-1). They start with the most stringent ozone bias/error performance goals of $\pm 15\%/35\%$, which are followed by $\pm 30\%/50\%$ bias/error performance goals that we believe a good-performing PM model should achieve, and they conclude with $\pm 60\%/75\%$ bias/error criteria that, if equaled or exceeded, suggest potential problems with the model simulation. Note that we are not suggesting that these performance goals/criteria be generally adopted or that they are the most appropriate to use. Rather, we are using them just to frame and put the PM model performance into context and to facilitate model performance intercomparison across episodes, species, models, and sensitivity tests.

Table 6-1. Model performance goals/criteria used to help interpret modeling results.

Fractional Bias	Fractional Error	Comment
$\leq \pm 15\%$	$\leq 35\%$	If these ozone model performance goals are met, PM model performance would be considered good. Note that for many PM species, measurement uncertainties may exceed these goals.
$\leq \pm 30\%$	$\leq 50\%$	Proposed PM model performance goals that we would hope each PM species could meet.
$\leq \pm 60\%$	$\leq 75\%$	If these proposed PM criteria are exceeded, that indicates potential fundamental problems with the modeling system.

As noted in EPA's draft fine PM modeling guidance, less abundant PM species should have less stringent performance goals. Accordingly, we are also using performance goals that are a continuous function of average observed concentrations, as proposed by Dr. James Boylan at the Georgia Department of Natural Resources (Boylan, 2004), which have the following features:

- Asymptotically approaching proposed performance goals/criteria (i.e., the $\pm 30\%/50\%$ and $\pm 60\%/75\%$ bias/error levels listed in Table 6-1) when the mean of the observed concentrations is greater than $2.5 \mu\text{g}/\text{m}^3$.
- Approaching 200% error and $\pm 200\%$ bias when the mean of the observed concentrations approaches zero.

On "bugle plots," bias and error are plotted as a function of average observed concentrations. As the mean observed concentration approaches zero, the bias performance goals and criteria flare out to $\pm 200\%$, creating a horn shape (hence the plot name). Dr. Boylan has defined three zones of model performance: Zone 1 meets the $\pm 30\%/50\%$ bias/error performance goals and is considered "good" model performance; Zone 2 lies between the $\pm 30\%/50\%$ performance goals and $\pm 60\%/75\%$ performance criteria and is an area where concern for model performance is raised; and Zone 3 lies above the $\pm 60\%/75\%$ performance criteria and is an area of questionable model performance.

Note that Dr. Boylan's chosen observed concentration ($2.5 \mu\text{g}/\text{m}^3$) where the performance goals/criteria begin to flare toward $\pm 200\%$ may be more appropriate for the eastern U.S., where concentrations are higher and visibility impairment greater; it may be too high for the western U.S., which has lower concentrations. For now we are using his chosen concentration in our evaluation, but the issue should be re-examined for the western states.

6.1.4 Performance time periods

In this 2002 CMAQ pre02d evaluation, model performance evaluation statistics and graphical displays were generated for monthly time periods using the native averaging times of each monitoring network (i.e., 24 hours for IMPROVE and STN; one week for CASTNet and NADP). We did not attempt to evaluate the model using longer-term averages (e.g., seasonal and annual

averages). The monthly performance evaluation does provide some indications of seasonal trends in performance. We could have used longer-term averaging in the model evaluation by converting the predicted and observed short-term concentrations into longer-term averages, but using that procedure can mask some performance problems and may introduce compensating errors, with overpredictions compensating for underpredictions. For example, in the WRAP 1996 multimodel evaluation we saw that the three models (CMAQ, REMSAD, and CAMx) exhibited low sulfate bias for annual averages, but that was due to a winter overestimation bias being compensated for by a summer underestimation bias. We therefore avoided using longer-term averages so that we did not defeat one of the purposes of the CMAQ 2002 pre02d base case evaluation: to uncover flaws and problems that should be corrected in revised CMAQ base cases.

6.1.5 Performance measures

The UCR model performance analysis tools generate hundreds of graphical displays over 20 statistical measures of model performance for each species, network, subdomain, and time period comparison (see <http://pah.cert.ucr.edu/aqm/308/cmaq.shtml>). As we reviewed the CMAQ performance, we found that the fractional bias and fractional gross error, along with graphical displays including scatter- and time-series plots, contain the best descriptive power for evaluating PM species. We also focus much of our discussion on the performance for four months that represent the different seasons: January, April, July, and October (although fractional bias and error are presented for all 12 months of 2002).

6.2 Operational Evaluation of CMAQ Base Case D (pre02d) in the WRAP States

In the following discussions we use selected monthly scatterplots, time-series plots, and model performance statistical measures in an operational evaluation of the model for PM species. As noted above, we focus on the six main components of PM that are used to project visibility: SO₄, NO₃, OC, EC, soil, and CM. We also briefly examine NH₄ model performance.

6.2.1 Sulfate (SO₄)

Figure 6-1 displays scatterplots of predicted and observed sulfate concentrations for IMPROVE, CASTNet, STN, and NADP sites in the WRAP states for January, April, July, and October 2002. In January, the CMAQ 36-km simulation exhibits SO₄ fractional bias levels of 42%, 28%, and -7% across monitors in the IMPROVE, CASTNet, and STN networks, respectively, in the western U.S. When a 12-km grid is used, the fractional bias across the same three networks is much higher: 65%, 63%, and 60%, respectively. The use of the higher-resolution grid results in higher SO₄ concentrations and a degradation in the SO₄ model performance. The January performance for wet SO₄ deposition is also degraded when the 12-km grid is used, from a 10% fractional bias using a 36-km grid (not shown) to a 69% bias using a 12-km grid (Figure 6-1a). The fractional error for January SO₄ performance degrades by approximately 20 percentage points when going from the 36-km to 12-km grid (e.g., IMPROVE SO₄ January fractional error increases from ~60% to ~80%).

Better SO₄ performance is exhibited across the WRAP IMPROVE sites in April, with a relatively low bias of -6% and 7% and error 39% and 43% using the 36-km and 12-km grid, respectively (Figure 6-1b). The CASTNet bias (-24% at 36-km and -1% at 12-km) and STN bias (-14% at 36-km and 13% at 12-km) suggest fairly good model performance using both grid resolutions. The fractional errors for April SO₄ concentrations are also fairly low (34% to 43%) using both grid resolutions. The April SO₄ concentrations are higher using a 12-km grid than a 36-km grid, but because the model SO₄ bias straddles zero, the model performance between the 36-km and 12-km grid resolutions is comparable. Wet SO₄ deposition in April across the western U.S. indicates a slight underprediction bias of -16% using the 36-km grid and slight overprediction bias of 26% using the 12-km grid, with comparable errors of 93% and 86%.

The model also estimates higher SO₄ levels in July using the higher resolution grid, with fractional bias across the IMPROVE, CASTNet, and STN networks of 4%, -1%, and -23% using a 36-km grid, increasing to 14%, 23%, and -9% using a 12-km grid. With the exception of the STN network, there is a slight degradation in July SO₄ model performance when the 12-km grid is used. However, the July SO₄ model performance is still fairly good. The July wet SO₄ deposition bias increases from -38% using the 36-km grid to 28% using the 12-km grid, with both simulations exhibiting ~100% error.

In October 2002, use of the 12-km grid slightly degrades model performance across the more rural IMPROVE and CASTNet monitors in the western U.S. but improves it across the STN monitors, with fractional bias levels across the three networks increasing from 13%, 3%, and -19% using a 36-km grid to 26%, 21%, and 13% using a 12-km grid. Wet SO₄ deposition using a 36-km grid exhibits low bias (6%) but high error (84%); results for this metric using the 12-km grid are not available.

The time series of monthly fractional bias and gross error for SO₄ at sites in the WRAP states for the 2002 CMAQ pre02d 36-km and 12-km simulations (Figure 6-2) confirm the results from the scatterplots for the four months; SO₄ is overestimated in the winter and underestimated in the summer, and the fractional bias levels using the 12-km grid are always higher than when using a 36-km grid. With the exception of June 2002, the SO₄ model performance using the IMPROVE network exhibits better bias (i.e., closer to zero) and lower error when using a 36-km grid versus using a 12-km grid, with the differences in the model performance using the two grid resolutions greater in winter than in summer.

Figure 6-3 displays the SO₄ bugle plots for the 2002 CMAQ pre02d 12-km simulation and the IMPROVE, CASTNet, and STN networks. The monthly average fractional bias for SO₄ concentrations in the western U.S. mostly resides in the Zone 1 area of “good” model performance (bias/error of less than ±30%/50%), although there are four network-month combinations that reside in the Zone 2 area between the performance goals and criteria, which is an area of concern. SO₄ performance never exceeds the performance criteria. The poorer winter SO₄ model performance occurs under lower SO₄ concentrations, so the bias and error points reside in the horn of the bugle plot, where goals and criteria are relaxed. As noted previously, the relaxing of performance goals at around 2 µg/m³ may be appropriate for the eastern U.S., but more stringent goals/criteria should be defined at these levels for the western U.S. due to the lower concentrations present in the west.

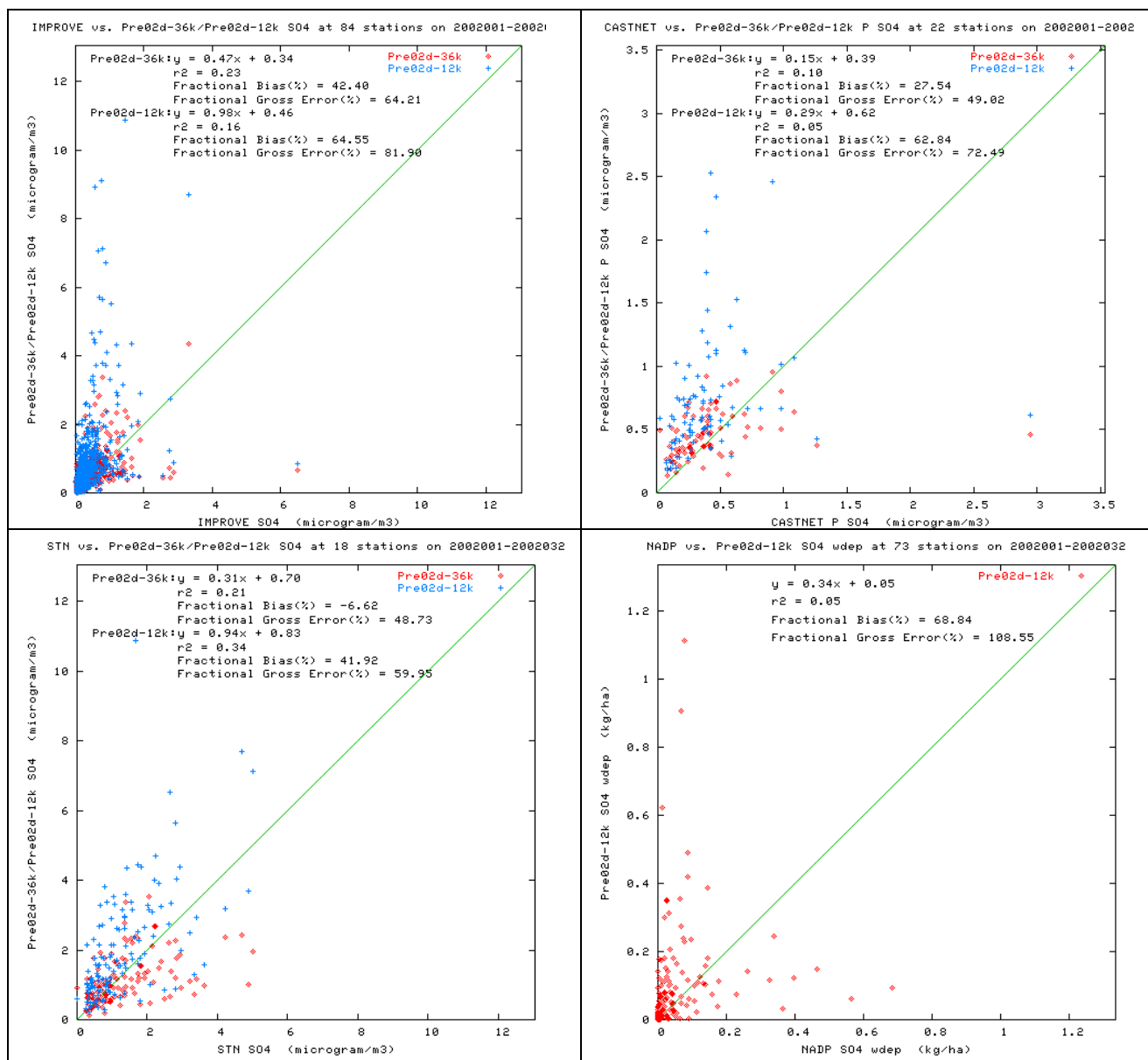


Figure 6-1a. CMAQ 2002 pre02d base case simulation SO₄ model performance in the WRAP states for January 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and NADP (bottom right) monitoring networks. (NADP measures wet SO₄ deposition, whereas the other three networks measure ambient air SO₄ concentrations.)

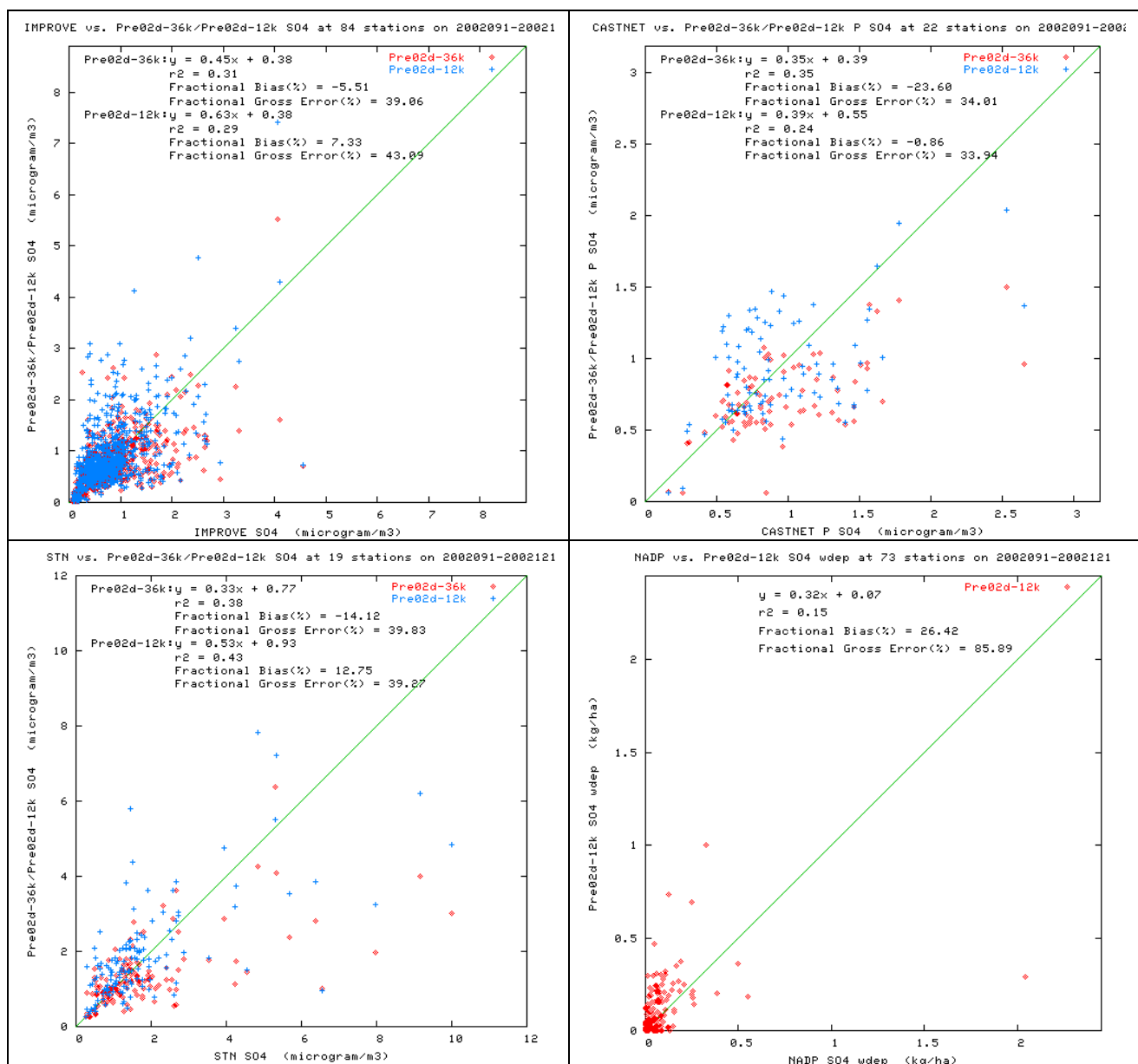


Figure 6-1b. CMAQ 2002 pre02d base case simulation SO₄ model performance in the WRAP states for April 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and NADP (bottom right) monitoring networks. (NADP measures wet SO₄ deposition, whereas the other three networks measure ambient air SO₄ concentrations.).

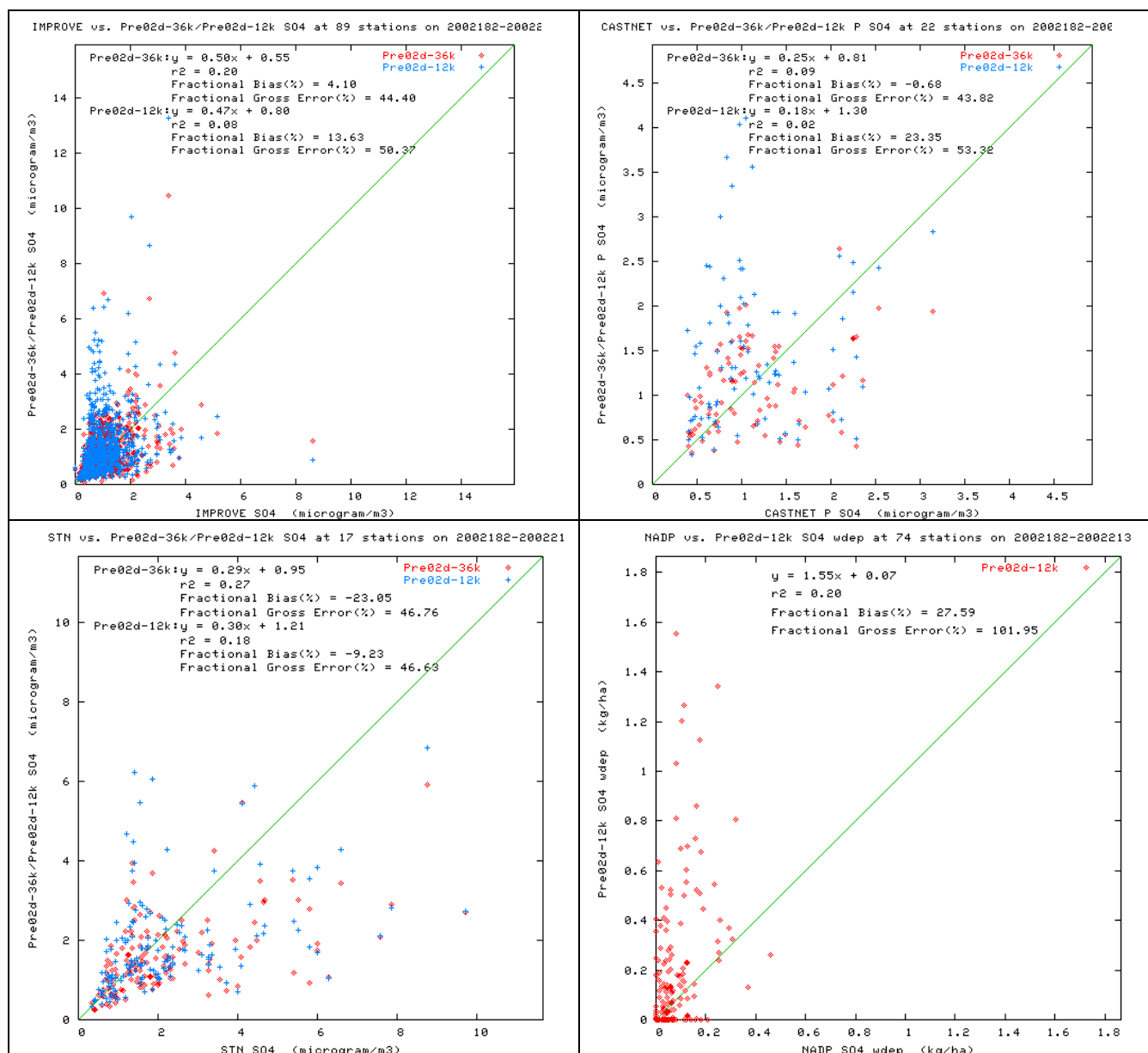


Figure 6-1c. CMAQ 2002 pre02d base case simulation SO₄ model performance in the WRAP states for July 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and NADP (bottom right) monitoring networks. (NADP measures wet SO₄ deposition, whereas the other three networks measure ambient air SO₄ concentrations.)

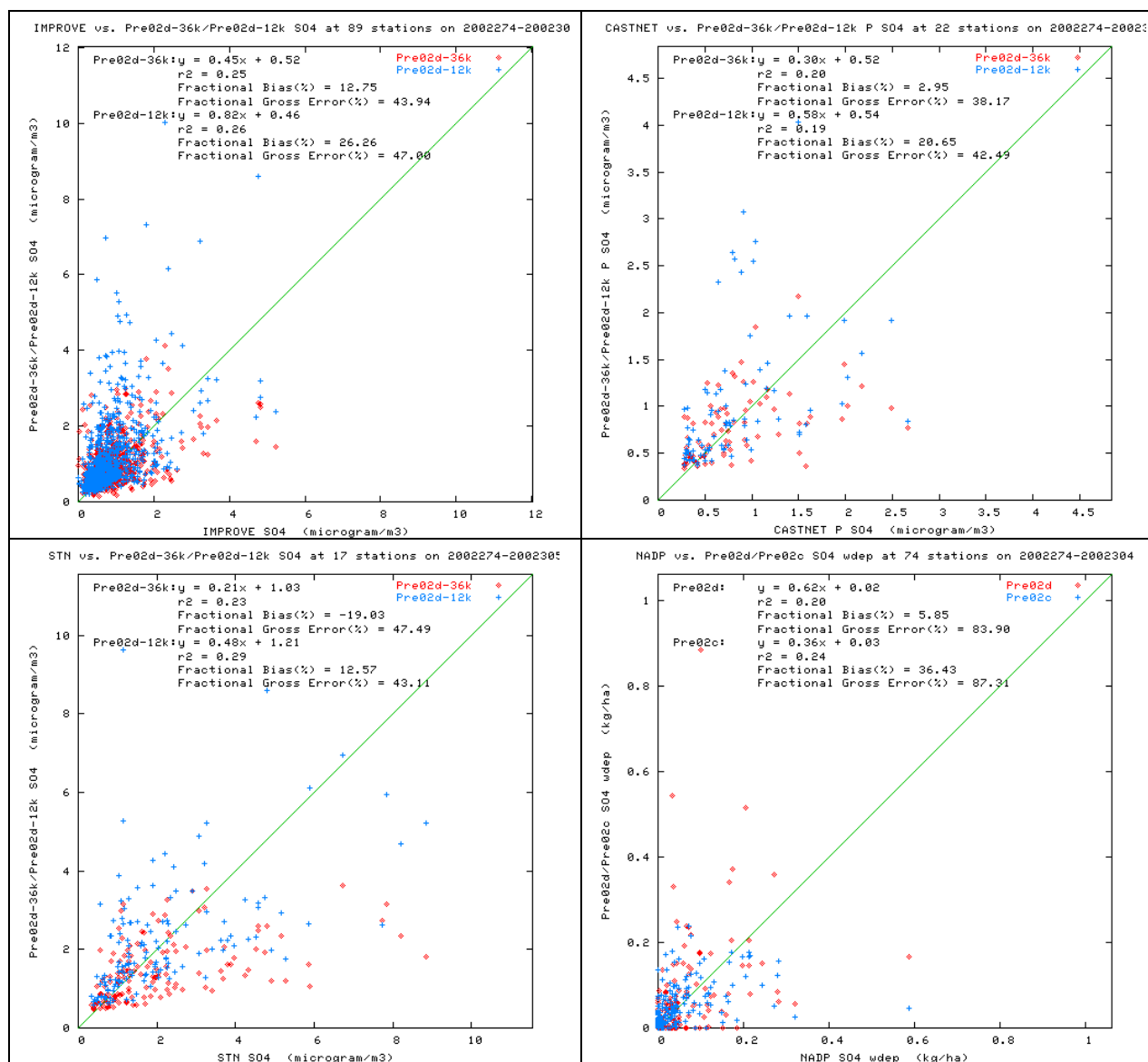


Figure 6-1d. CMAQ 2002 pre02d base case simulation SO₄ model performance in the WRAP states for October 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and NADP (bottom right) monitoring networks. (NADP measures wet SO₄ deposition, whereas the other three networks measure ambient air SO₄ concentrations.)

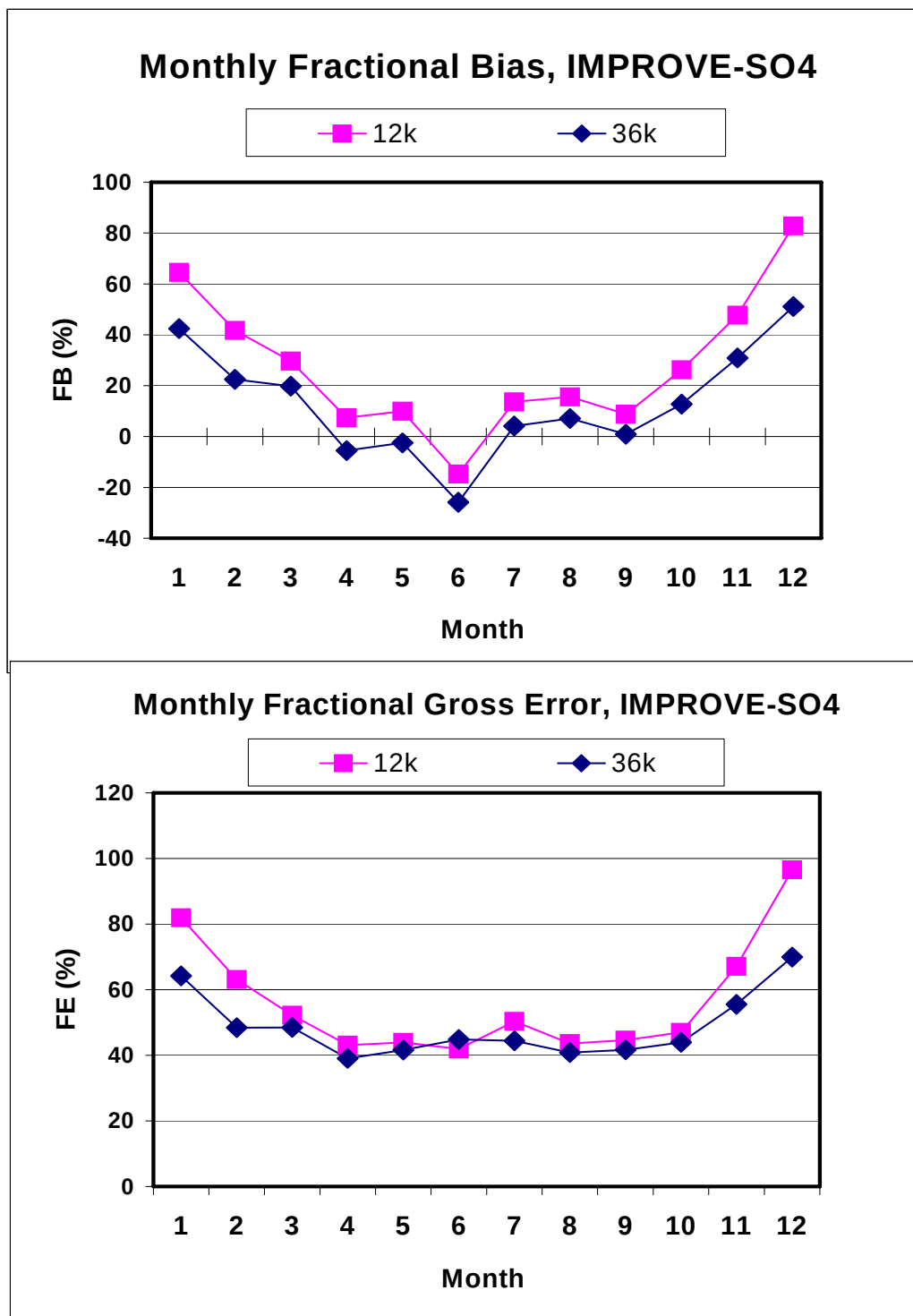


Figure 6-2. Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d 36-km and 12-km base case SO₄ model performance across IMPROVE sites in the WRAP states.

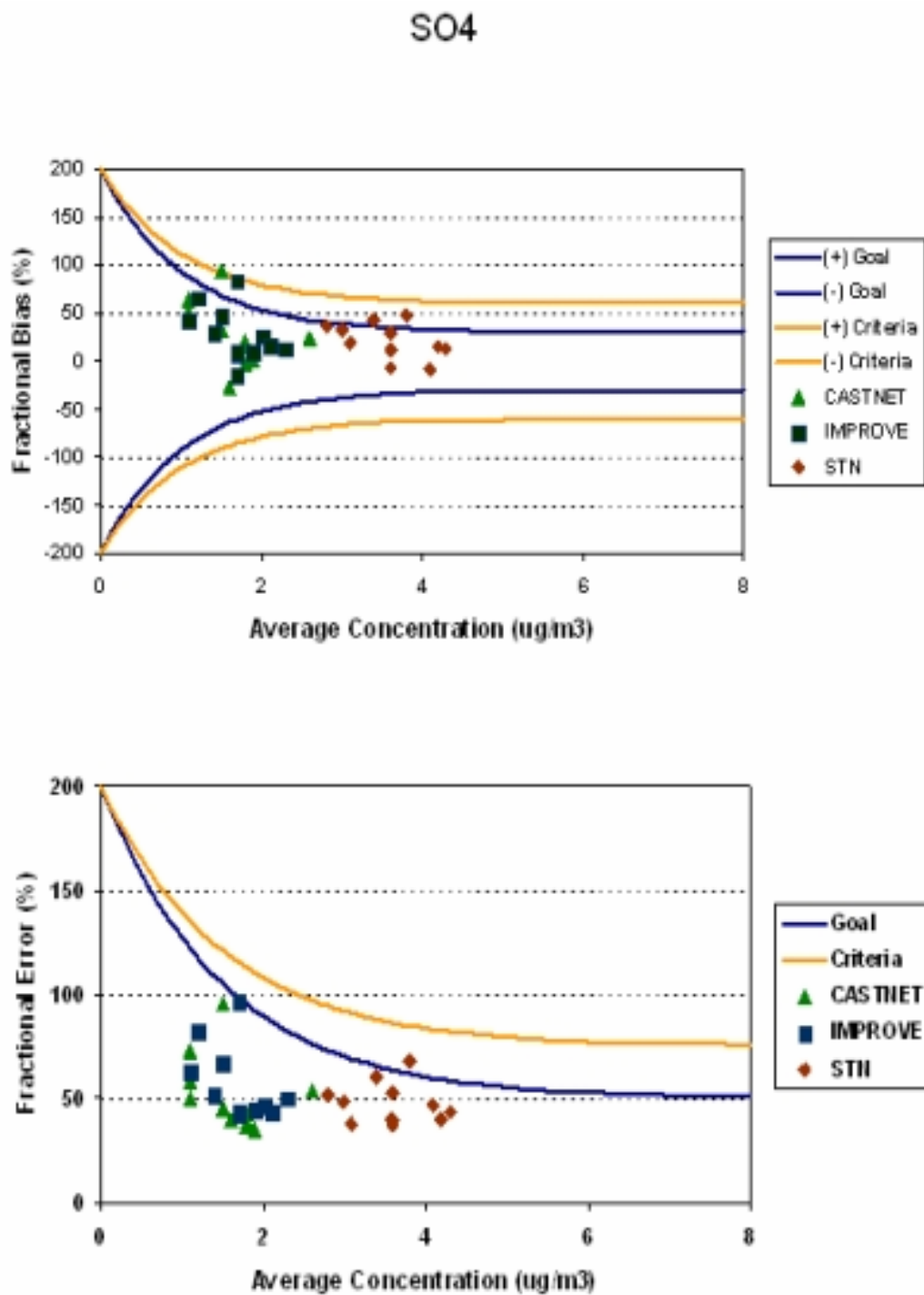


Figure 6-3. Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d base case SO₄ model performance as a function of observed concentration.

6.2.2 Nitrate (NO₃)

The plots of nitrate (NO₃) model performance are shown in Figures 6-4 through 6-6. Except for the STN network, which exhibits an average NO₃ underestimation tendency throughout the year, the CMAQ pre02d base case simulation tends to overestimate NO₃ in the winter and underestimate it in the summer. The 12-km base case tends to estimate slightly higher NO₃ levels that exacerbate the NO₃ overestimation tendency in the winter, but improve the underestimation tendency in the summer. As seen in the bugle plots (Figure 6-6), the winter overestimation generally occurs at concentration levels twice that of the summer underestimation and causes the fractional bias and error points for the IMPROVE and CASTNet networks to reside in the Zone 3 area of serious model performance concern. At the more urban STN sites, the NO₃ underprediction bias occurs throughout the year and is more pronounced in the summer, when its performance also resides in the Zone 3 area of model performance concern (See Figures 6-4c and 6-6). The NADP wet NO₃ deposition bias is higher using the 12-km than the 36-km grid, with 36-km values for January and July being -11% and -73% and corresponding values using the 12-km grid being 21% and 43%.

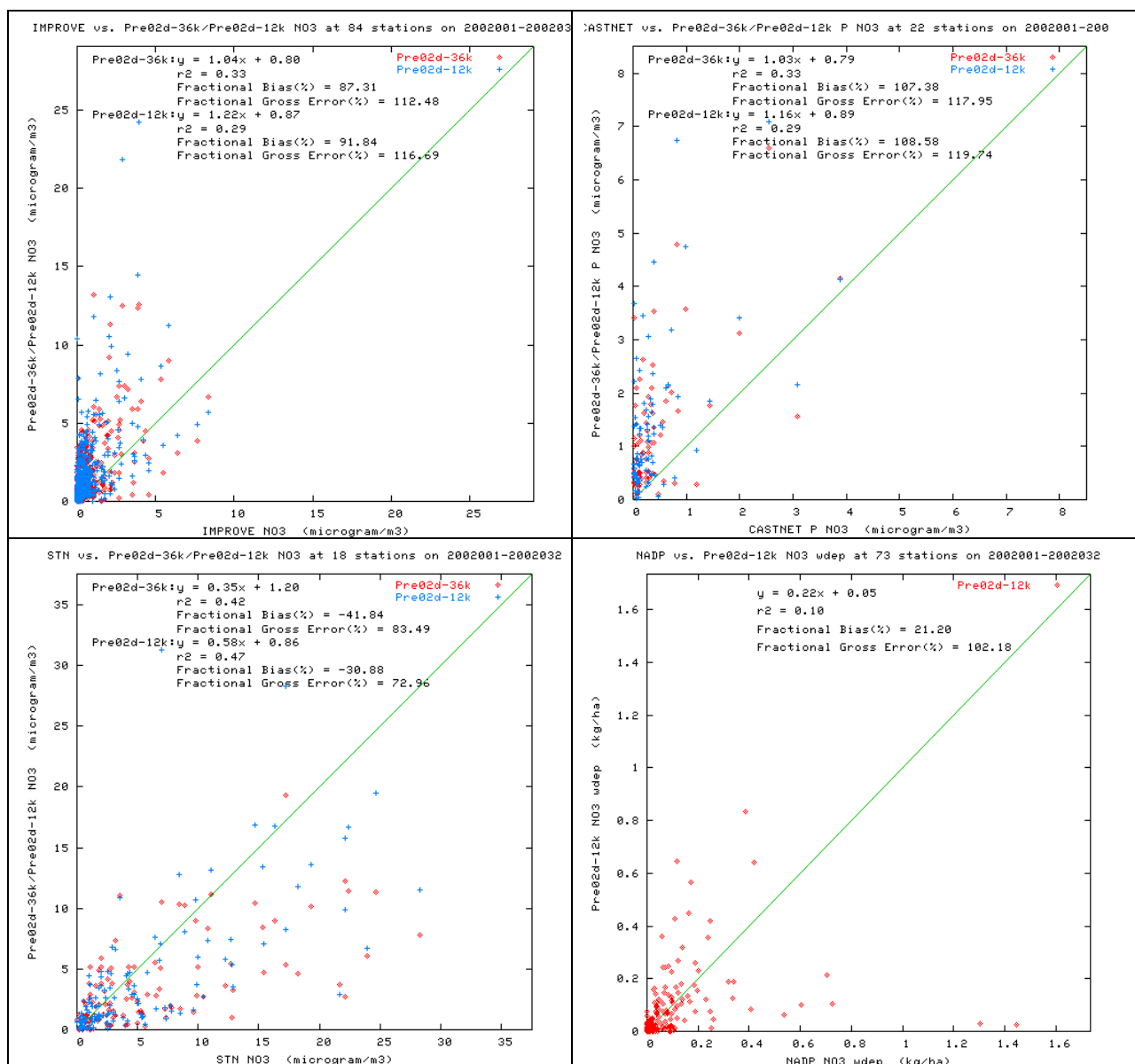


Figure 6-4a. CMAQ 2002 pre02d base case simulation NO₃ model performance in the WRAP states for January 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and NADP (bottom right) monitoring networks.

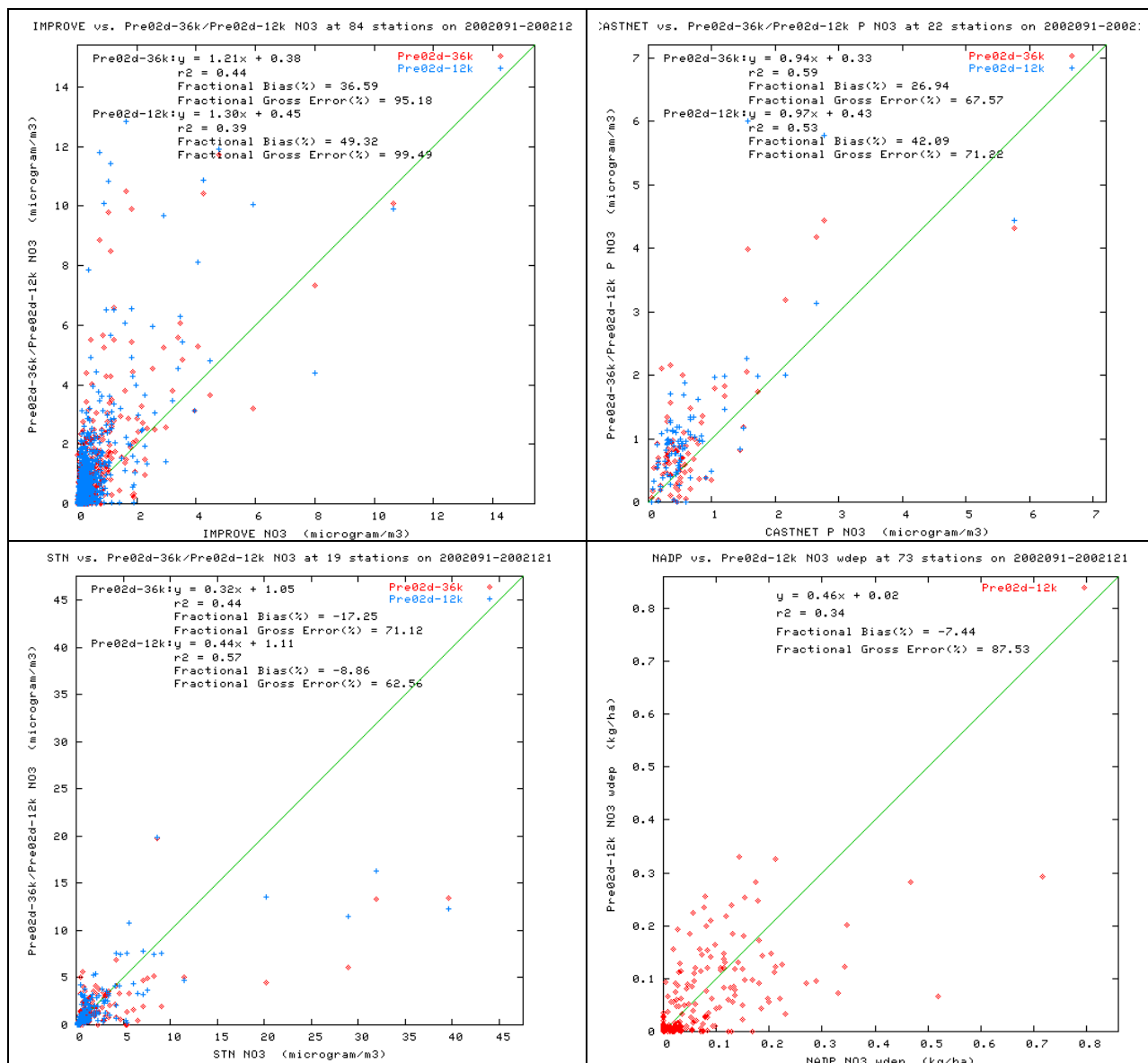


Figure 6-4b. CMAQ 2002 pre02d base case simulation NO₃ model performance in the WRAP states for April 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and NADP (bottom right) monitoring networks.

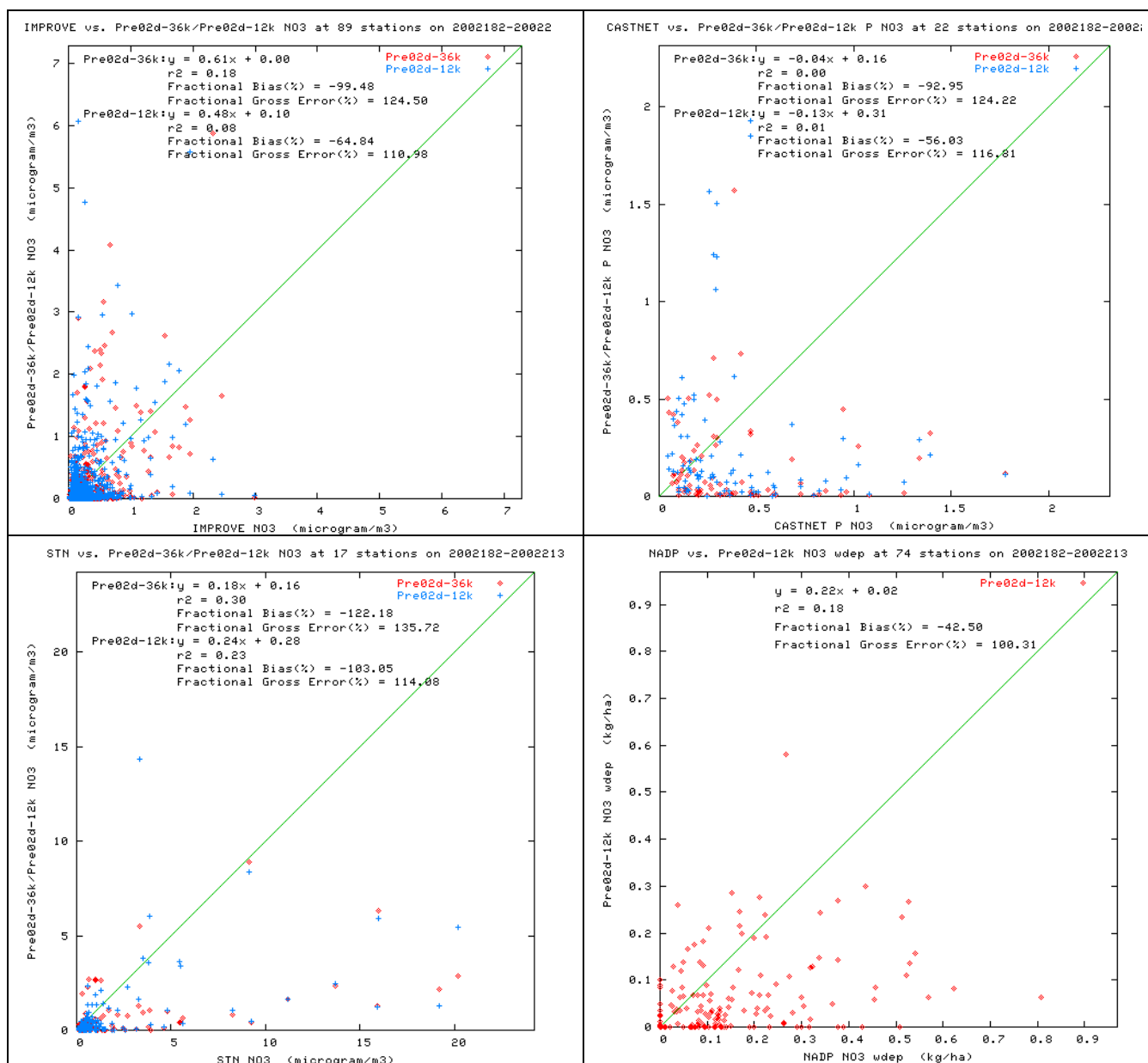


Figure 6-4c. CMAQ 2002 pre02d base case simulation NO₃ model performance in the WRAP states for July 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and NADP (bottom right) monitoring networks.

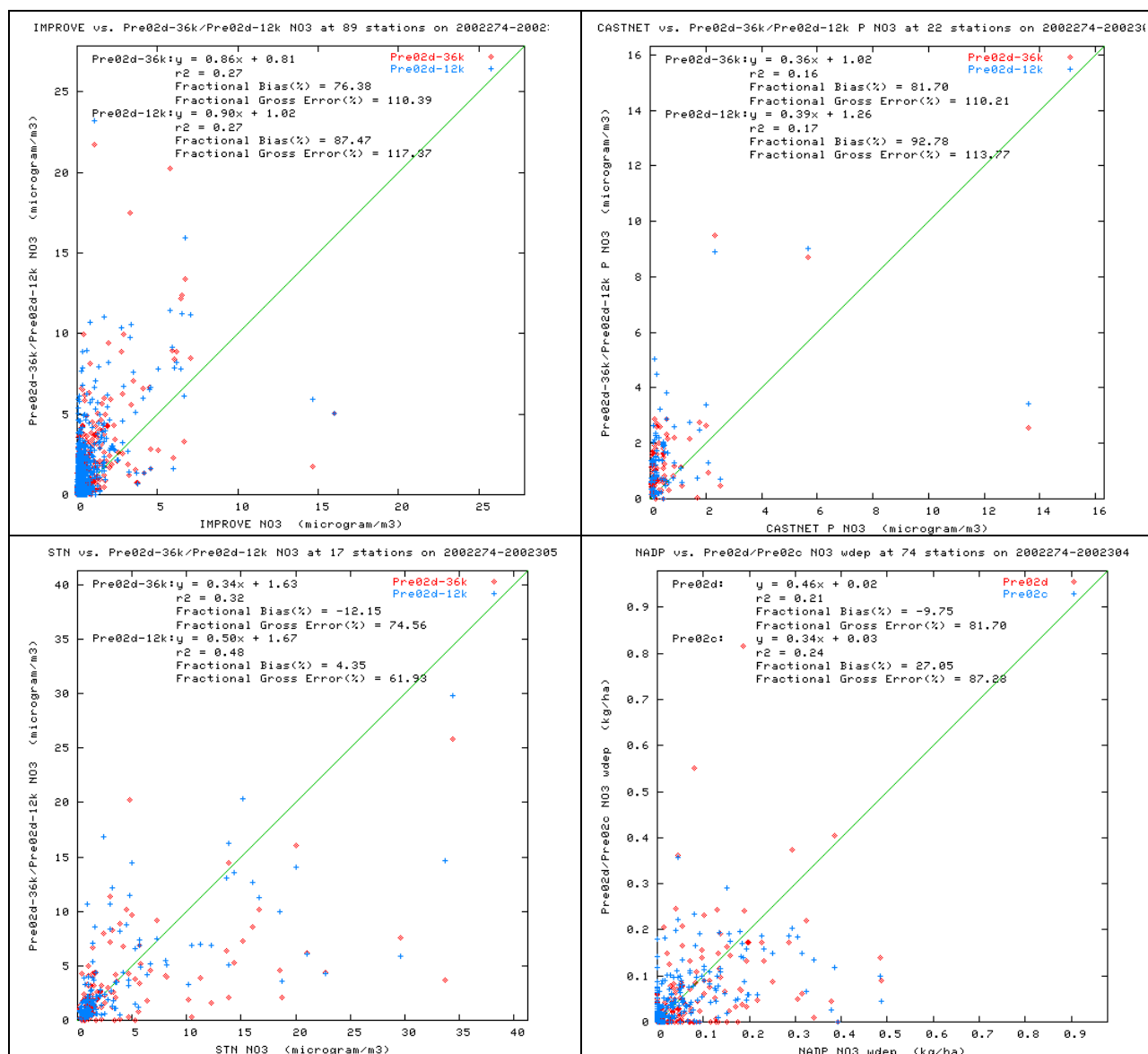


Figure 6-4d. CMAQ 2002 pre02d base case simulation NO₃ model performance in the WRAP states for October 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and NADP (bottom right) monitoring networks.

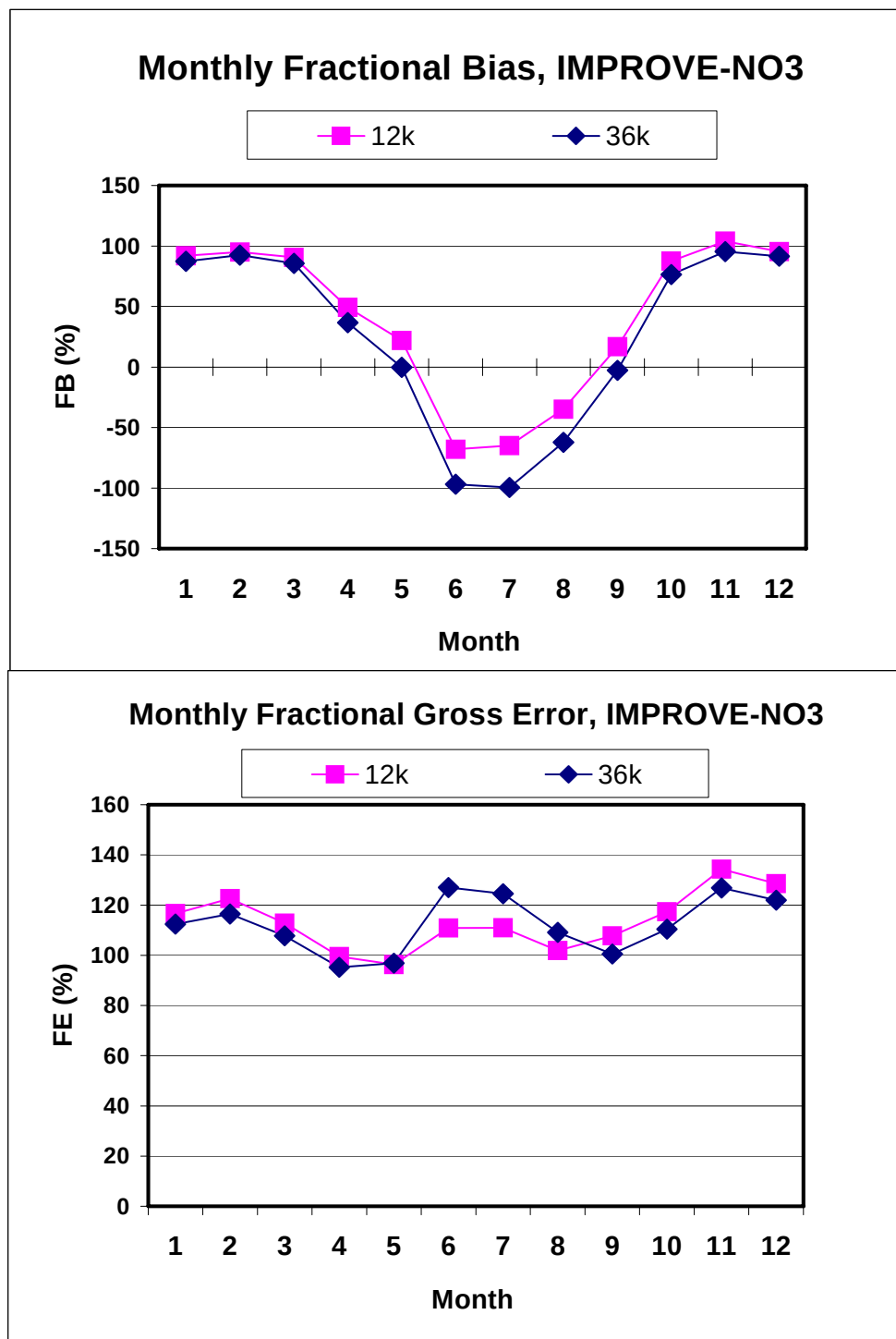


Figure 6-5 Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d 36-km and 12-km base case NO₃ model performance across IMPROVE sites in the WRAP states.

NO₃

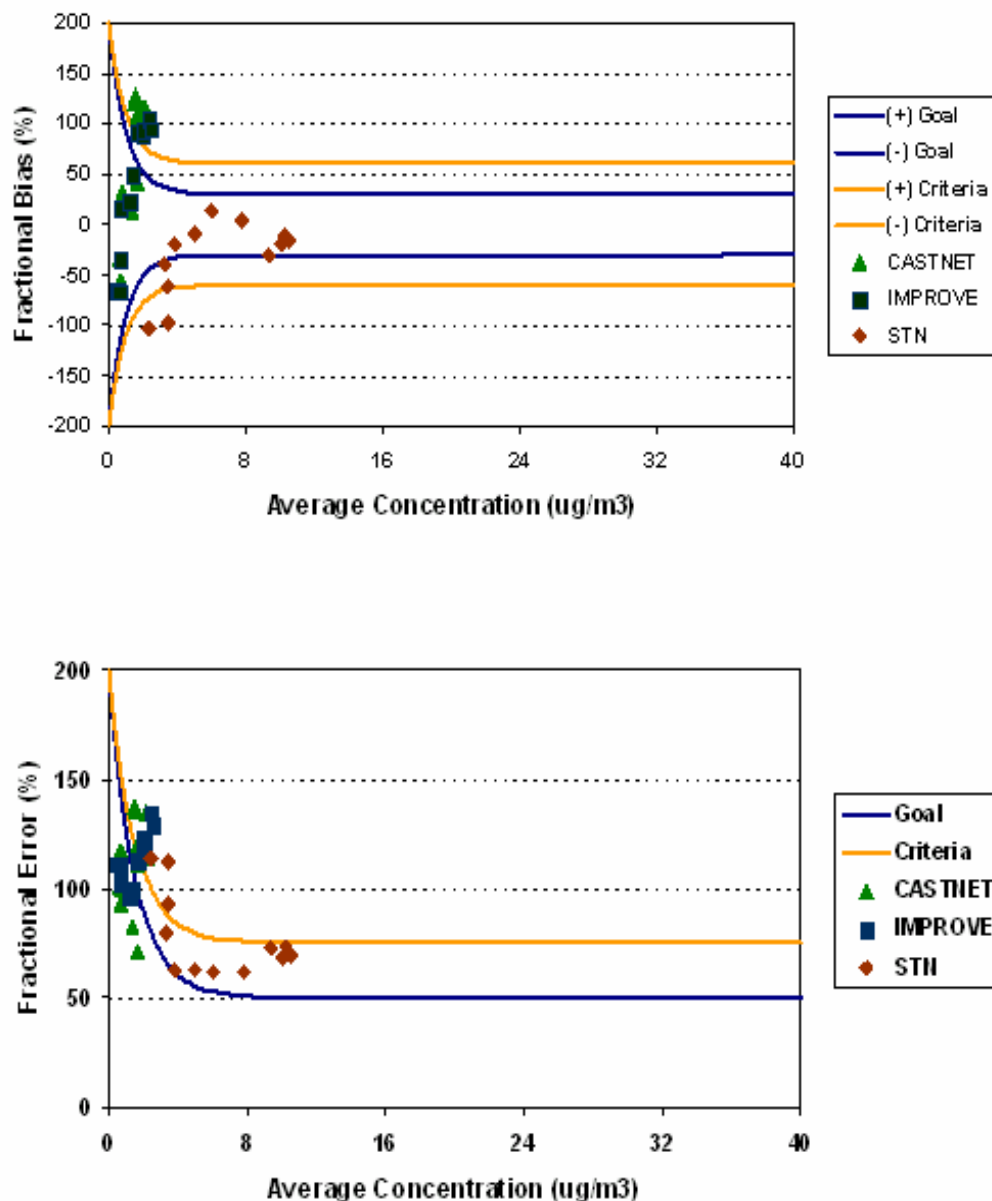


Figure 6-6. Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d 36-km and 12-km base case NO₃ model performance as a function of observed concentration.

6.2.3 Ammonium (NH₄)

The IMPROVE network does not directly measure NH₄. Consequently, we use “derived” NH₄ concentrations in the IMPROVE model performance evaluation whereby the “observed” NH₄ is assumed to be the level of NH₄ needed to completely neutralize SO₄ and NO₃. During the winter this is likely an adequate assumption; during the warmer months, however, this may overstate NH₄ concentrations. The NH₄ evaluation should thus be considered qualitative, so only bugle plots are presented for NH₄ (Figure 6-7). The bugle plots suggest that NH₄ is overestimated, with the overestimation severe enough that the fractional bias and error exceed the model performance goal and the fractional bias exceeds the model performance criterion for CASTNet for several months.

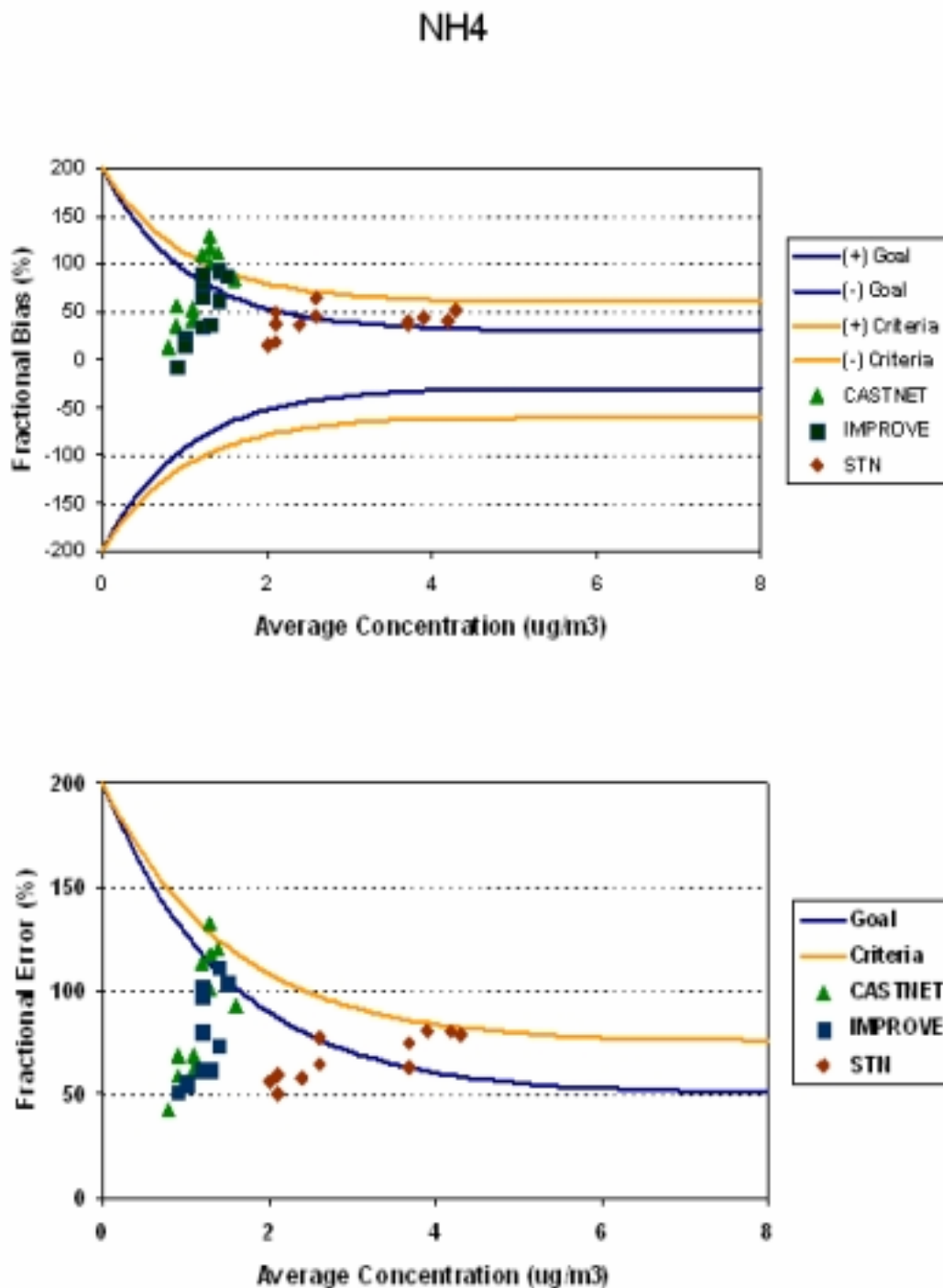


Figure 6-7. Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d base case NH₄ model performance as a function of observed concentration.

6.2.4 Organic carbon (OC)

The CMAQ 2002 pre02d base case simulation exhibits very different OC model performance across the IMPROVE and STN networks in the WRAP states (Figures 6-8 through 6-10). Whereas OC is overestimated across the IMPROVE sites, it is underestimated across the STN sites. We believe this is due to (1) higher OC concentrations at the more urban STN sites versus the more rural IMPROVE sites; and (2) different OC measurement technologies, whereby the STN measurement technology is believed to understate OC and overstate EC.

During April 2002, a very high observed OC value occurs ($\sim 115 \mu\text{g}/\text{m}^3$), which was traced to an observation on April 5 at Bryce Canyon. Unusually high EC ($\sim 17 \mu\text{g}/\text{m}^3$) was also observed at this site on this day, suggesting that biomass burning may have contributed (e.g., wildfire or prescribed burn).

The time series of monthly fractional bias and error for the IMPROVE network are shown in Figure 6-9 and suggest a winter overestimation bias and summer underestimation bias for OC in the western US. Unlike SO_4 and NO_3 , where the 12-km modeling results showed higher concentrations than those obtained using the 36-km grid, for OC the 36-km bias values are substantially larger than those obtained using the 12-km grid. In the summer, when the model underestimates, this results in improved OC model performance using a 36-km grid, whereas in the winter, when the model overestimates, OC model performance is worse using a 36-km grid. For example, in January and July the OC bias using the 36-km grid is 35% and 8%; the corresponding values using the 12-km grid are 25% and -28%. The bugle plots using the 12-km grid are shown in Figure 6-10 and suggest that the summer OC underestimation is a performance area of concern, whereas the winter overestimation occurs under conditions of lower OC levels so may not be as much of a concern.

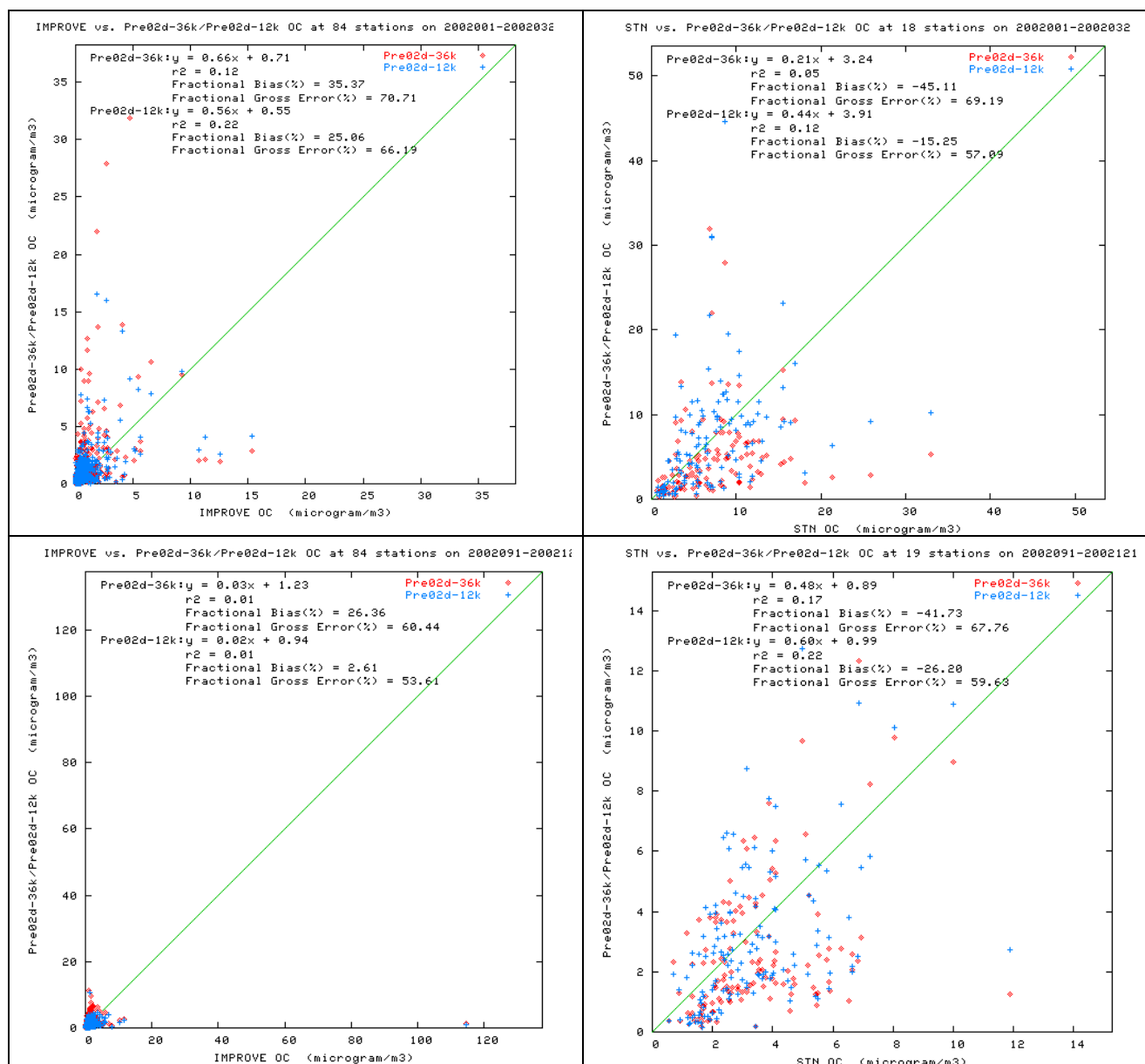


Figure 6-8a. CMAQ 2002 pre02d base case simulation OC model performance in the WRAP states for January (top) and April (bottom) using the IMPROVE (left) and STN (right) monitoring networks.

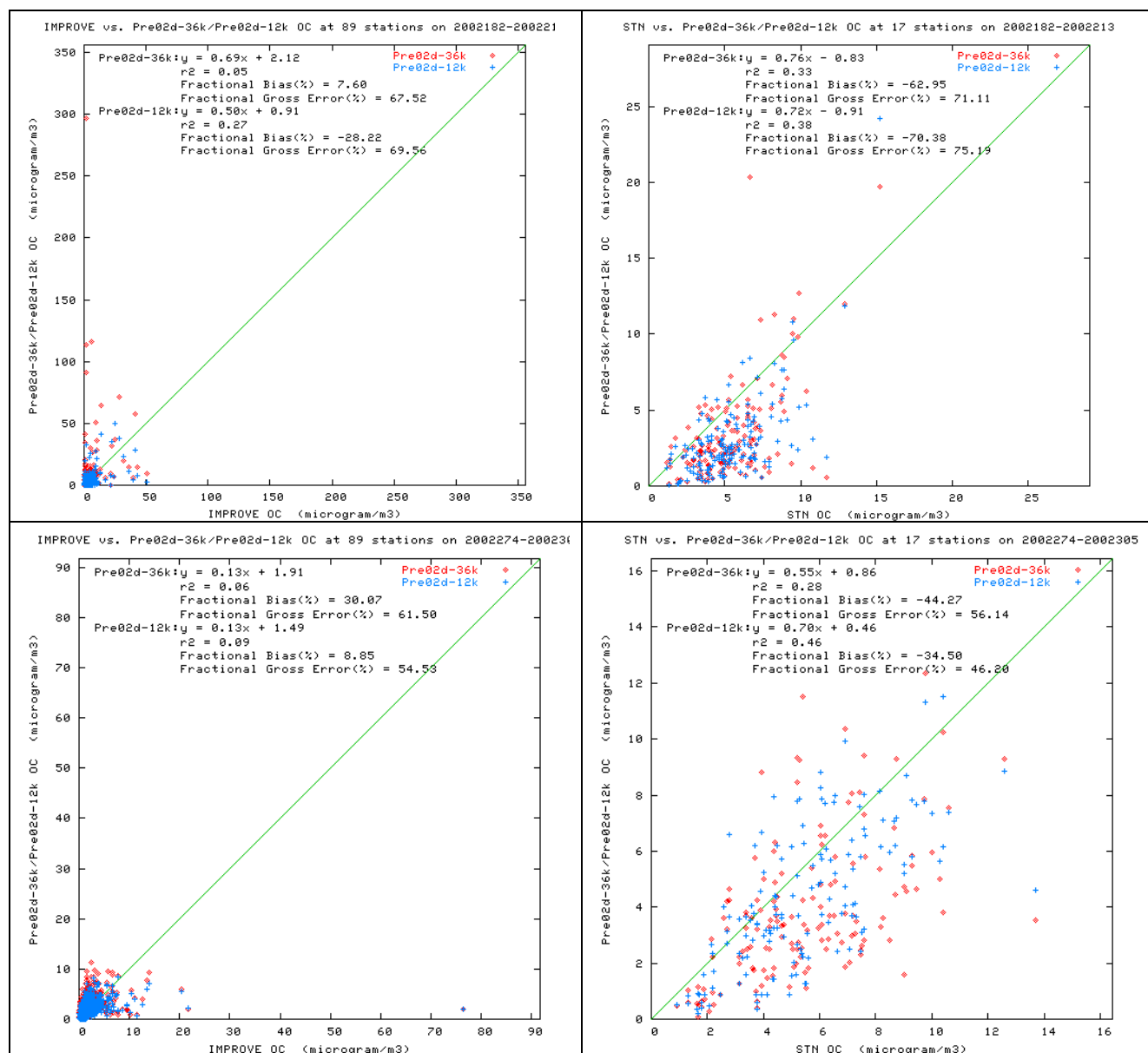


Figure 6-8b. CMAQ 2002 pre02d base case simulation OC model performance in the WRAP states for July (top) and October (bottom) using the IMPROVE (left) and STN (right) monitoring networks.

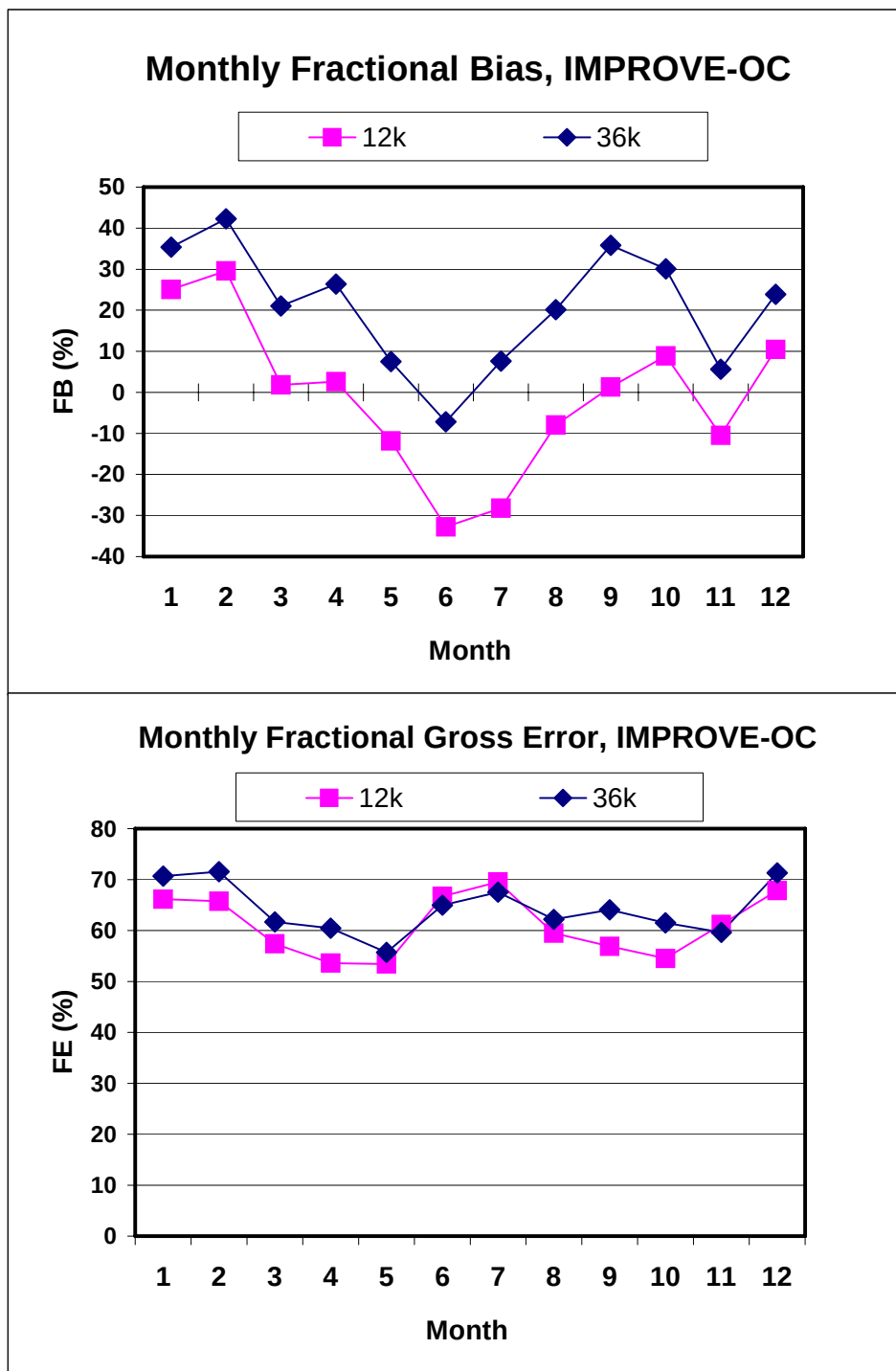


Figure 6-9. Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d base case OC model performance across IMPROVE sites in the WRAP states.

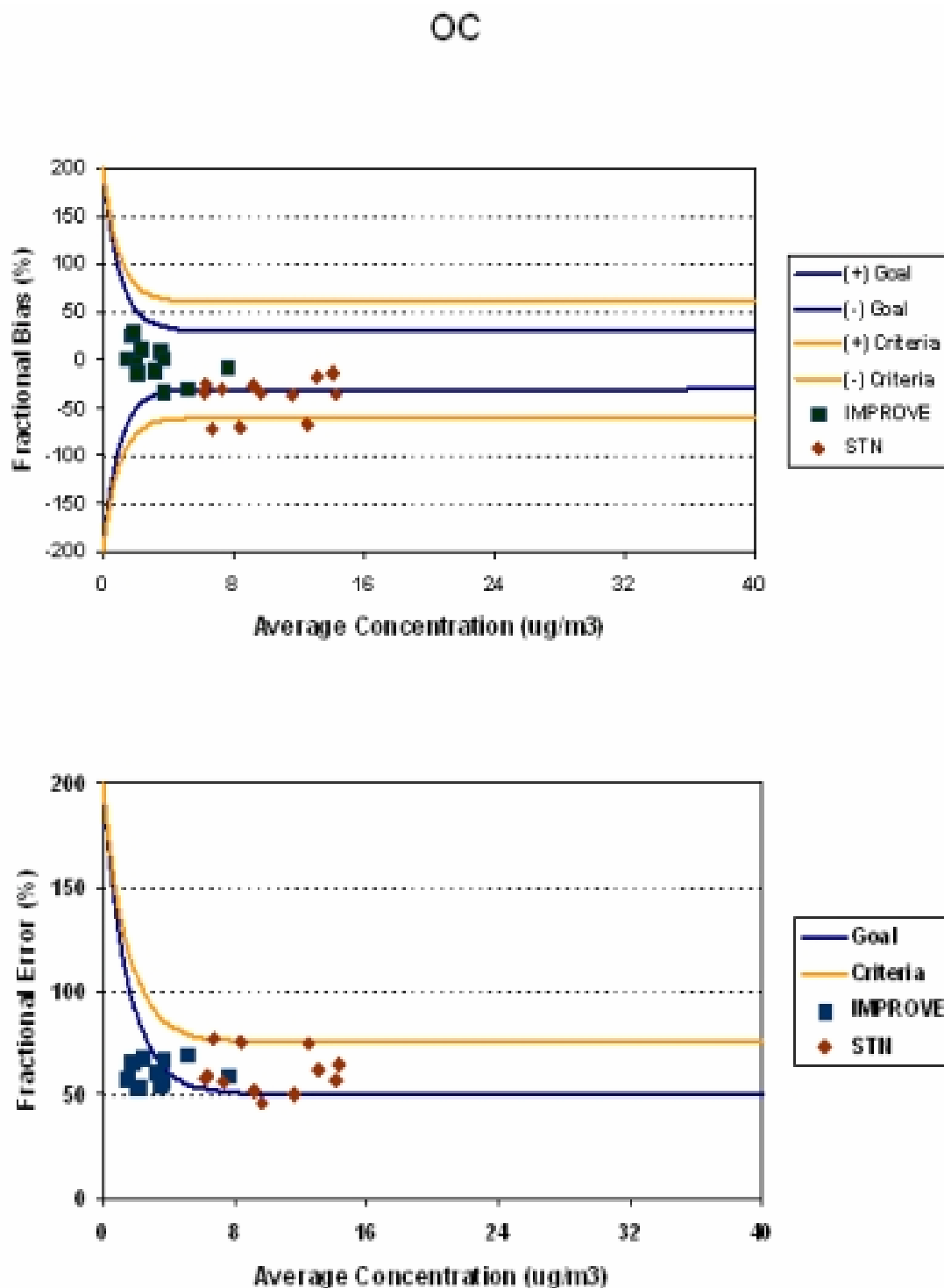


Figure 6-10. Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d base case OC model performance as a function of observed concentration.

6.2.5 Elemental carbon (EC)

The EC performance (Figures 6-11 through 6-13) across the IMPROVE network exhibits fairly low bias, without as strong a seasonal variation as was exhibited by the other species. For the STN network, EC tends to be overestimated during most months, although the bias is still low relative to the other species. As seen in the scatterplots and bugle plots, EC measurements at the IMPROVE sites tend to be fairly low, except when there are incursions of plumes from fires. As seen for OC, but in contrast to SO_4 and NO_3 , the CMAQ 12-km EC estimates are lower than their 36-km counterparts. For example, during the first six months of 2002 the EC fractional bias for the IMPROVE monitoring sites is approximately -20% using the 36-km grid and approximately -30% using the 12-km grid (Figure 6-12). The bugle plots show that the EC concentrations are typically very low across the IMPROVE network, so that the model performance meets the expanding performance goal in the horn of the bugle plot (Figure 6-13).

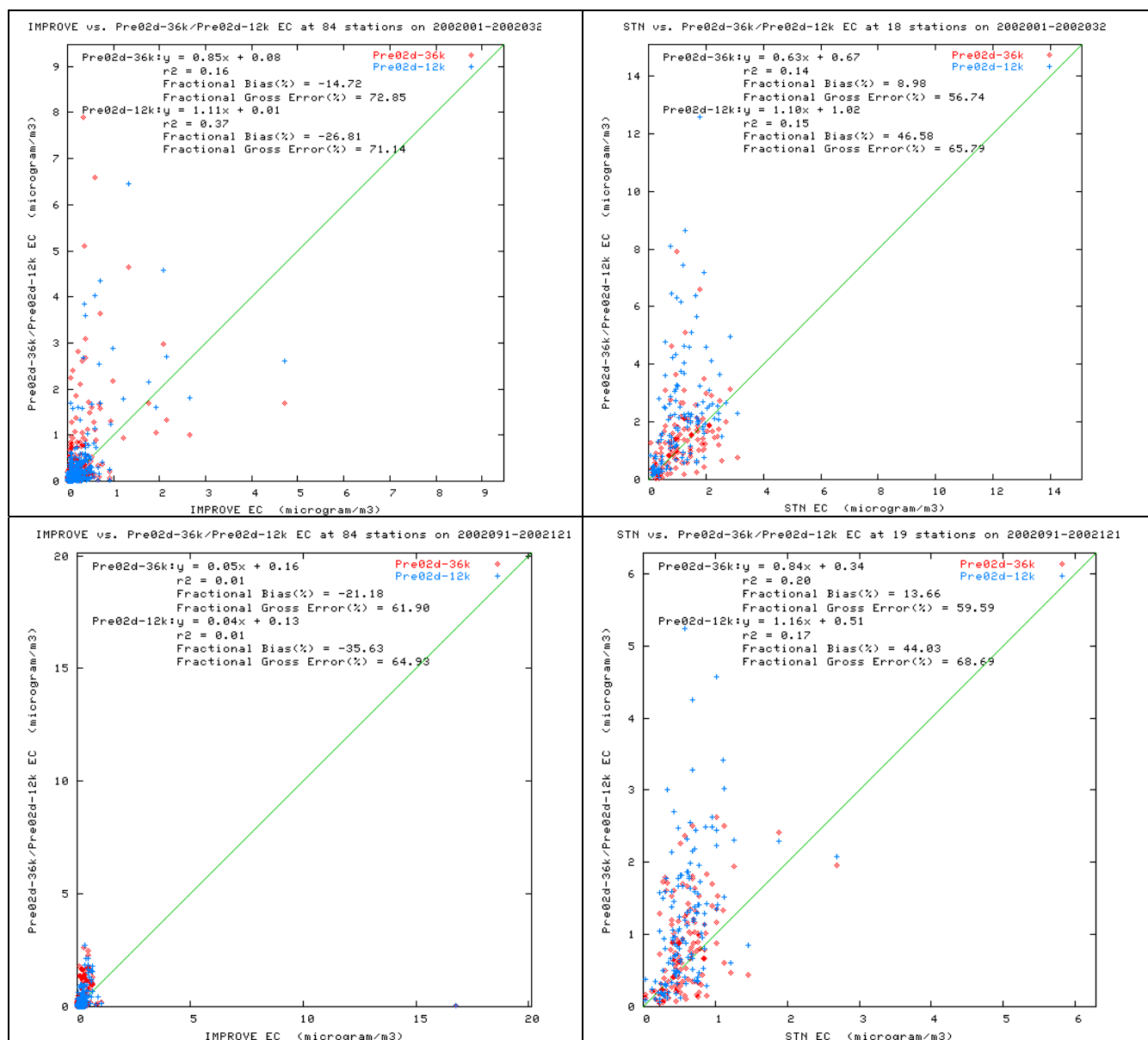


Figure 6-11a. CMAQ 2002 pre02d base case simulation EC model performance in the WRAP states for January (top) and April (bottom) using the IMPROVE (left) and STN (right) monitoring networks.

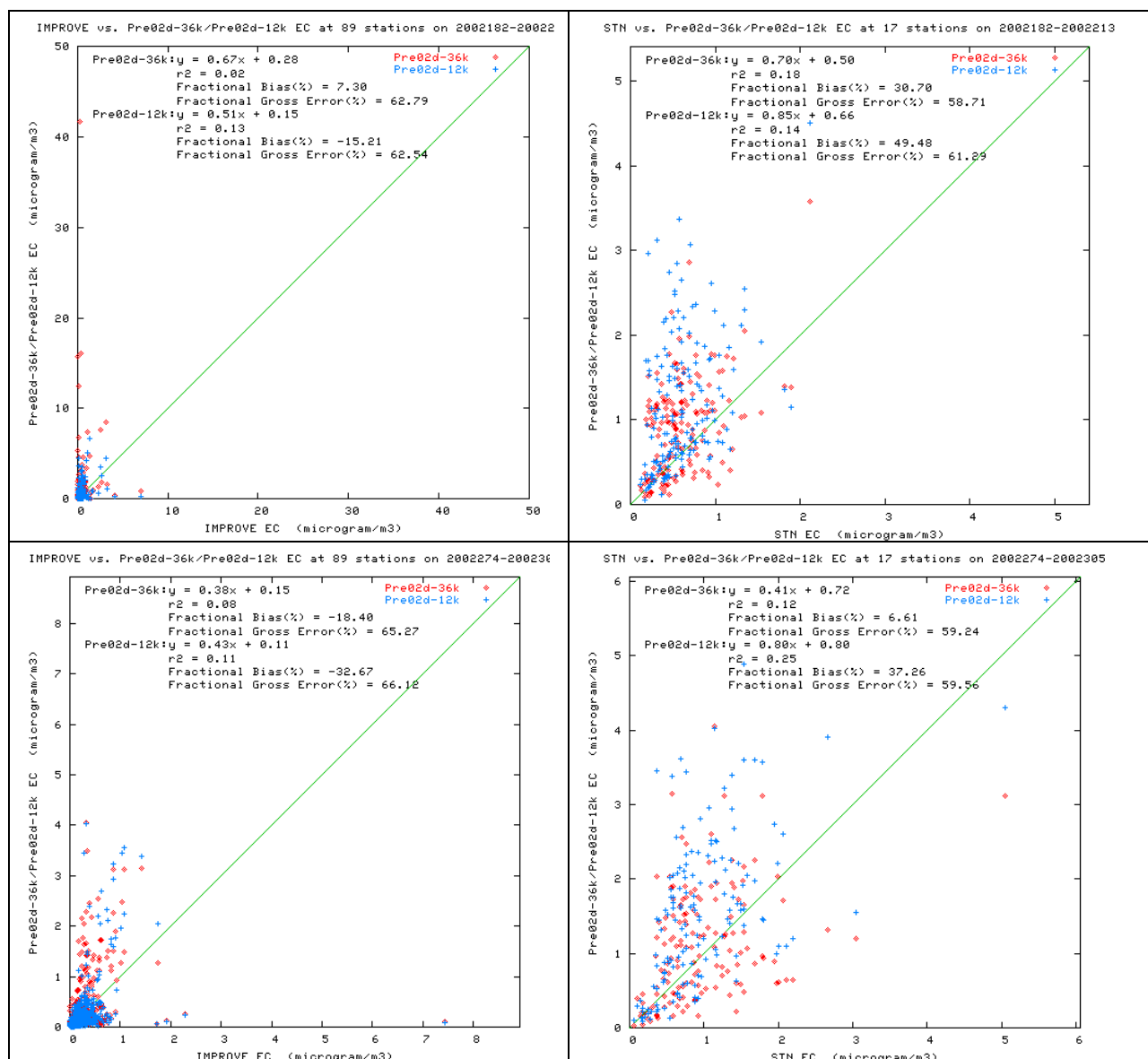


Figure 6-11b. CMAQ 2002 pre02d base case simulation EC model performance in the WRAP states for July (top) and October (bottom) using the IMPROVE (left) and STN (right) monitoring networks.

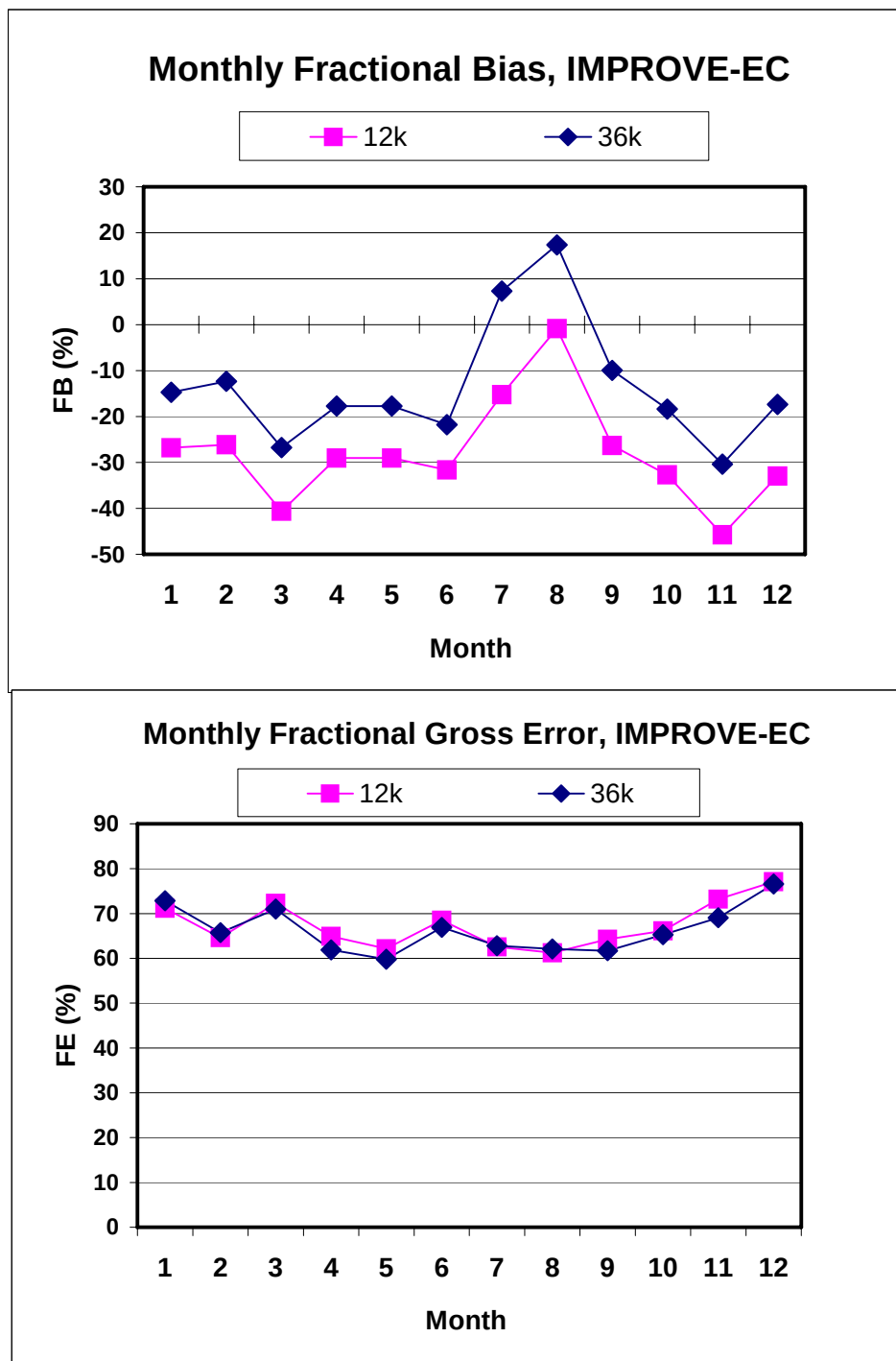


Figure 6-12. Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d base case EC model performance across IMPROVE sites in the WRAP states.

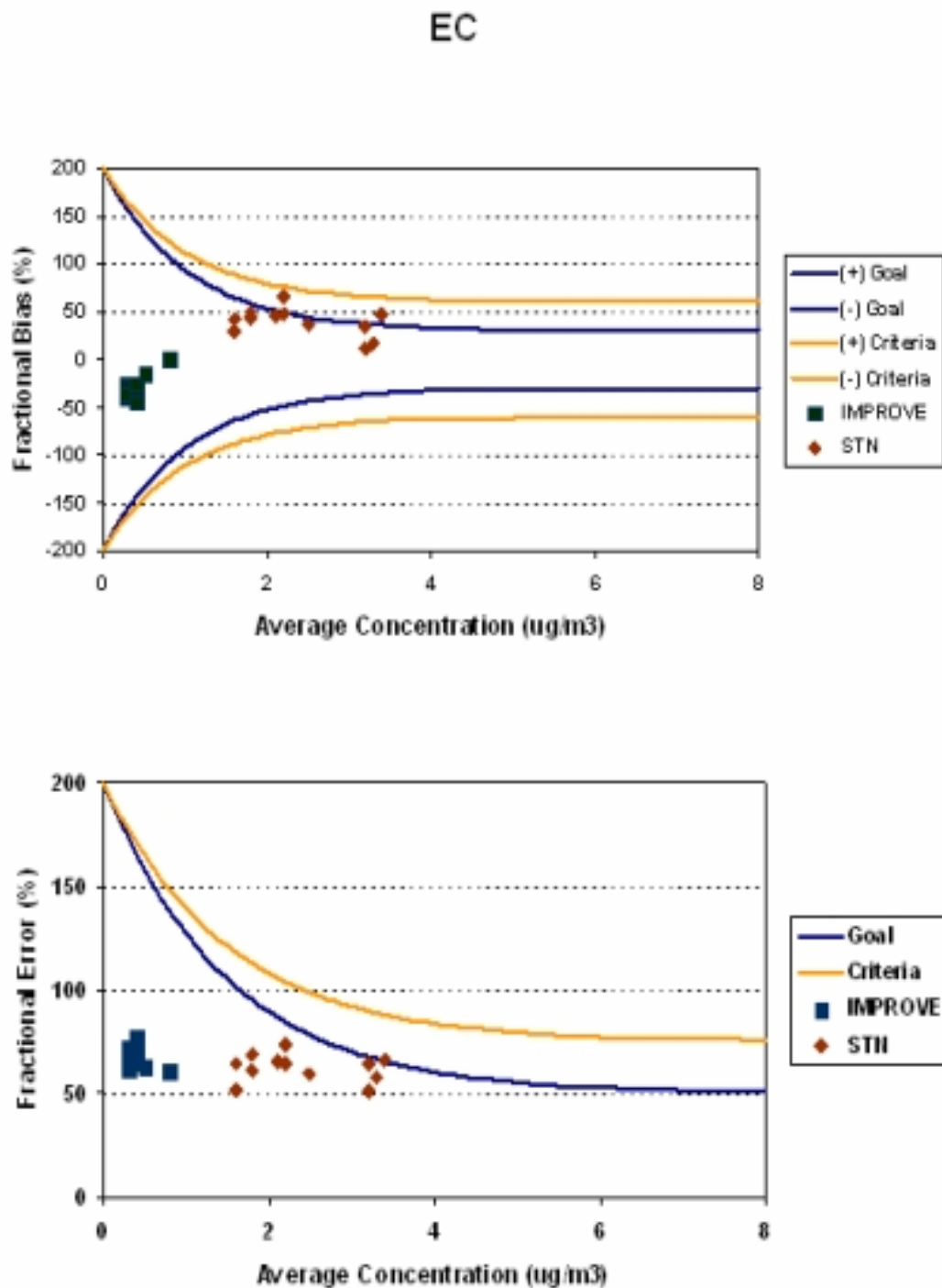


Figure 6-13. Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d base case EC model performance as a function of observed concentration.

6.2.6 Other fine PM (soil) and coarse mass (CM)

Figures 6-14 and 6-15 display scatterplots of predicted and observed other fine PM (soil) and coarse mass (CM), respectively, across the IMPROVE network in the western U.S. for the CMAQ 2002 36-km and 12-km pre02d base case simulations. The time series of monthly bias and error for soil and CM are given in Figures 6-16 and 6-17, respectively. Soil is overestimated in January by approximately 100%, with the bias dropping almost linearly to an underestimation bias of -33% (36-km) and -24% (12-km) in April. The soil bias is then $<\pm 20\%$ from May to September, when both the 36-km and 12-km base cases exhibit near zero bias. The soil bias then increases linearly from zero in September to $\sim 80\%$ in December. Unlike the other species, for soil the 36-km and 12-km performance statistics track each other very closely in the winter, early spring, and late fall, and in the summer the 12-km results are lower than when a 36-km grid is used, resulting in slightly worse performance with the 36-km grid than the 12-km grid.

The performance for CM, on the other hand, exhibits a severe underprediction bias throughout the year that is worse (exceeding -100%) in summer than in winter. The January-December CM fractional bias is approximately -40%; it then decreases as one moves toward summer, with the lowest fractional bias of approximately -120% (12-km) and -130% (36-km) occurring in June-July. The reasons for the CM underestimation bias are unclear but are likely due to missing dust sources and subgrid-scale local dust impacts that are not simulated by the model.

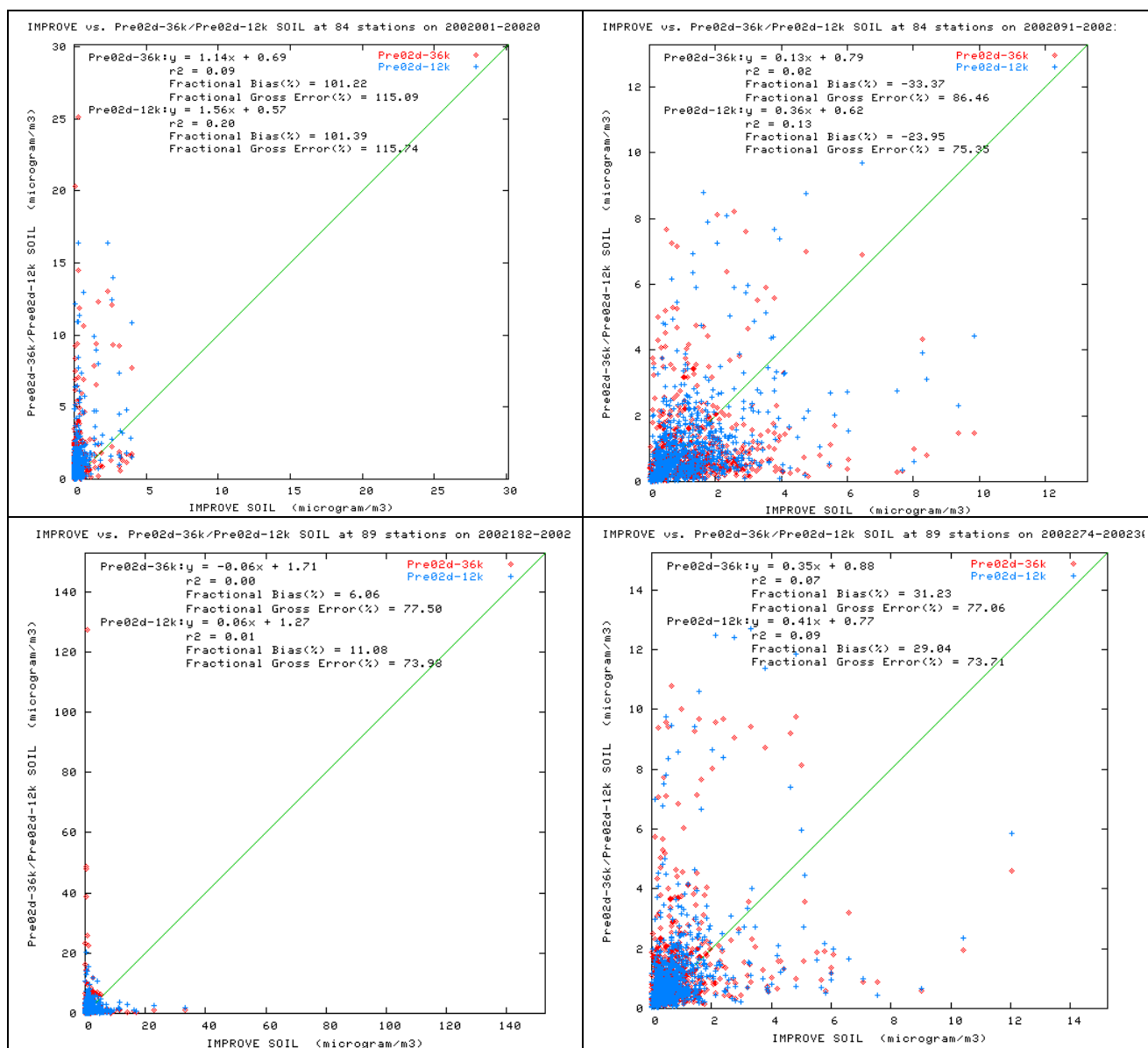


Figure 6-14. CMAQ 2002 pre02d base case simulation "other fine PM" (soil) model performance in the WRAP states for January (top left), April (top right), July (bottom left), and October (bottom right) using the IMPROVE monitoring network.

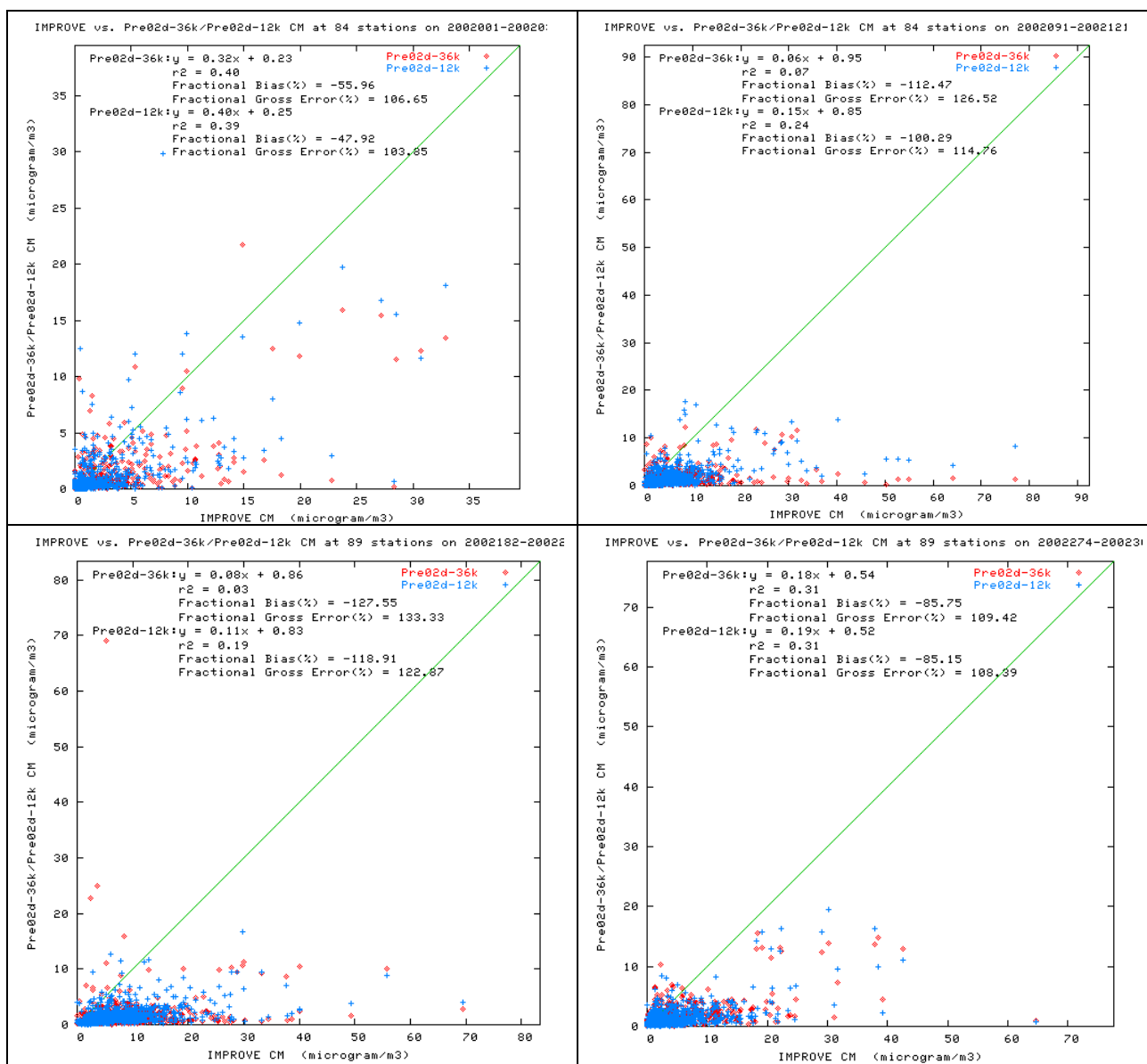


Figure 6-15. CMAQ 2002 pre02d base case simulation CM model performance in the WRAP states for January (top left), April (top right), July (bottom left), and October (bottom right) using the IMPROVE monitoring network.

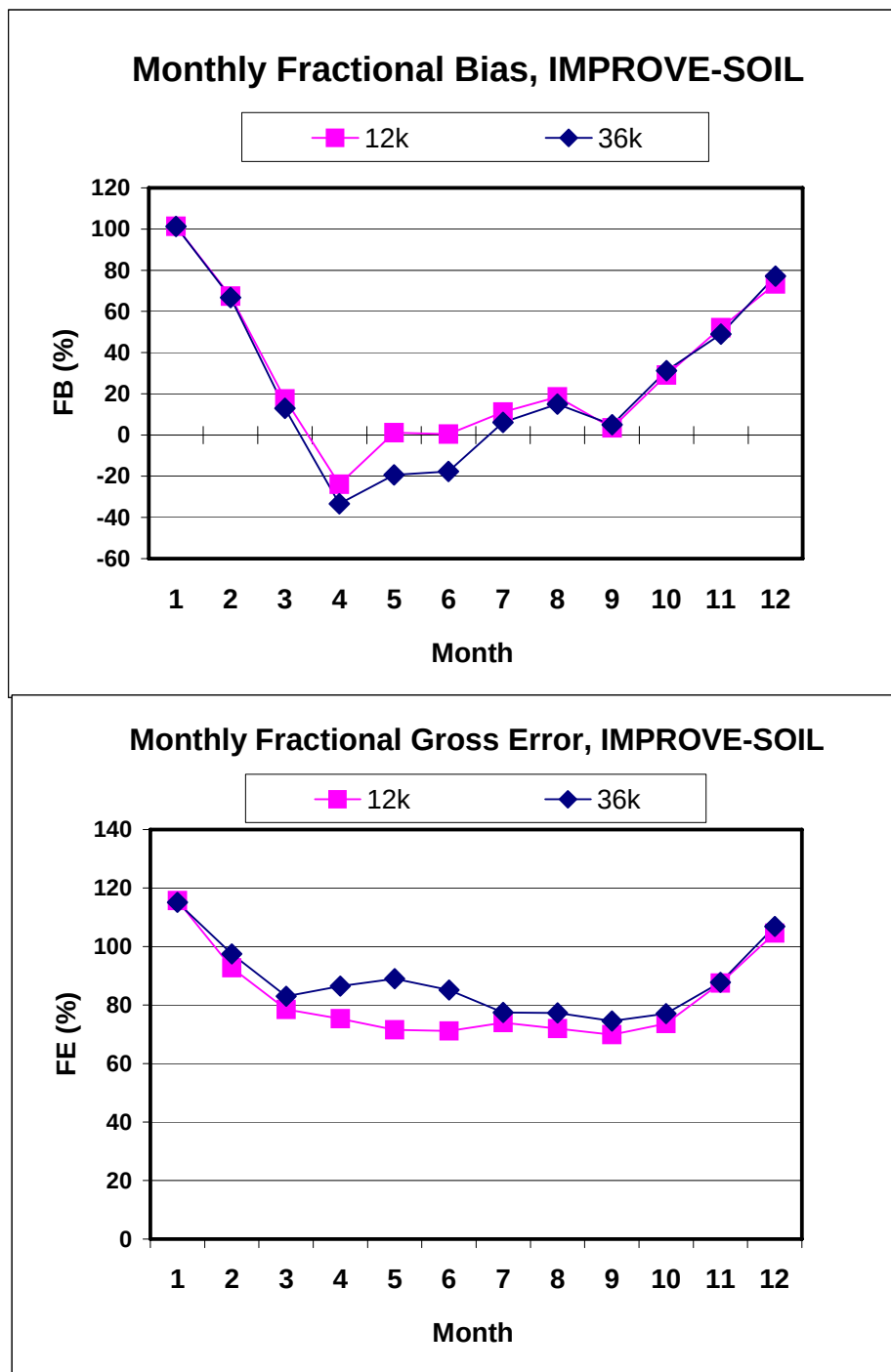


Figure 6-16. Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d base case “other fine PM” (soil) model performance across the IMPROVE sites in the WRAP states.

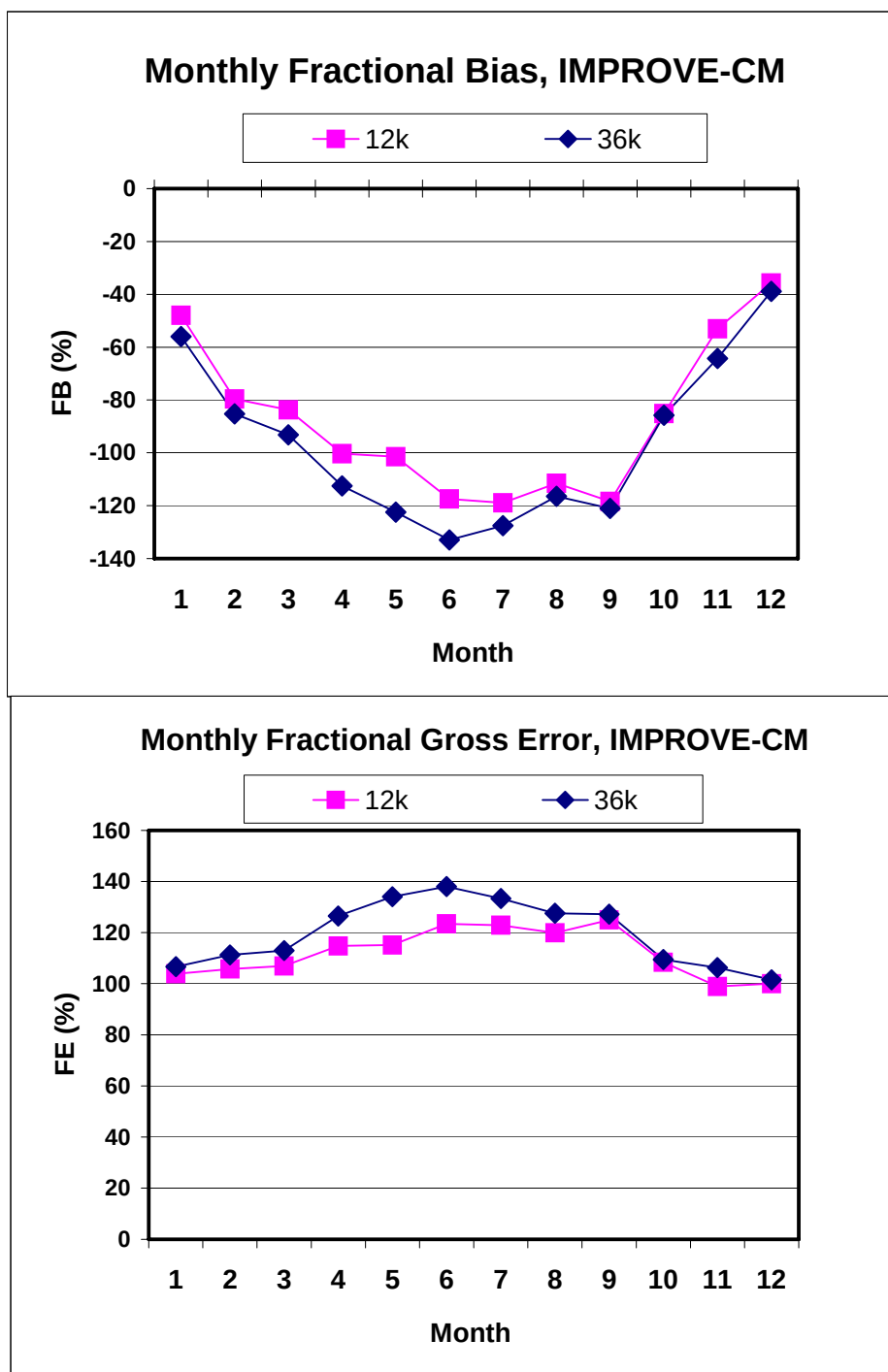


Figure 6-17. Monthly fractional bias (top) and fractional gross error (bottom) for the CMAQ 2002 pre02d base case CM model performance across the IMPROVE sites in the WRAP states.

6.3 Evaluation of CMAQ at Class I Areas for the Best-20% and Worst-20% Days

The 2007/2008 RHR SIP/TIP will be the first progress SIP/TIP that must demonstrate progress toward achieving natural conditions at Federally mandated Class I areas by 2064. The 2000-2004 five-year baseline is used as the starting point for the visibility projections, with the first future-year progress demonstration year being 2018. For the 2007/2008 SIP/TIP, visibility is projected at Class I areas for the worst-20% visibility days and the best-20% visibility days to achieve the following goals:

- demonstrate progress toward natural conditions in 2064 for the worst-20% visibility days, and
- demonstrate no worsening in visibility conditions for the best-20% days.

6.3.1 Procedures for projecting visibility improvements

Visibility is projected using modeling results in a relative fashion to scale the observed components of light extinction for the worst/best-20% days (U.S. EPA, 2001). The species-dependent and Class-I-area-dependent scaling factors are referred to as relative reduction factors (RRFs). Although the exact procedures for projecting visibility are undergoing analysis and refinement and will depend on the amount of modeling results available, the steps that would be taken using 2002 annual CMAQ modeling results to project current-year to 2018 future-year visibility conditions would likely be as follows (U.S. EPA, 2001):

1. Identify the worst-20% and best-20% observed visibility days at each Class I area during each year within the 2000-2004 baseline.
2. Calculate the average CMAQ estimated concentrations of SO₄, NO₃, OC, EC, soil, and CM for the worst-20% days and the best-20% days (separately) for the 2002 “typical year base case” and the 2018 emissions scenario, then calculate the species- and Class-I-area-dependent RRFs as the ratio of average future to current year modeling results (2018/2002) across the observed worst-20% or best-20% days from 2002.
3. Apply the model-derived RRFs for the worst-20% days to the current observed concentrations at each Class I area for each of the worst-20% days from the years 2000-2004 to obtain projected 2018 PM species concentrations for the worst-20% days from 2000-2004.
4. Calculate visibility extinction from the 2018 projected concentrations for each of the observed worst-20% days from 2000-2004 using the reconstructed mass extinction equation and monthly-average Class-I-area-specific relative humidity adjustment factors.
5. Convert the 2018 projected daily average total visibility extinction for each of the worst-20% days from 2000-2004 to deciview (dV) and average across each year to obtain the five average 2018 deciviews for 2000-2004.
6. Average the five annual worst-20% 2018 deciviews to obtain the five-year-average 2018 deciview.

7. Repeat steps 3 through 6 for the best-20% days.
8. Compare the 2018 projected five-year average deciviews with the visibility progress goal for each Class I area.

The key modeling components used to project future-year visibility are the Class-I-area- and species-specific RRFs that are based on the model-estimated average concentrations for the worst-20% and best-20% observed visibility days. Consequently, the CMAQ model performance for the worst-20% and best-20% days is very important.

6.3.2 Evaluation for best/worst-20% days

In this section we provide examples of the CMAQ model performance for extinction on the best-20% and worst-20% visibility days during 2002. Note that in this evaluation we used results from the previous CMAQ Base Case C rather than pre02d results. Base Case C is one iteration previous to the pre02d scenario, but since Base Case C produced model performance similar to pre02d's (see <http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#pre02d>) our evaluation results provide insights to the CMAQ pre02d performance.

The evaluation was conducted by comparing the predicted and observed average extinction for each component of light extinction in the IMPROVE aerosol mass extinction equation using the Class-I-area-specific monthly relative humidity adjustment factors. The extinction is averaged across the worst-20% and best-20% observed visibility days during 2002.

6.3.2.1 Performance across IMPROVE sites for average of worst-20% days

Figure 6-18 compares the predicted and observed extinction averaged for the worst-20% days at western U.S. IMPROVE sites for the six components of light extinction due to SO₄, NO₃, OC, EC, soil, and CM. The model estimates the observed average extinction due to SO₄ on the worst-20% days fairly well, although there is an underestimation tendency when the observed extinction due to SO₄ is above ~15 Mm⁻¹.

At most of the IMPROVE sites the model exhibits little bias in the extinction due to NO₃ at western U.S. IMPROVE sites for the worst-20% days, although there is a lot of scatter. However, there do appear to be three sites where the model underestimates the average extinction due to NO₃ on the worst-20% days by a factor of 2 to 3 (Figure 6-18a, top right).

With the exception of one very large overestimation outlier, the extinctions due to OC and EC on the worst-20% days appear to be reproduced reasonably well (Figure 6-18a, middle). The one outlier is the Kalmiopsis site, which was highly influenced by fires during August 2002.

Extinction due to CM is understated by the model for the worst-20% days. However, both the model and observations indicate that CM is a minor contributor to the total extinction on the worst-20% days. There do appear to be three predicted and observed CM extinction points for the average of the worst-20% days that stand out from the rest (Figure 6-18a, bottom left): (1) a point lying above the 1:1 line at around 10 Mm⁻¹ predicted/observed value, which is Kalmiopsis; (2) a point with a 10 Mm⁻¹ predicted and 20 Mm⁻¹ observed, which is Phoenix; and (3) a point with about 2 Mm⁻¹ predicted and 17 Mm⁻¹ observed, which is Saguaro National Park.

With the exception of the 40 Mm^{-1} point that is Kalmiopsis, the model and observations agree that soil is also a minor contributor to the extinction budget at IMPROVE monitors in the western U.S. during the worst-20% days.

6.3.2.2 Performance across IMPROVE sites for average of best-20% days

On the best-20% days (Figure 6-18b), the agreement between the predicted and observed average extinction across the six species is not as good as it was for the worst-20% days. Extinction due to SO_4 , NO_3 , and OC is overstated for the average of the best-20% days. For around a half-dozen IMPROVE monitors, extinction due to OC, EC, and soil is greatly overstated on the average of the best-20% days, whereas extinction due to CM is generally understated at most monitors on the best-20% days.

6.3.2.3 Example predicted and observed Class I area extinction budgets for worst-20% and best-20% days

Figure 6-19 displays comparisons of predicted and observed stacked bar charts of total extinction averaged across the worst-20% days at several of the IMPROVE monitors at Class I areas in the western U.S. These stacked bar charts are shown without including Rayleigh background, which would add a constant 10 Mm^{-1} to all plots if it were included. A comparison of the average predicted and observed extinction for the worst-20% days at Grand Canyon National Park (Figure 6-19a, top) reveals fairly good agreement with the total extinction. Although extinction due to SO_4 and NO_3 is slightly underestimated, this is compensated for by slightly overstated extinction due to OC. However, the extinction due to CM is greatly understated at the Grand Canyon for the worst-20% days.

Results for the average of the worst-20% days at Chiricahua National Monument in southeastern Arizona are not as good, with the observed total extinction of approximately 35 Mm^{-1} underestimated by approximately a factor of 3 (Figure 6-19a, bottom). Every component of extinction for the worst-20% days is underestimated at Chiricahua, with the underestimation of extinction due to CM being over an order magnitude lower. We suspect that issues associated with the Mexican inventory, missing fugitive dust sources (e.g., windblown dust), and local impacts are contributing to the poor extinction performance at Chiricahua for the worst-20% days.

At Bandelier National Monument in north central New Mexico (Figure 6-19b, top), the total extinction on the worst-20% days is underestimated by approximately 20% due to an understatement of the extinction that is due to SO_4 , NO_3 , EC, soil, and especially CM. Extinction due to OC is overstated at Bandelier for the worst-20% days.

For Rocky Mountain National Park the total extinction for the worst-20% days is underestimated by approximately 35% (Figure 6-19b, bottom). Again, extinction due to SO_4 , NO_3 , EC, soil, and CM is understated, with the underestimation of the extinction due to CM being about a factor of 10. The extinction due to OC is reproduced quite well by the CMAQ Base Case C simulation at Rocky Mountain National Park for the worst-20% days.

At Yellowstone National Park (Figure 6-19c, top), the model overstates the total extinction on the worst-20% days by approximately 60% due to an overstatement of the extinction caused by OC and EC, where extinction due to these two components is overstated by a factor of 2 and 3,

respectively. Extinction due to soil is also overstated, although soil is a minor contributor to total extinction for the worst-20% days at Yellowstone. As seen at the other Class I areas, extinction due to CM is understated by the model.

At Glacier National Park in northwestern Montana, total extinction on the worst-20% days is understated by approximately 30%, with underestimation of the extinction due to SO₄, EC, and CM contributing the most to this bias (Figure 6-19c, bottom).

At Mount Rainier National Park (Figure 6-19d, top) the amount of extinction due to NO₃ is overestimated by the model by almost a factor of 5, resulting in a net overestimation bias for total extinction of 65%. Extinction due to OC and soil is also overstated, whereas extinction due to SO₄ and CM is understated at Mount Rainier for the worst-20% days.

The overstated OC and EC impacts at Kalmiopsis (Figure 6-19d, bottom) due to the August 2002 fires in southwestern Oregon are clearly evident in the extinction budgets for the worst-20% days at this site. The observed total extinction (187 Mm⁻¹) is overestimated by a factor of 3 by the model (581 Mm⁻¹). Even though Kalmiopsis has the highest observed total extinction of any site examined in Figures 6-19a-e, the model still greatly overstates it.

The final two IMPROVE sites with predicted and observed extinction comparisons for the worst-20% days are Point Reyes and San Geronio in California (Figure 6-19e). The high NO₃ contributions in both the observed and estimated extinction budgets are clearly evident. At San Geronio the model estimates the extinction due to NO₃ reasonably well, overstates the extinction due to EC and OC, and understates it due to CM, resulting in a good agreement in total extinction for the worst-20% days (within 10%). At Point Reyes, however, the model underestimates extinction due to SO₄ and NO₃ by approximately a factor of 2, resulting in an understatement of total extinction by 33%.

Finally, Figure 6-20 presents two fairly typical examples of the CMAQ Base Case C extinction performance for the *best*-20% days. The model overstates total extinction at Grand Canyon and Yellowstone on the best-20% days by approximately a factor of 2, with overstated extinction due to SO₄, NO₃, and OC contributing to this bias. Clearly the model has difficulty in simulating the clearest-visibility days.

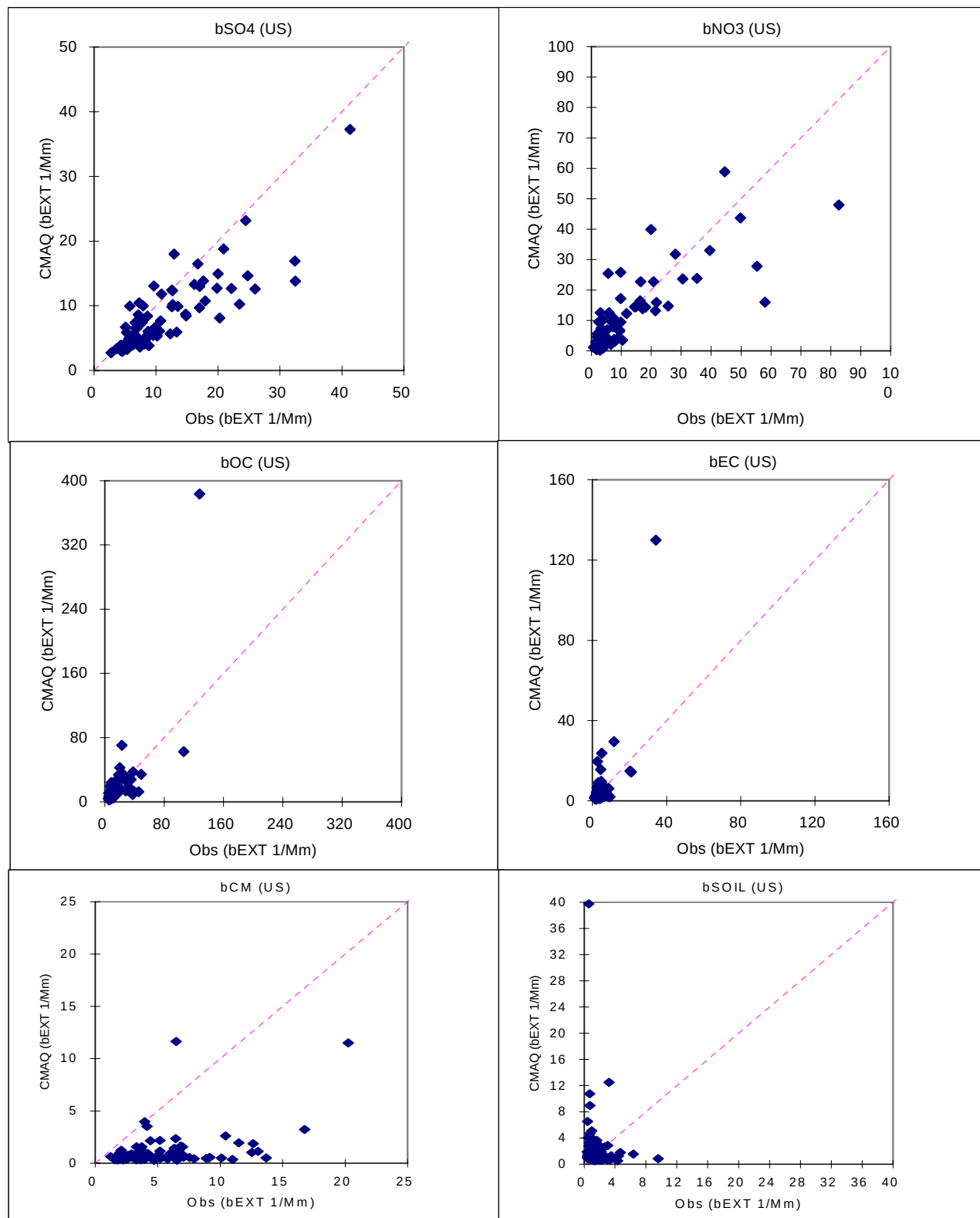


Figure 6-18a. Comparison of predicted and observed average extinction for the worst-20% visibility days in 2002 at IMPROVE monitors for SO₄, NO₃, OC, EC, CM, and soil.

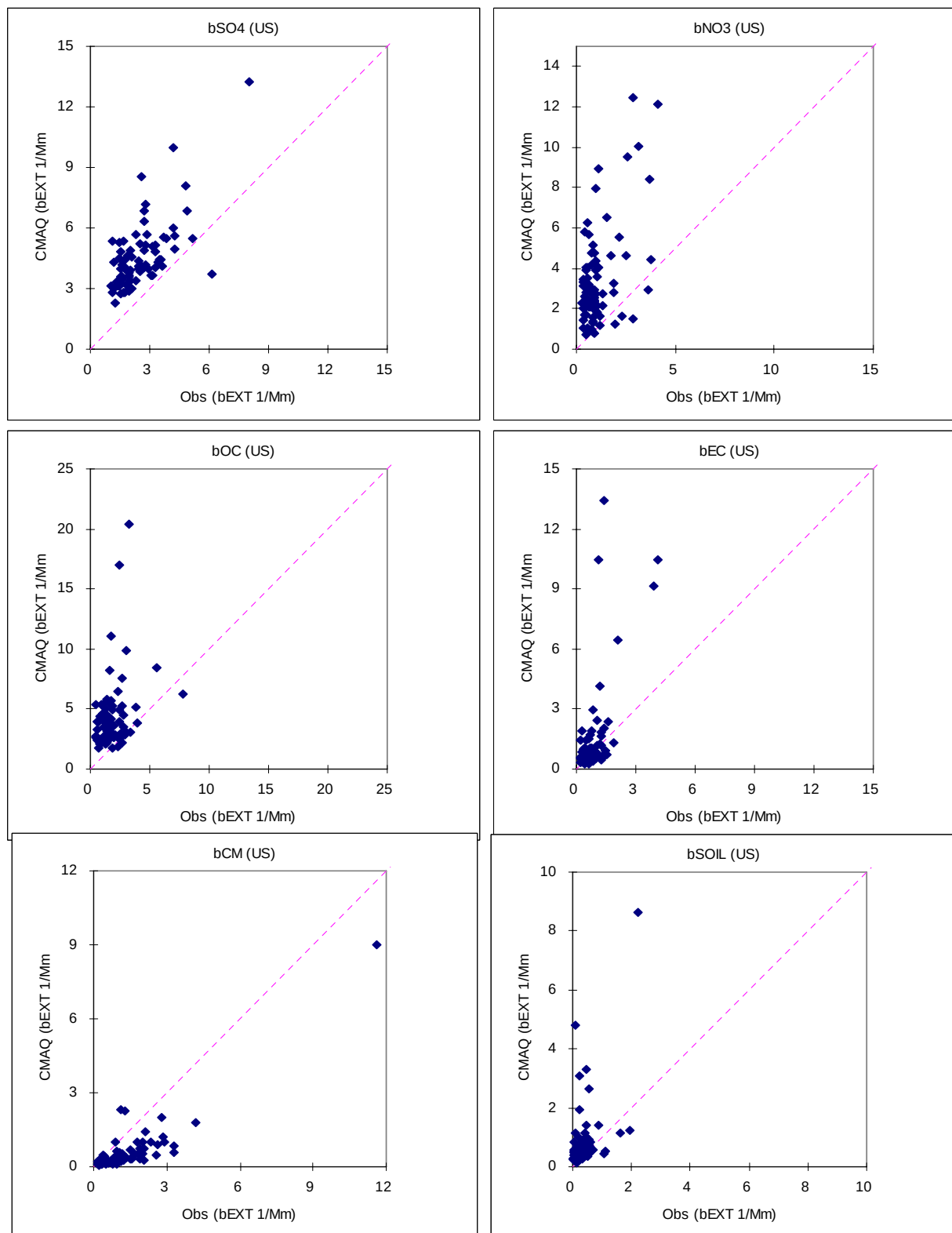


Figure 6-18b. Comparison of predicted and observed average extinction for the best-20% visibility days in 2002 at IMPROVE monitors for SO₄, NO₃, OC, EC, CM, and soil.

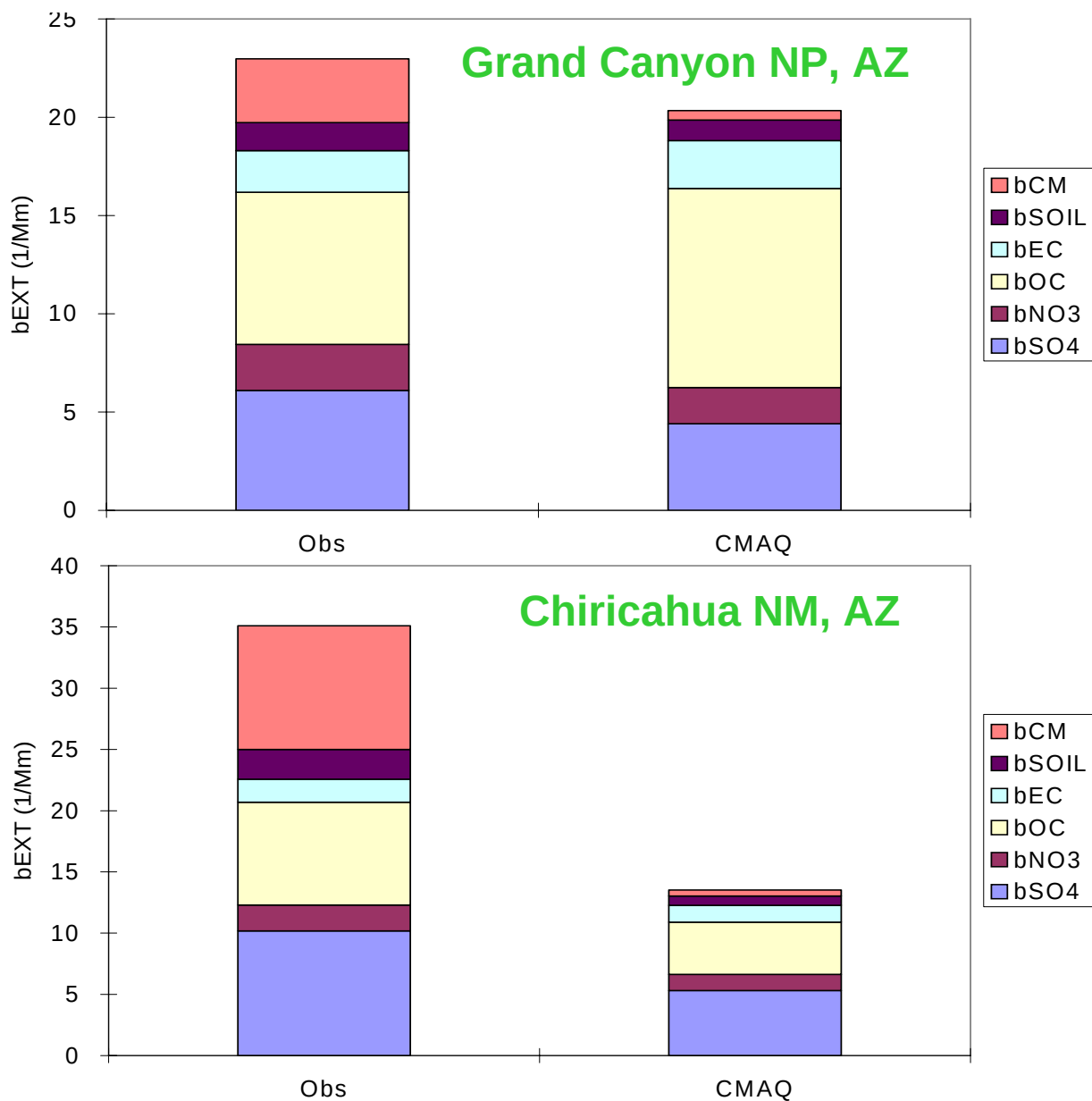


Figure 6-19a. Comparison of predicted (right) and observed (left) average extinction for the worst-20% visibility days in 2002 at the Grand Canyon (top) and Chiricahua (bottom) Class I areas.

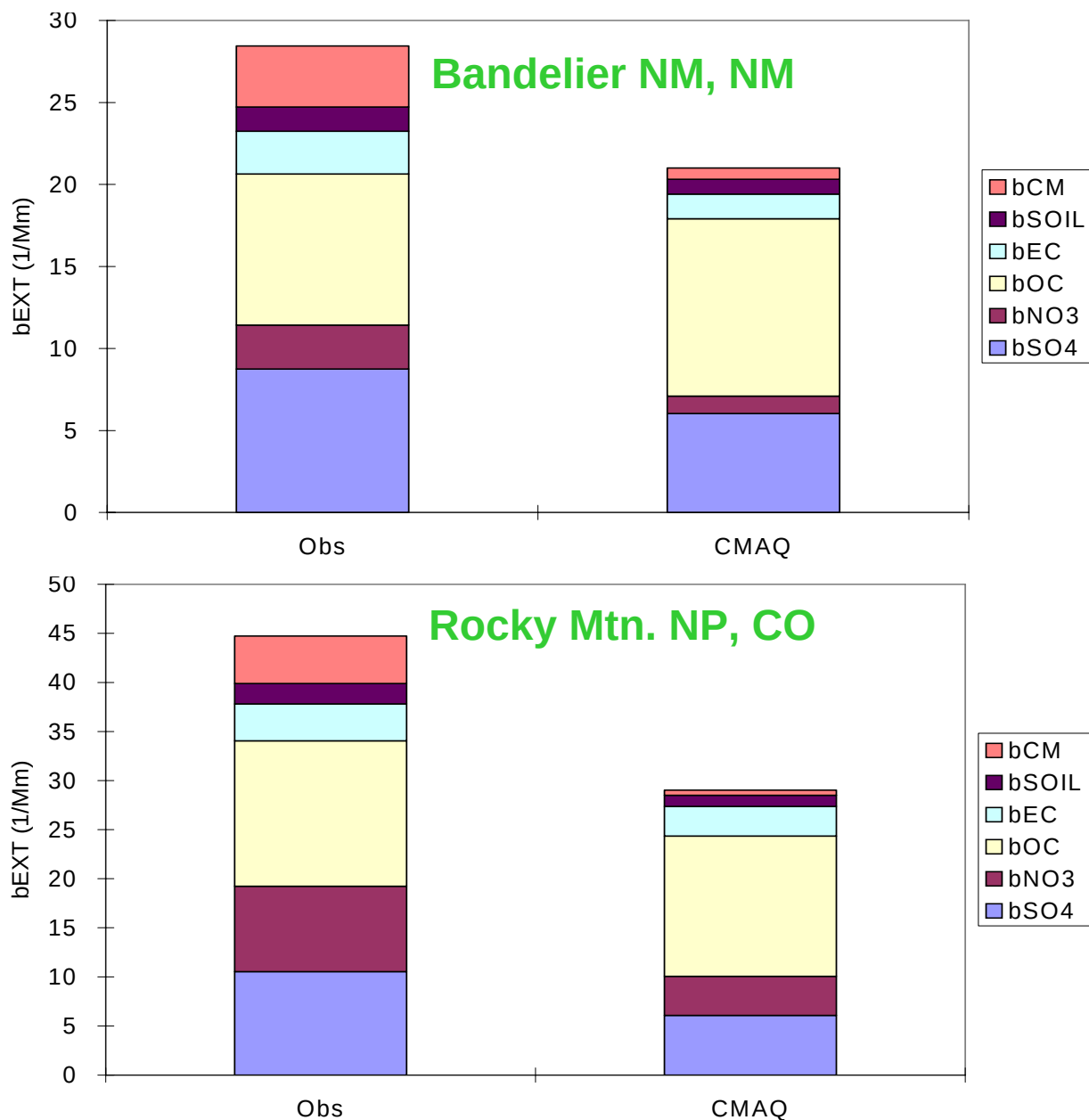


Figure 6-19b. Comparison of predicted (right) and observed (left) average extinction for the worst-20% visibility days in 2002 at the Bandelier (top) and Rocky Mountain National Park (bottom) Class I areas.

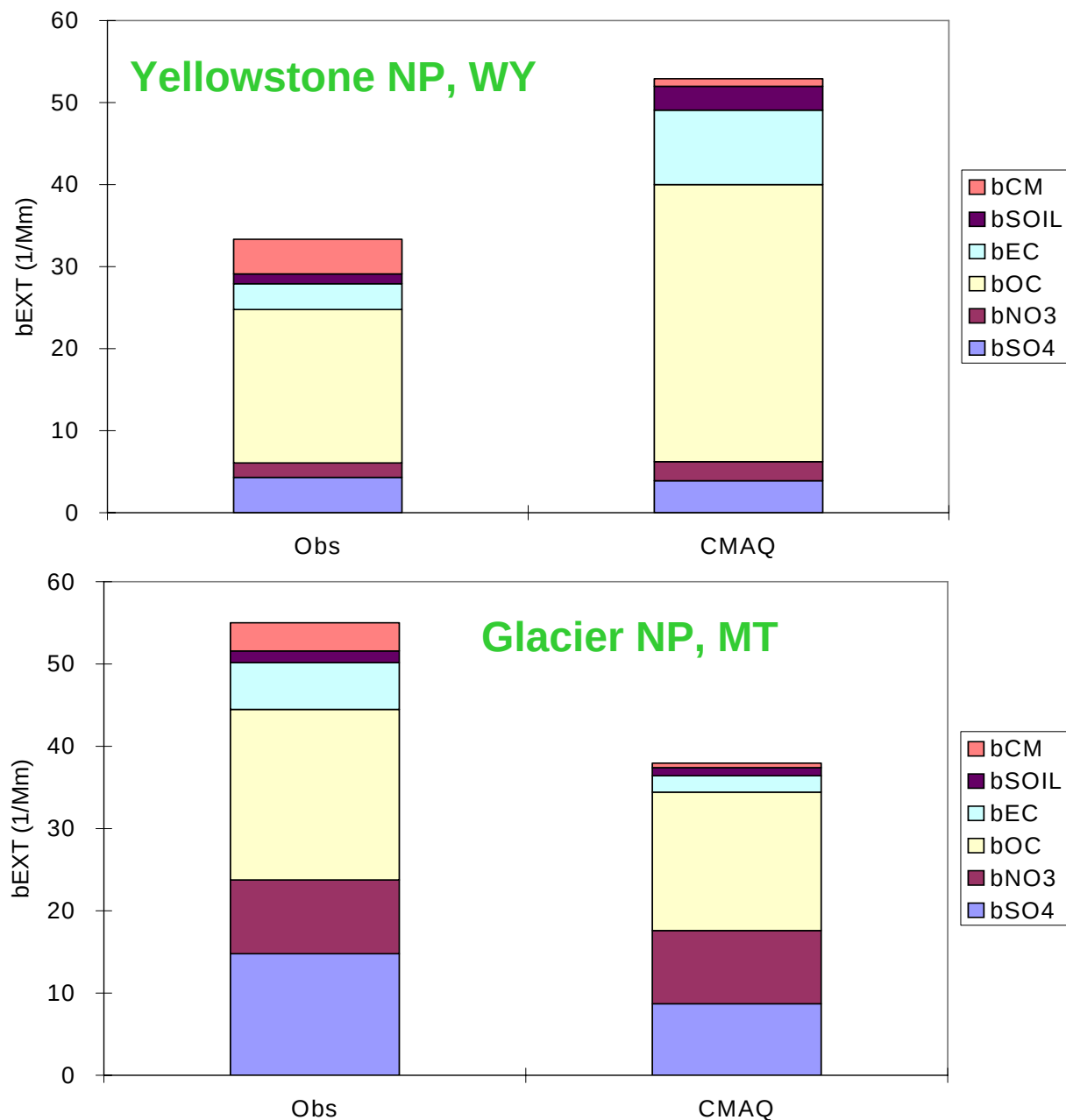


Figure 6-19c. Comparison of predicted (right) and observed (left) average extinction for the worst-20% visibility days in 2002 at the Yellowstone (top) and Glacier (bottom) Class I areas.

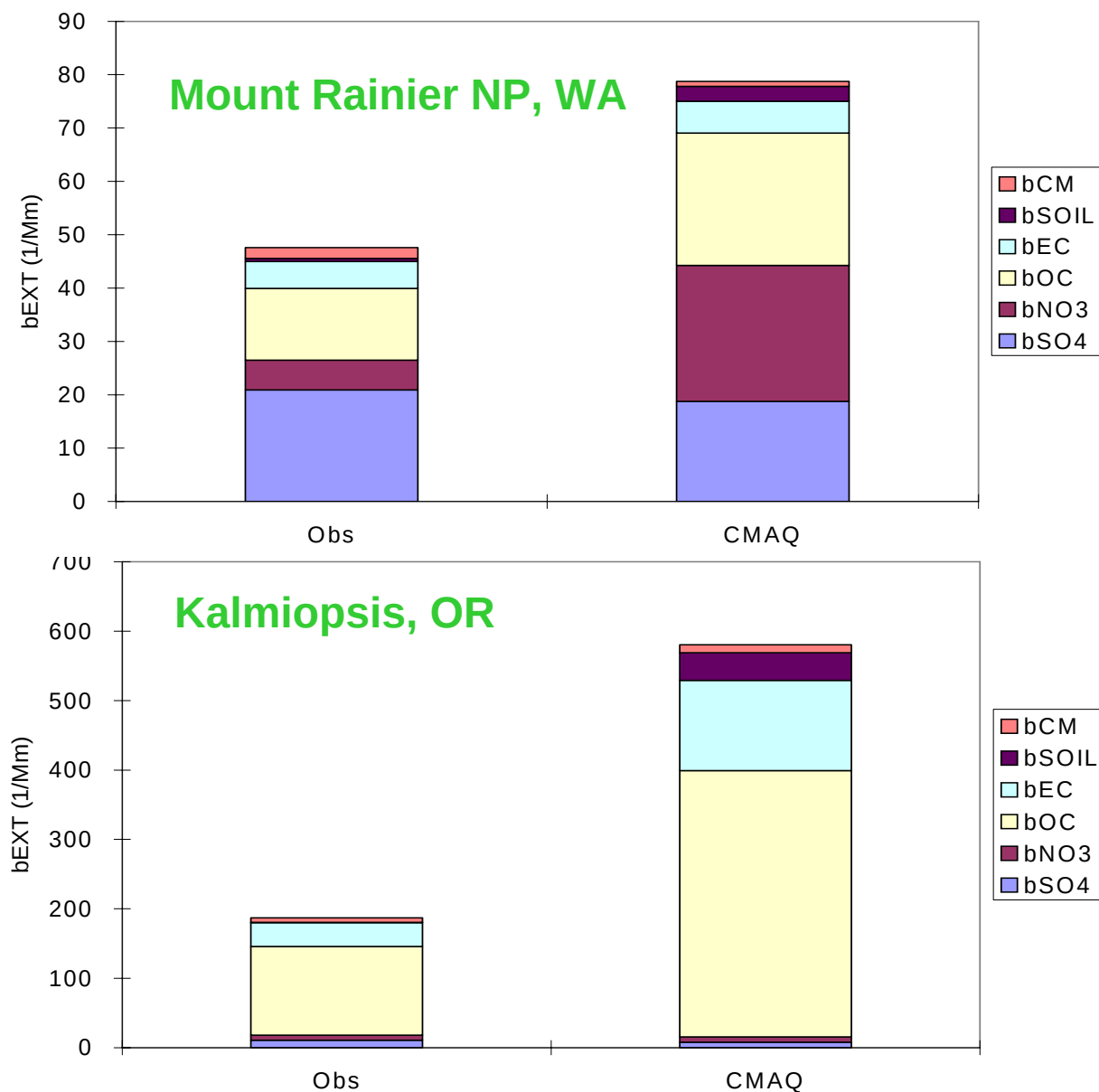


Figure 6-19d. Comparison of predicted (right) and observed (left) average extinction for the worst-20% visibility days in 2002 at the Mount Rainier (top) and Kalmiopsis (bottom) Class I areas.

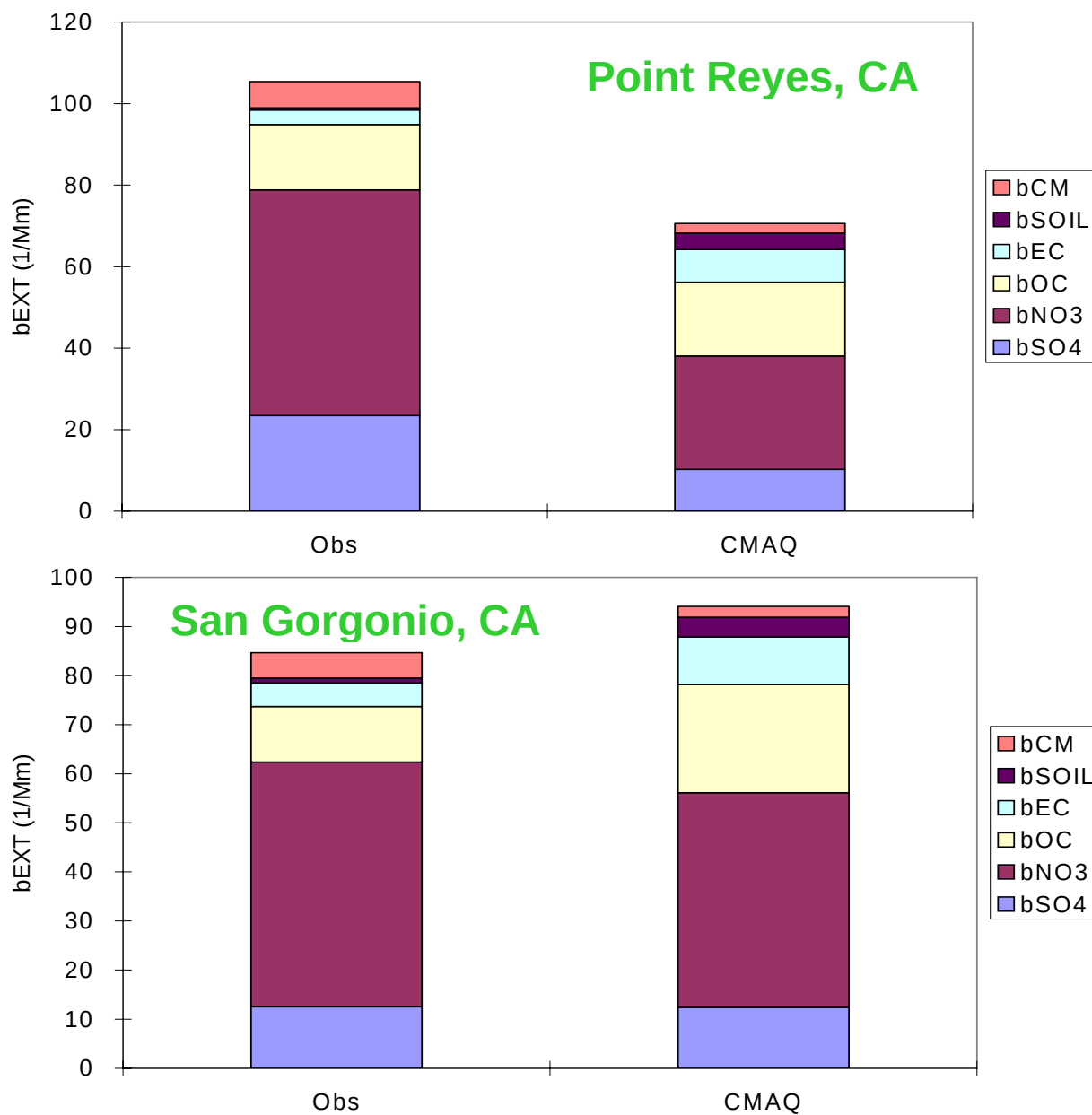


Figure 6-19e. Comparison of predicted (right) and observed (left) average extinction for the worst-20% visibility days in 2002 at the Point Reyes (top) and San Geronio (bottom) Class I areas.

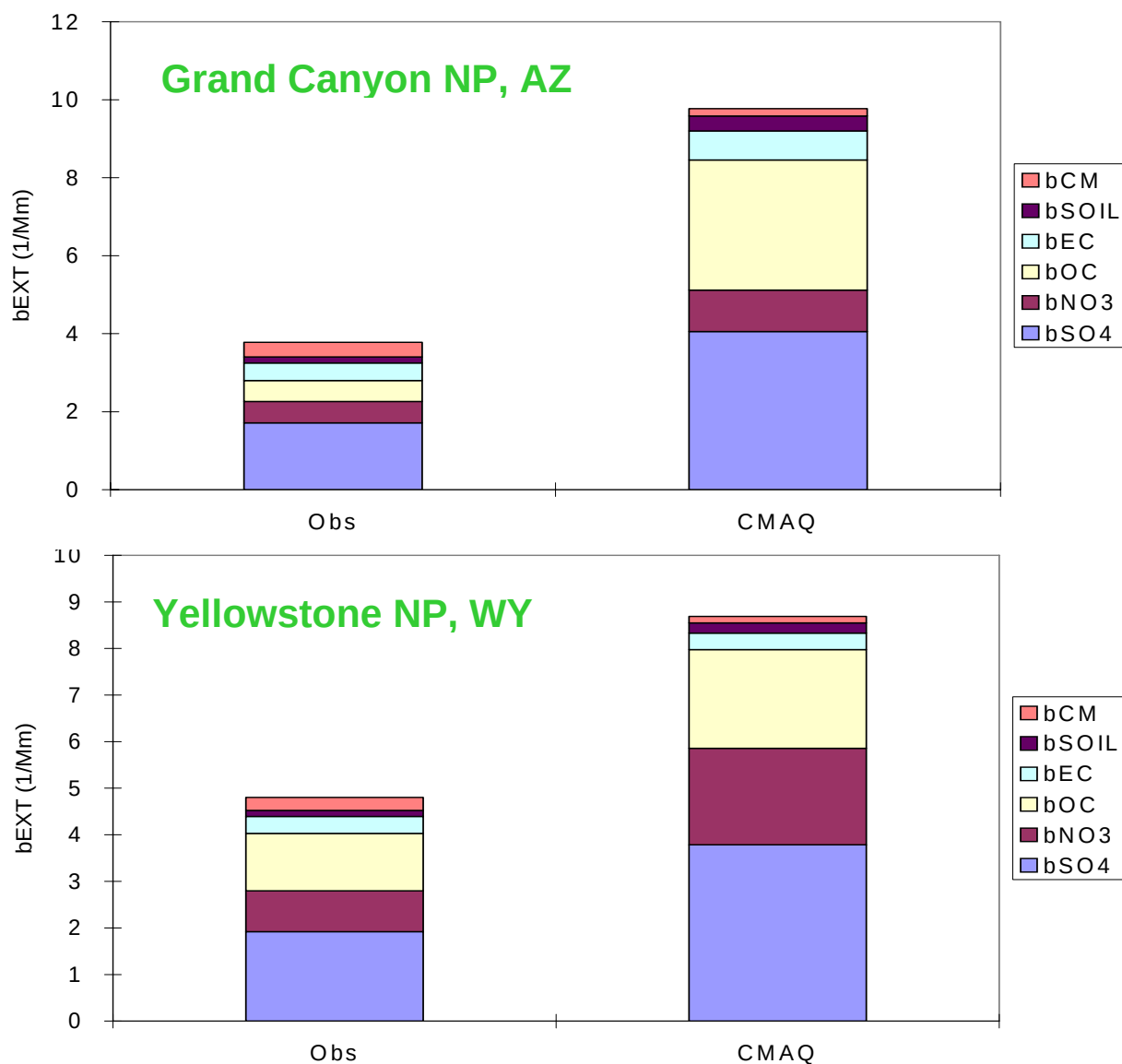


Figure 6-20. Comparison of predicted (right) and observed (left) average extinction for the best-20% visibility days in 2002 at the Grand Canyon (top) and Yellowstone (bottom) Class I areas.

6.4 Conclusions of CMAQ 2002 pre02d 36-km and 12-km Base Case Model Performance Evaluation

Performance for the CMAQ 2002 pre02d 36-km and 12-km base case simulation for sulfate across the western states is reasonably good, albeit with a summer underestimation and winter overestimation bias; the biases in the spring and fall are near zero. The summer SO₄ underestimation bias affects the model performance for visibility for the worst-20% days. One of the biggest changes between the previous CMAQ Base Case C simulation and the new CMAQ

pre02d base case was the inclusion of the new MM5 meteorological modeling results (see Section 4). WRAP expended extensive effort finding a more optimal MM5 configuration for simulating meteorological conditions in the western U.S. In particular, a summer overestimation of the precipitation in the southwestern U.S. led to overstated wet deposition and understated concentrations in previous CMAQ base case simulations. Figure 6-21 compares the SO₄ wet deposition across NADP sites in the WRAP states for the previous Base Case C and current pre02 2002 36-km CMAQ simulations. Using the older MM5 meteorology, wet SO₄ deposition is overstated by Base Case C during these four months by 36%, 61%, 55%, and 57%. However, using the new MM5 meteorology, wet SO₄ deposition is understated for the same four months by smaller amounts: -25%, -15%, -38% and -34%; also, in each month this deposition exhibits lower bias and the same or lower error. The CMAQ 2002 pre02d 12-km simulation produced higher SO₄ concentrations than the 36-km simulation. Comparisons of 36-km and 12-km wet SO₄ deposition were not available.

Nitrate performance exhibits a large winter overestimation and summer underestimation bias, with large errors throughout the year. During the summer the model and observations both show low NO₃ values, so the NO₃ underestimation does not drastically affect visibility model performance for the worst-20% days. However, the winter NO₃ overestimation bias can affect performance the best-20% days. The 12-km base case produced higher NO₃ concentrations than the 36-km base case, resulting in slightly improved model performance in the summer and slightly degraded model performance in the winter when a 12-km grid is used.

Organic carbon at the IMPROVE sites has a positive bias in the winter and near zero (36-km) or negative (12-km) bias in the summer. There were large differences in the CMAQ OC performance using the 36-km and 12-km grids, with the 12-km modeling results estimating lower OC than did the 36-km results. On at least one documented case of large fire impacts (August 2002 in southwestern Oregon), the model greatly overstated the amount of both OC and EC at the monitors. Other than that, EC bias across the IMPROVE sites was relatively low, with an approximately -20% (36-km) and -30% (12-km) bias during the nonsummer months and bias <±20% during the summer.

Coarse mass was understated throughout the year, with the understatement greatest during the summer, late spring, and early fall, exceeding -100% for some months. Other fine PM (soil) was overstated in the winter (60% to 100%) and understated in the summer (0% to -40%).

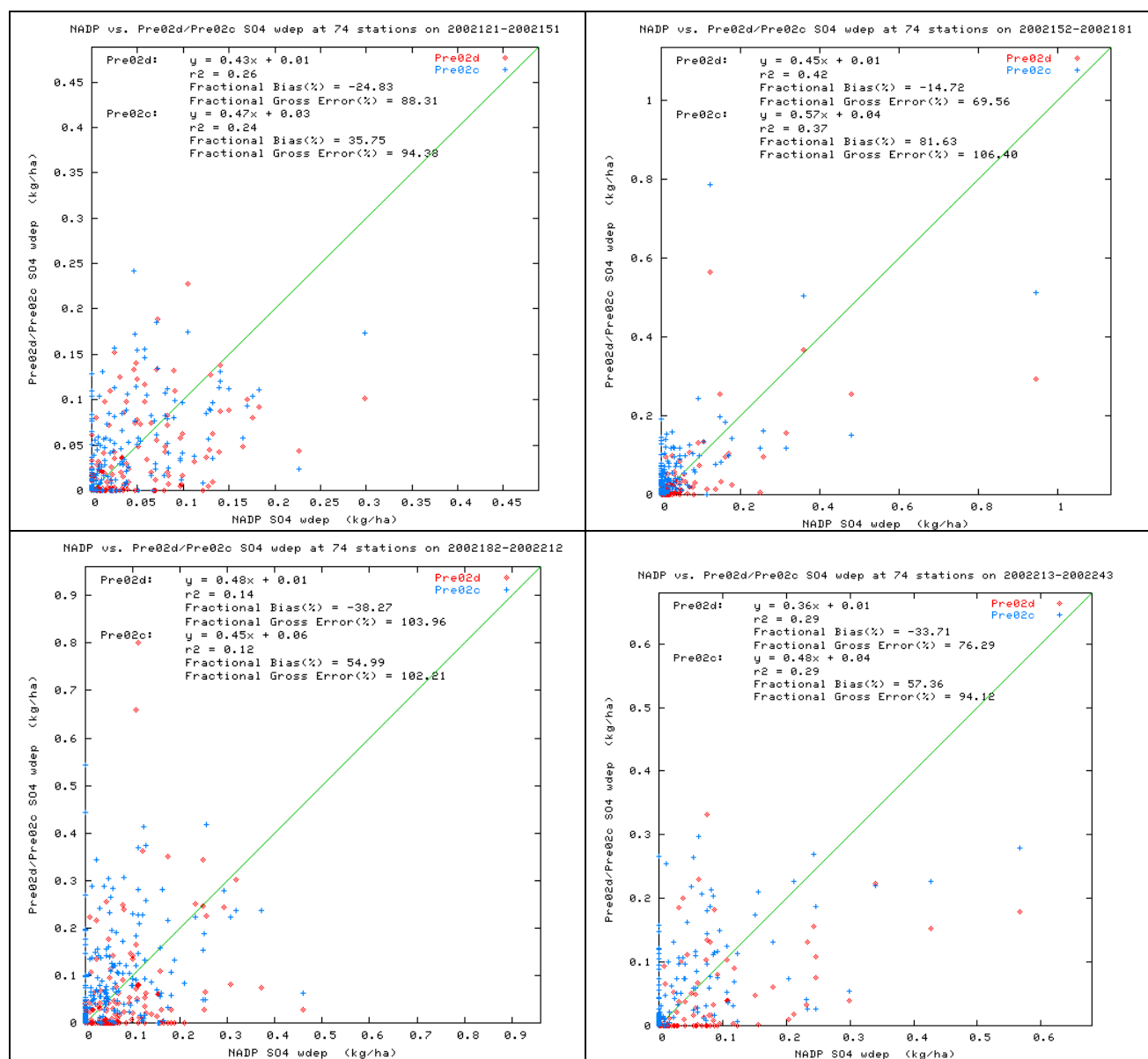


Figure 6-21. Comparison of CMAQ 2002 36-km pre02d and Base Case C wet SO₄ deposition model performance in the WRAP states for May (top left), June (top right), July (bottom left) and September (bottom right).

6.5 Status of Task 4 Deliverables

The table below gives the status of each Task 4 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 6-2. Status of the Task 4 deliverables.

Deliverable	Status
CMAQ pre02b (Base B) Base Case Performance Evaluation	Posted January 2004: http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#pre02b
Comparison of CMAQ V4.3 with CMAQ V4.4beta model performance	Posted June 2004: http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#compare
CMAQ pre02c (Base C) Base Case Performance Evaluation	Posted July 2004: http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#pre02c
Comparison of CMAQ V4.4beta with final CMAQ V4.4 (October 2004 release)	Posted November 2004: http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#beta
CMAQ pre02d (Base D) Base Case Performance Evaluation	Posted January and April 2005: http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#pre02d

7. Task 5: Preparation and Reporting of Geographic Source Apportionment Results

7.1 Overview

A primary motivation for using air quality models is the attempt to identify the particular emissions sources that contribute to pollutant exposure at a particular receptor site. This source attribution information can then be used to develop the most effective emissions reduction strategy for attaining air quality goals at that site.

A variety of modeling and data analysis methods have been used to perform source attribution (also sometimes referred to as “source apportionment”). Model sensitivity simulations have been used in which a “base case” model simulation is performed and then a particular source is “zeroed out” of the emissions. The importance of that source is assessed by evaluating the change in pollutants at the receptor site, calculated as pollutant concentration in the sensitivity case minus that in the base case. This approach is known as a “brute force” sensitivity because a separate model simulation is required for each sensitivity.

Although sensitivity approaches are widely used and provide valuable information, they also have some disadvantages. For small sources, the model used may lack sufficient numerical precision to represent the effect of the source at a receptor site. More importantly, the chemical reactions of some precursor species have a nonlinear dependence on ambient species concentrations and are subject to positive and negative feedback effects when a model input parameter is changed. Thus, the change in pollutant concentration at a receptor site in the sensitivity case might not accurately reflect the contribution of that source to the receptor in the base case. The concern regarding nonlinearity primarily affects NO_x, O₃, and nitrate, with a smaller effect on organic aerosols and sulfate. (Nonlinearity is not a concern for nonreactive or slowly reacting species.) Another limitation of brute force sensitivity approaches is that very large numbers of sensitivity simulations must be completed to develop source attribution for all of the emissions source categories and source regions of interest. More efficient sensitivity approaches, e.g., the decouple direct method (DDM), are available for gas-phase sensitivities and are being developed for aerosols.

Mass-tracking approaches such as a tagged-species algorithm represent a second approach for performing source attribution. Mass-tracking approaches do not attempt to predict how the pollutant concentrations will change at a receptor site; instead, they attempt to identify the mass contributions of each source to the pollutant at the receptor site in the base case model simulation. Thus, these mass-tracking approaches for performing source attribution have the potential to evaluate the contribution or “responsibility” for all sources in a single model simulation. These approaches have not been widely used in air quality modeling because of the complexity and difficulty of implementing a mass-tracking algorithm. A tagged species approach using tracers to track the contributions of particular emissions sources is probably the most easily implemented type of mass tracking approach. EPA has previously used tagged-species methods

to do source attribution for sulfate in regional acid deposition modeling. ENVIRON's CAMx model uses a source attribution algorithm for ozone (OSAT). ENVIRON has recently implemented a particulate source attribution algorithm in CAMx, known as PM Source Apportionment Technology (PSAT). It is still uncertain whether sensitivity approaches or source attribution approaches are more useful for attributing responsibility to emissions sources. It is likely that a combination of both approaches will be most useful for developing optimal emission control strategies. The key difference between the approaches is that source attribution estimates the contribution of a source to pollutants at a receptor, while sensitivity simulations estimate the change in pollutants at receptor when an individual source is changed by a particular amount.

During 2003 and 2004, UCR developed a new algorithm in CMAQ to assess source attribution. The Tagged Species Source Apportionment (TSSA) algorithm uses a system of tracers or "tagged species" to track the chemical transformations, transport, and removal of emissions from particular source categories or source locations. This algorithm has been implemented and tested for NO_x-NO₂-nitrate chemistry, sulfate, and ammonium. The algorithm was initially implemented in CMAQ version 4.2.2 using the Sparse-Matrix Vectorized Gear (SMVGEAR) gas-phase chemistry solver. During 2004 we implemented the TSSA algorithm in a beta release of CMAQ 4.4 and adapted it for use with a more computationally efficient Quasi Steady State Approximation (QSSA) gas-phase chemistry solver in CMAQ. The algorithm is written in Fortran 90 and supports multiprocessor usage. The results of this algorithm were first demonstrated at the WRAP Technical Workshop in January 28-29, 2004, using the RMC's preliminary 2002 modeling with CMAQ 4.2.2. In this section we describe the implementation of the algorithm and summarize results for modeling with the beta CMAQ 4.4 using the Pre02c 2002 simulation discussed in Section 5.

During the testing of the TSSA algorithm in CMAQ 4.4beta, we discovered significant mass conservation errors in the algorithm. These errors were likely the result of a bug that affected mass conservation in CMAQ 4.4beta. However, it is also possible that the vertical advection algorithm in CMAQ introduces errors in mass conservation in the TSSA algorithm. During 2004 we experimented with several different methods to handle problems with mass conservation in CMAQ. Nonetheless, large fractions of mass of PM species could not be attributed to the source categories. Additional development and testing of the TSSA algorithm are required. This effort is currently underway with separate funding from EPA using a new release of CMAQ 4.4 in which the mass conservation error was corrected.

Although there are concerns regarding the *absolute* mass attributions in the CMAQ TSSA results, comparisons with brute force sensitivity tests and alternate models have made us more confident that the *relative* mass attributions are correct. As noted above, a similar source attribution algorithm has been implemented in the CAMx model by ENVIRON. The CAMx PSAT was released in 2004 and uses a system of tracers similar to the system used in the TSSA algorithm to attribute particulate mass at receptor sites to emissions source categories or source regions. To compare CMAQ TSSA results with CAMx PSAT results, we performed CAMx PSAT simulations for two months: February and July, 2002. Results for both models are described in Section 7.3. The CAMx and CMAQ results are not directly comparable because updated versions of the emissions and meteorology data were used in the CAMx PSAT simulation. However, we would expect the results to be generally similar, so the CAMx results provide a useful test to evaluate the usefulness of the CMAQ results.

In summary, the CAMx PSAT results are generally consistent with the relative source attributions in CMAQ. However, the PSAT much more accurately accounts for the total mass of PM at receptor sites. In the CMAQ results large fractions of mass were either not attributed to emissions sources at some receptor sites or were attributed to a combination of emissions categories, such as fires and area sources, that were not individually tracked. Although work is in progress to develop a new version of the TSSA algorithm in CMAQ, we do not expect this to be completed in time for additional WRAP source attribution studies in 2005. We therefore plan to complete additional source attribution simulations in 2005 using the CAMx model with PSAT.

7.2 Description of TSSA Method

7.2.1 Initialization of tagged species

The CMAQ TSSA methodology uses tagged species to track the temporal evolution of emissions, chemical transformations, transport, and dispersion of mass across the model's spatial domain. Tracers are defined for a subset of key chemical species and for certain predefined subregions and emissions source categories. In addition, tracers are included to represent mass contributions from the initial conditions (ICs) and from transport into the model domain from the boundary conditions (BCs). The tracers are all initialized with zero values, except for the IC tracer, which is identical to the initial species concentrations. Then, the tracer concentrations are updated at each model time step over the entire model simulation period.

For each species, the “bulk concentration” is defined to be the model-predicted concentration of the species for each grid cell. Thus, a three-dimensional (3-D) array is required to represent the concentration of the bulk species. For the TSSA method, the source attribution requires the addition of one additional 3-D array for each source category or source region that is tracked by the algorithm. For example, if source attribution is performed for three emissions categories (e.g., point, mobile, and biogenic) and 10 different source regions (e.g., 10 different state or tribal areas), a total of 32 new 3-D tracers must be added to represent the 30 combinations of source category and region plus the ICs and BCs. By definition, the sum of the tracers must always be identical to the bulk species concentration because the tracers are defined to represent the sources that compose the bulk species, as shown in Equation 7-1:

$$C_{bulk}^j = \sum_{m,n}^{M,N} C_{m,n}^j + C_{IC}^j + C_{BC}^j \quad (7-1)$$

where j represents the chemical species, m represents emissions source categories, and n represents geographical source regions.

The 3-D concentration fields for each tracer are output at the same time interval (typically hourly) that is used for the CMAQ bulk concentration output files. Thus, tracer output files provide three-dimensional fields showing the time-varying contribution of each tagged source (where a “tagged source” is defined by the use of a set of tagged species to identify the contributions from that source) in all spatial regions throughout the model domain. For example, Figure 7-1 shows

the 3-D concentration field for a tracer for aerosol nitrate attributed to California mobile-source emissions at 24:00 UTC on January 14, 2002.

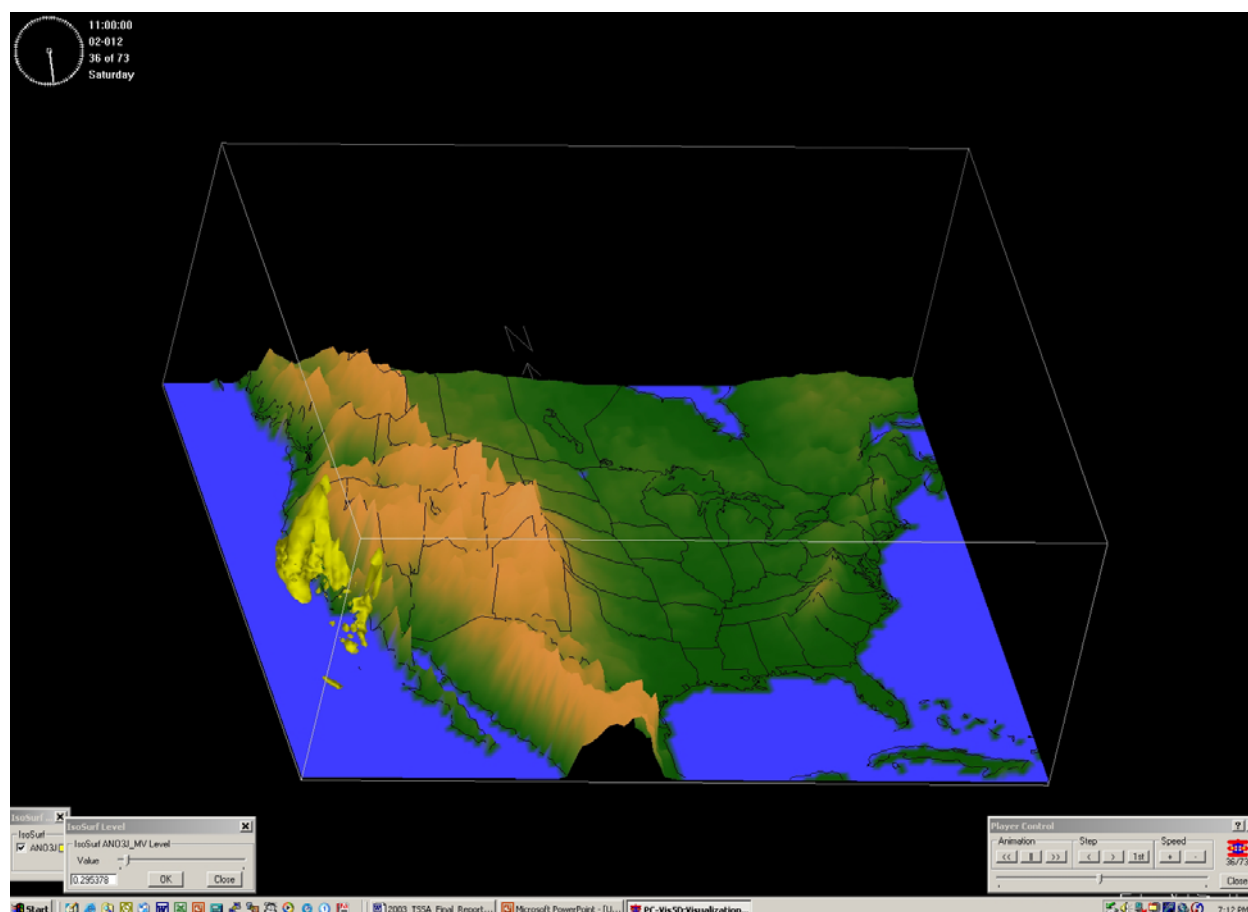


Figure 7-1. Three-dimensional plot of aerosol nitrate attributed to California mobile-source emissions on January 14, 2002.

Currently, the tagged species implemented in CMAQ include the family of nitrogen model species, including NOX (the “reactive N” family), HNO₃, PAN, RNO₃, ANO₃I, and ANO₃J. The reactive NOX species is defined as the sum of NO, NO₂, NO₃, 2*N₂O₅, and HONO. We note that this definition of “big NOX” differs from the usual definition of NO_x as the sum of NO and NO₂. We use the expanded definition of big NOX because these short-lived, reactive forms of nitrogen are in fairly rapid chemical equilibrium, and we achieve a substantial computation cost reduction by using a single family to represent the sum of reactive N.

7.2.2 Definition of source regions

Tracers are defined for selected, predefined geographical regions. Source regions are defined by assigning a unique numeric code to the model grid cells that compose each source area. The

source region can be defined to be a single grid cell or any number of grid cells up to the total number of cells used in the spatial domain. Typically, a source region is composed of a group of contiguous cells, but a source region could also be composed of noncontiguous cells. Figure 7-2a illustrates the TSSA regions for each state within the WRAP 36-km modeling domain. In this figure, California is assigned the number 1, Nevada is assigned 2, etc. The entire source regions of Canada and Mexico are assigned the numeric codes of 91 and 92, respectively. All U.S. states outside of the WRAP region are grouped together. The boundaries of California, Oregon, and Washington were extended westward so that offshore shipping would be included in the source attribution for those states. The map in Figure 7.2a is truncated, so portions of Canada, Mexico, and the easternmost U.S. states are not shown, but the full model domain is included in the algorithm.

The state and national boundaries can be only coarsely represented in this map because the resolution is limited by the 36-km grid used in the modeling. We assigned each grid cell to whichever state accounted for the largest area of the grid cell. Thus, emissions sources near political boundaries might be incorrectly located in an adjacent state.

A 12-km grid definition would allow better representation of political boundaries. Alternatively, the digital map could easily be modified to change the source region definitions by simply editing the numeric values in the ASCII text file that contains the source region definitions. For example, if a border cell is located primarily in California but includes a large point source located in Nevada, that grid cell could easily be reassigned to Nevada by changing the cell's numeric code. The ASCII file can also be edited to define new source regions as needed.

Figure 7.2b shows the boundaries of the source regions used in the CAMx PSAT model. It appears that the boundaries are not always correctly represented, possibly because of the map projection used. These should be adjusted in future simulations.

[illegible]

Figure 7-2a. Source area mapping file as used in the CMAQ TSSA algorithm, with each source region distinguished by a unique numeric code.

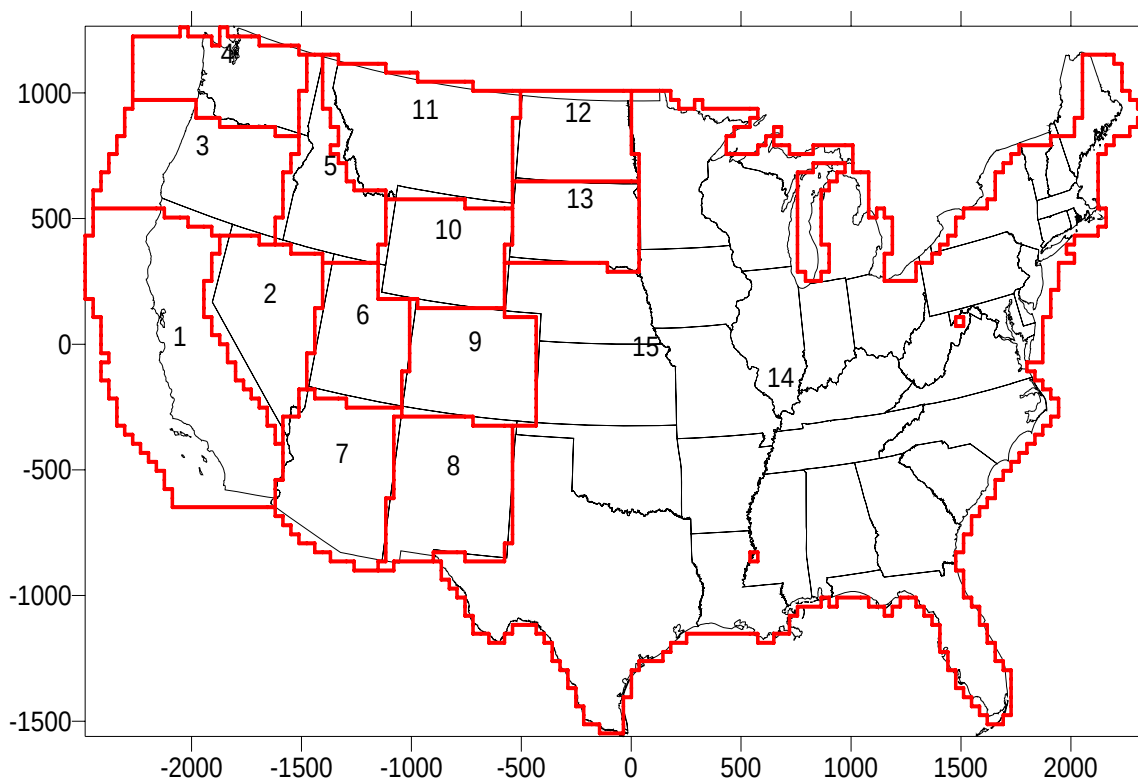


Figure 7 2b. Source area mapping file as used in CAMx PSAT showing the boundaries for each state/region.

7.2.3 Definition of source categories

The source categories include initial and boundary conditions; individual types of emissions sources, such as motor vehicles, point sources, area sources, and fires; and “other” sources, which include all sources other than those that are explicitly defined. Lumping all unassigned sources together in the “other” category allows the total mass of tracers to be identical to the bulk species concentration, as required by Equation 7-1.

In the SMOKE/CMAQ modeling system, all emissions are merged into a single emissions file that is read by CMAQ. However, all information regarding the source categories is lost in this merging step. The TSSA method therefore requires that emissions files be read by CMAQ for each individual emissions source category that is included among the tagged sources. Because of the file structure used in CMAQ, this can require a vast increase in disk storage cost for the emissions, because sparse data storage is not employed in the CMAQ emissions files.

Table 7-1 gives details on the tagged-sources naming scheme that is used in the algorithm and displayed in some of the plots showing model simulation results. Source category codes in column 2 of the table are combined with two-letter state abbreviations to create identifiers for particular source categories within a given state.

Table 7-1. Combinations of source categories and geographic regions that are typically included in a TSSA simulation.

Types	Source Category [†]	Notes
ICON	ICON	Initial concentration
BCON	BCON	Boundary concentration
Emissions	MV_*	Mobile sources of any state
	BG_*	Biogenic sources of any state
	RD_*	Road dust of any state
	NR_*	Nonroad dust of any state
	PN_*	Point sources without SO ₂ of any state
	PS_*	Point sources with SO ₂ of any state
	AR_*	Area sources of any state
	WF_*	Wildfire sources of any state
	AG_*	Agricultural fire sources of any state
	RX_*	Prescribed fire sources of any state
	MX_*	Mexico fire
	ET_*	Total emission of any state
	*_WRAP	Any type of emission of WRAP domain
Others	OTHERS	Any sources other than those listed above

[†]The asterisks can be the two-letter state code for any state in the WRAP region (or for Canada [CN] or Mexico [MX]), or all states in the WRAP region.

7.2.4 Updating of tracers in CMAQ science algorithms

The CMAQ Chemical Transport Model (CCTM) is a three-dimensional, regional-scale, nonhydrostatic air quality model based on the mass conservation equation to simulate transport, transformation, dry and wet deposition, and aerosol formation of pollutants. The governing equation can be rewritten in generalized coordinates where the turbulent flux terms are expressed with eddy diffusion theory (further described in Byun and Ching [1999]). Through operator splitting, or the use of fractional time steps, modularity is achieved in CCTM and computationally efficient algorithms are applied to solve each science process (e.g., advection, chemistry). The TSSA routine is implemented into each science process to account for the change in species concentration and update the tracer species accordingly. Figure 7-3 illustrates the TSSA implementation in CCTM science processors. The TSSA routine checks for mass conservation at each advection time step and adjusts mass (renormalizes) if needed. The program will halt if large errors are detected during the mass conservation check.

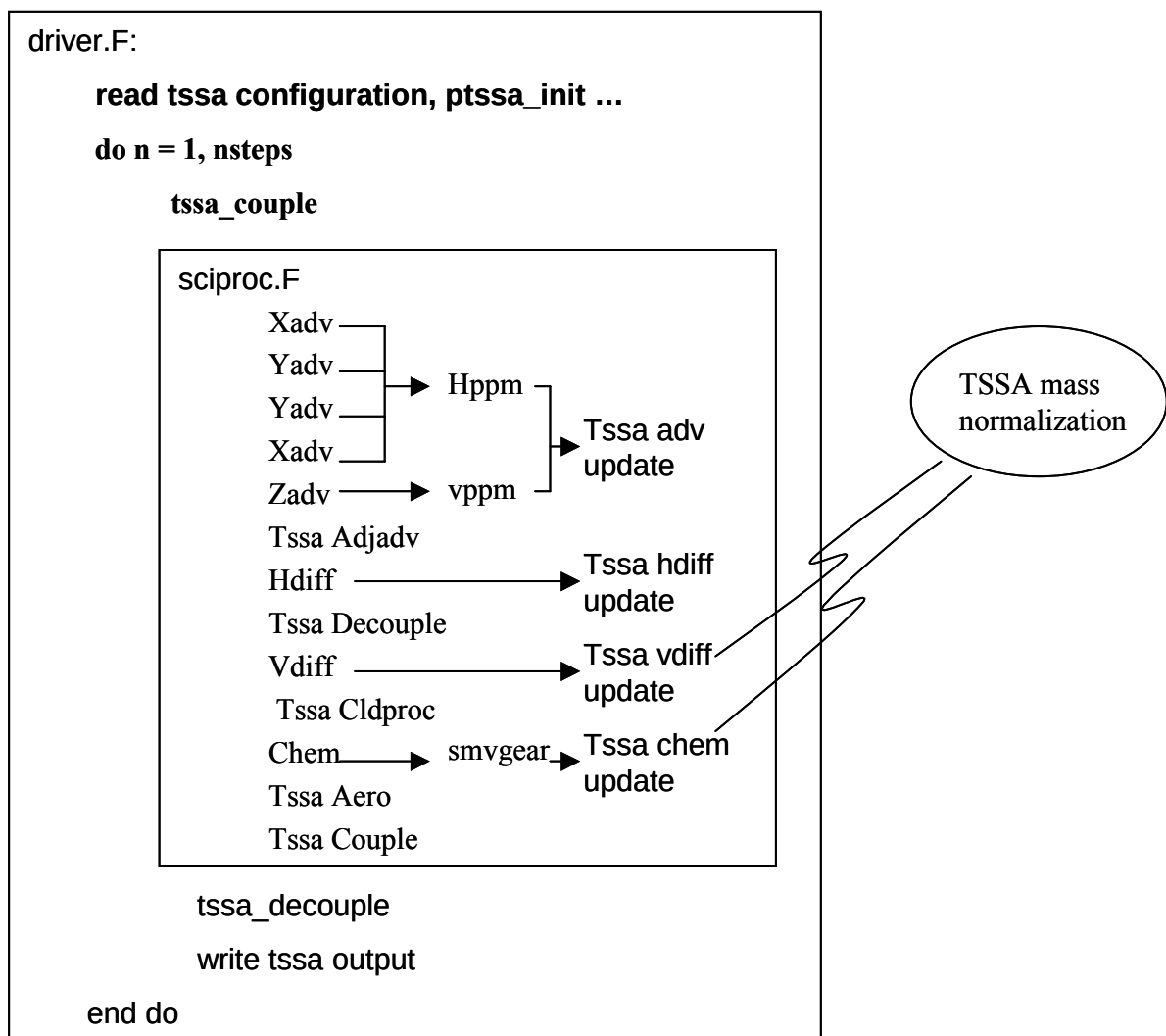


Figure 7-3. Flowchart of the TSSA implementation in CMAQ's CCTM.

The TSSA initialization stage takes place at the beginning of the model simulation. The tagged species are initialized with concentrations from the initial conditions input file. The TSSA algorithm also updates the tagged species at the boundary with concentrations from the boundary conditions input file.

The equation below is the mass continuity equation that defines the processes that are solved for in the CMAQ model. We added new computer code to CMAQ to track the changes in tagged species at each time step for each of the processes represented in the equation.

$$\begin{aligned}
& \frac{\partial(\overline{\varphi}_i J_\xi)}{\partial t} + m^2 \nabla_\xi \bullet \left(\frac{\overline{\varphi}_i \widehat{\nabla}_\xi J_\xi}{m^2} \right) + \frac{\partial(\overline{\varphi}_i \widehat{\nabla}^3 J_\xi)}{\partial \hat{x}^3} \\
& - m^2 \frac{\partial}{\partial \hat{x}^1} \left[\frac{\overline{\rho} J_\xi}{m^2} (\hat{K}^{11} \frac{\partial \overline{q}_i}{\partial \hat{x}^1}) \right] - m^2 \frac{\partial}{\partial \hat{x}^2} \left[\frac{\overline{\rho} J_\xi}{m^2} (\hat{K}^{22} \frac{\partial \overline{q}_i}{\partial \hat{x}^2}) \right] - \frac{\partial}{\partial \hat{x}^3} \left[\overline{\rho} J_\xi (\hat{K}^{33} \frac{\partial \overline{q}_i}{\partial \hat{x}^3}) \right] \\
& - m^2 \frac{\partial}{\partial \hat{x}^1} \left[\frac{\overline{\rho} J_\xi}{m^2} (\hat{K}^{13} \frac{\partial \overline{q}_i}{\partial \hat{x}^3}) \right] - m^2 \frac{\partial}{\partial \hat{x}^2} \left[\frac{\overline{\rho} J_\xi}{m^2} (\hat{K}^{23} \frac{\partial \overline{q}_i}{\partial \hat{x}^3}) \right] \\
& - \frac{\partial}{\partial \hat{x}^3} \left[\overline{\rho} J_\xi (\hat{K}^{31} \frac{\partial \overline{q}_i}{\partial \hat{x}^1} + \hat{K}^{32} \frac{\partial \overline{q}_i}{\partial \hat{x}^2}) \right] \\
& = J_\xi R_{\varphi_i}(\overline{\varphi}_1, \dots, \overline{\varphi}_N) + J_\xi Q_{\varphi_i} + \frac{\partial(\overline{\varphi}_i J_\xi)}{\partial t} \Big|_{cld} + \frac{\partial(\overline{\varphi}_i J_\xi)}{\partial t} \Big|_{aero} + \frac{\partial(\overline{\varphi}_i J_\xi)}{\partial t} \Big|_{ping}
\end{aligned}$$

The terms in this equation are summarized below:

a. Time rate of change in species concentration	g. Off-diagonal vertical eddy diffusion
b. Horizontal advection	h. Production or loss from chemical reactions
c. Vertical advection	i. Emissions
d. Horizontal eddy diffusion (diagonal term)	j. Cloud mixing and aqueous-phase chemical production or loss
e. Vertical eddy diffusion (diagonal term)	k. Aerosol process
f. Off-diagonal horizontal eddy diffusion	l. Plume-in-grid process

7.2.5 Postprocessing of TSSA results

The tracer output files can be immediately visualized using the Program for the Analysis and Visualization of Environmental data (PAVE) and can also be converted into the format required by the Vis5D visualization software. This is useful for visualizing the transport of pollutants from a source across the model domain. However, the result of most interest is the source attribution at a particular receptor site. UCR has developed postprocessing software to read the 3-D TSSA output file and extract data for a list of IMPROVE sites, and create bar plots and ASCII files showing the 20 largest contributors at each site.

The source attribution can be calculated as the attribution averaged over a 24-h period (to match the temporal resolution specified in the IMPROVE monitoring protocol) or for some other averaging period. In particular, UCR has developed software to sort and identify for each receptor site the average source attribution for the best-20% and worst-20% visibility days, where the worst and best can be defined using either ambient IMPROVE data or model predictions.

Figure 7-4 shows an example bar plot created using the UCR postprocessing software. UCR also provides the ASCII data to Air Resource Specialists, another WRAP contractor, to develop other types of plots for displaying these results.

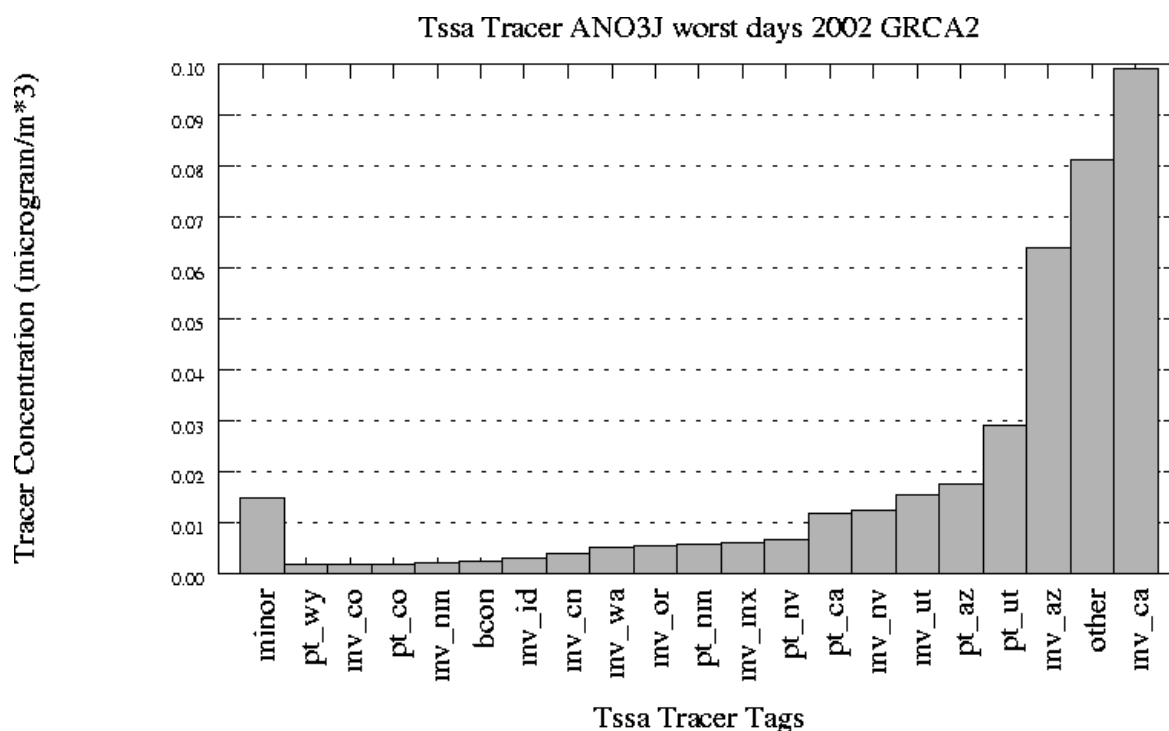


Figure 7-4. Example bar plot produced by UCR postprocessing software showing the largest 20 contributors to aerosol nitrate at a receptor site in the Grand Canyon. The x-axis labels are explained in Table 7-1.

7.2.6 Uncertainties in the TSSA results

While we have made considerable progress in developing and testing the TSSA algorithm in CMAQ, further work is needed. Most significantly, the algorithm should be implemented in the final release of CMAQ 4.4. The beta release contained a mass conservation error, which also introduced errors into the tracers used in the TSSA method. Although we experimented with a number of approaches for renormalizing to minimize the effects of mass errors, there are cases in which this introduces error terms into the TSSA algorithm that may accumulate over time. It is difficult to quantify the effect of these mass errors. In the current TSSA results for the 2002 modeling, we in some cases accumulated errors in the “other” category. The result of this

approach was that attributions to “other” were overestimated and attributions to mass transport at the domain boundary were probably underestimated. However, we believe that we obtained useful information from these model results by evaluating the relative contributions of the various source and emissions categories at each receptor site.

7.3 Source Attribution Modeling Results

During 2004 we completed three iterations of the source attribution modeling. Results were presented at WRAP Attribution of Haze Meetings in July, September, and November. These results represented three different approaches used in the CMAQ TSSA algorithm to account for mass conservation errors. Specifically, we tried two different algorithms to force mass conservation in the TSSA tagged species by renormalizing the sum of the tagged species to be identical to the bulk species concentration at each step in the CMAQ model:

- We first used a proportional renormalization scheme in which lost mass was added to each tagged species proportionally to the mass of each tag within a given grid cell. This method failed in grid cells with very low concentrations.
- We then used an equal-weighting scheme where lost mass was added equally to all tagged species within a given grid cell. This scheme produced unrealistic source attributions, for example, when mass was added to tracers for the boundary conditions.

We also experimented with several variations and hybrids of these two schemes, but no approach gave satisfying results. In the end, we simply allocated lost mass to an artificial tag labeled “other” and tracked this separately. The relative source attribution results were similar for each of these approaches, so we used the results in a relative sense, i.e., to rank the importance of each emissions source at the receptor sites. Here we describe example plots for the results that we presented at the September 2004 Attribution of Haze meeting. Complete results are on the RMC web page (see <http://www.cert.ucr.edu/aqm/308/cmaq.shtml#source>) and have also been further processed and reported by Air Resource Specialists.

Figure 7-5a shows an SO₄ concentration time series at the Ft. Peck IMPROVE site for part of July 2002. On July 2, the first day of the time-series, the model-simulated SO₄ was 0.5 µg/m³. Figures 7-5b and 7-5c show the CMAQ TSSA results for this site on July 2 using the proportional mass renormalization scheme (Figure 7-5b) and the method in which lost mass was attributed to an “other” category (Figure 7-5c). This site is representative of the sites that had larger disagreements between the TSSA algorithms, in which even the relative ranking differed.

In Figure 7-5b, boundary conditions (bcon) were ranked as the largest contributor, although this primarily represents the accumulation of mass error terms. Among the other source categories, point sources in the eastern U.S. and in North Dakota were ranked as the largest contributors, followed by smaller contributions from point sources in Canada and Washington and mobile sources in North Dakota and Washington. In Figure 7-5c, mass error terms were accumulated in the “other” tag, and point sources in North Dakota were ranked as the largest contributors, followed by contributions from point sources in the eastern U.S.

Due to the uncertainty of the results from the CMAQ TSSA algorithm, we also used the CAMx PSAT model to evaluate source attribution for February and July of 2002. Figure 7-6a shows CMAQ TSSA results for SO₄ at the Grand Canyon IMPROVE site on July 2, 2002. Point sources from Nevada were the single largest contributor, followed by smaller contributions from point sources in Arizona and Mexico. Figure 7-6b shows CAMx PSAT results for SO₄ for the same site and date. Point sources from Nevada were again the single largest contributor, followed by smaller contributions from point sources in Mexico and Arizona. The similarity in the relative rankings and in the magnitudes of the sources at the Grand Canyon site increased our confidence in the results of the CMAQ TSSA simulations.

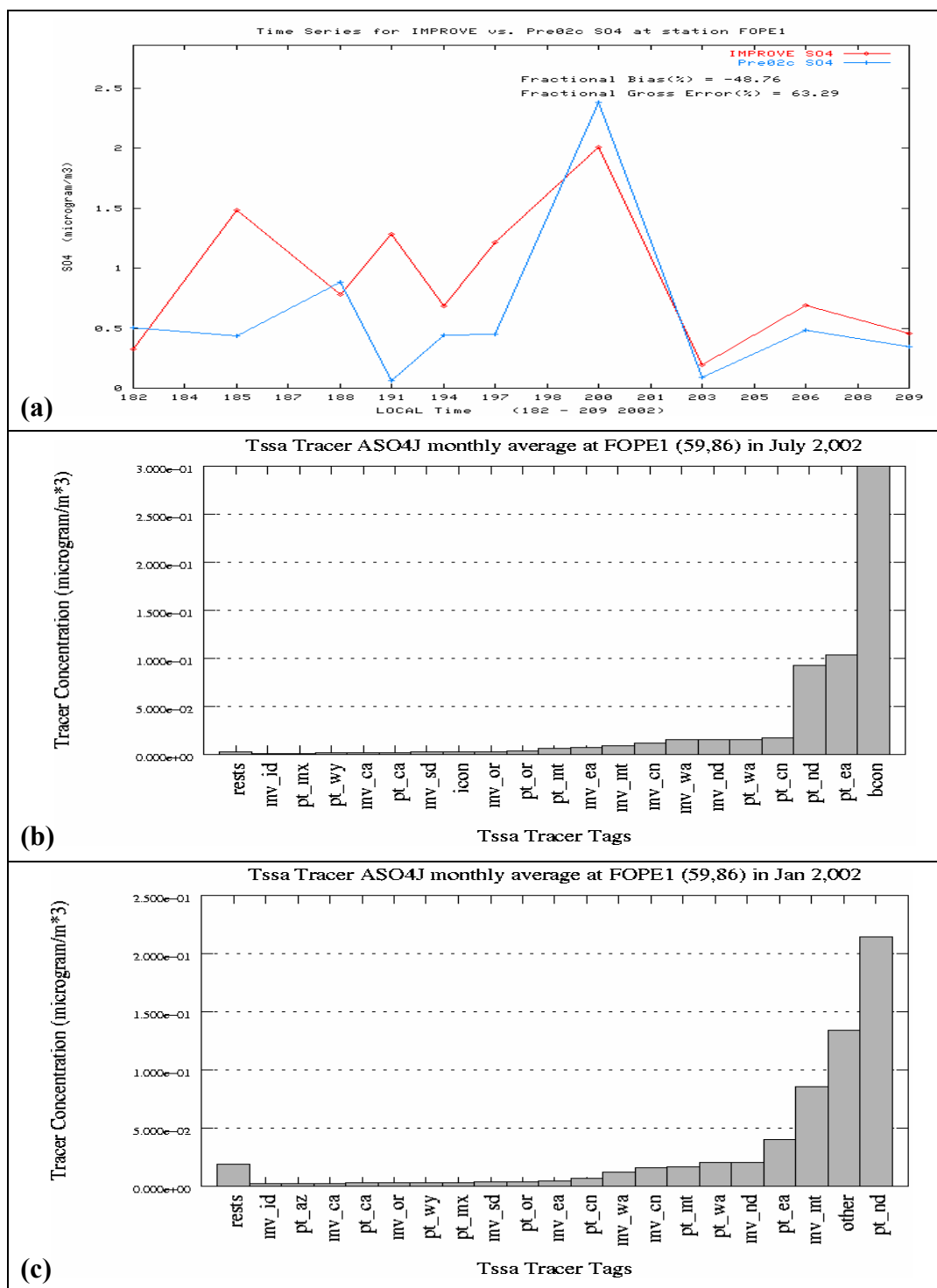


Figure 7-5. CMAQ source attribution results at the Ft. Peck IMPROVE site on July 2, 2002: (a) modeled and measured SO₄ concentrations; (b) TSSA results using proportional mass renormalization; (c) TSSA results with lost mass represented as “other.”

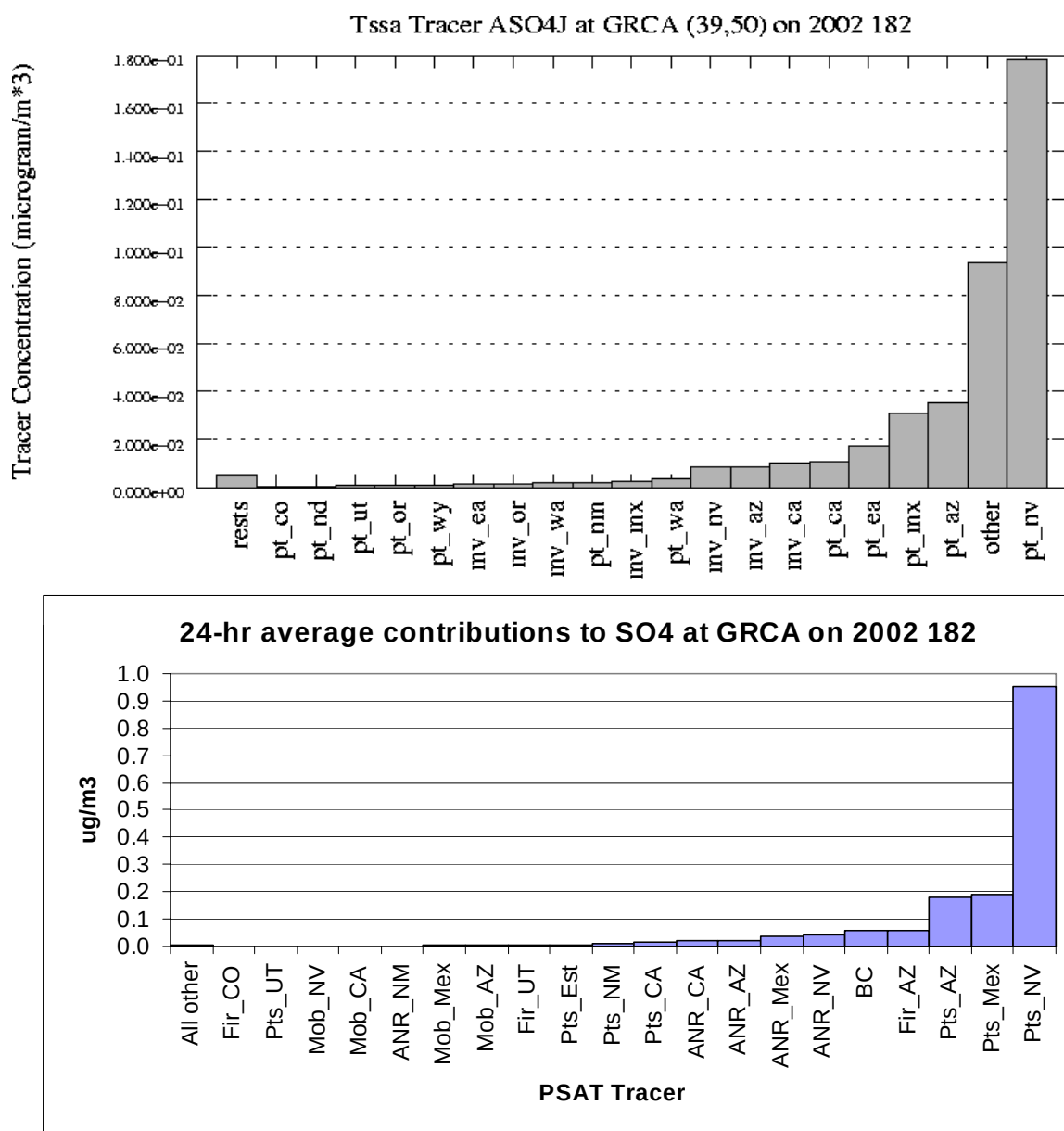


Figure 7-6. Source attribution results for SO₄ at the Grand Canyon IMPROVE site on July 2, 2002: (a) CMAQ TSSA results; (b) CAMx PSAT results.

7.4 Status of Task 5 Deliverables

Table 7-2 gives the status of each Task 5 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 7-2. Status of the Task 5 deliverables.

Deliverable	Status
Source attribution report using emissions and meteorology data available in early May	Because of problems with mass conservation in the CMAQ source code, we performed several iterations of CMAQ source attribution modeling. The final model simulations were completed in October 2004. Analysis products (bar charts showing source attribution at receptor sites) are available on the RMC web site, and ASCII results were provided to Air Resource Specialists for additional processing during September-October 2004. Plots for each receptor site are available here: http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#source Additional source attribution simulations with CAMx PSAT were completed for two months, February and July, to evaluate the CMAQ results. The CAMx PSAT source attribution results are available at http://pah.cert.ucr.edu/aqm/308/meetings/March_2005/03-08_09-05.SF_CA/ by clicking on Alternative_Model_Mar8-9_2005_MF_Meeting.ppt Simulation interim results and final results were presented as PowerPoint files at three meetings of the Attribution of Haze work group (below) and at the WRAP Modeling Forum Meeting. See http://pah.cert.ucr.edu/aqm/308/meetings.shtml. • Attribution of Haze Meeting, July 21-22, 2004, Denver, CO • Attribution of Haze Meeting, November 18-19, 2004 Las Vegas, NV: UCR_TSSA_results_Nov_2004 (ppt) • Attribution of Haze Meeting, September 22, 2004 Salt Lake City, UT: UCR TSSA Tracer Results (ppt files)

8. Task 6: Further Analysis of Model Performance in Regard to the Contribution of Natural Emissions to Visibility Impairment

In addressing the effects of regional haze on visibility, estimating reasonable progress goals and formulating the associated control strategies require an understanding of how two types of emissions sources contribute to haze: natural sources, and non-U.S. background sources. To develop this understanding, it is important to identify the natural emissions sources that impact regional haze. Combining guidance provided by EPA, analyses performed by other RPOs, publications in the primary literature, and the results of RMC modeling sensitivities, we have worked on identifying and quantifying the natural and non-U.S. background haze emissions sources in the WRAP region. This section summarizes the work completed from March 2004 through February 2005 to further our understanding of these sources of haze and their potential impacts on model performance evaluations and control strategy development in the WRAP states.

8.1 Background

One of the first phases of developing regional haze control strategies involves identifying the various sources of haze. During 2003, we began reviewing work by other groups and performing modeling sensitivities to identify and quantify the contributions of different sources of haze to visibility impairment in the WRAP region. We performed brute-force emissions sensitivities to study the effects of biogenic and wildfire emissions on visibility in the WRAP states. These simulations, in which we eliminated all anthropogenic emissions and included only biogenic and wildfire emissions, were insightful but somewhat incomplete in that the biogenic model did not include emissions estimates for some important sources, such as lightning NO_x. Also, the boundary conditions in these simulations did not differentiate between naturally derived and anthropogenic sources of haze, which is important for drawing conclusions about the influence of background haze on regional visibility. In addition to performing cursory model simulations, we have leveraged regional haze guidance from EPA and research completed by other RPOs to provide direction in identifying the research needs for addressing visibility issues in the WRAP region.

The Draft Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule (U.S. EPA, 2001) helps regional haze planning efforts by establishing default approaches for estimating the natural visibility conditions in the Class I areas. Through descriptions on how EPA interprets baseline haze and assesses visibility improvements, the guidance provides insight on what to consider when trying to identify natural and background sources of haze. Work by the VISTAS RPO (Tombach, 2004; Kumar, 2004; Brewer, 2004) has pointed out problems and recommended possible refinements to the EPA approach for calculating baseline and natural conditions, identified the importance of background or transported haze to the model domain boundary, and suggested definitions of controllable and uncontrollable haze sources.

8.2 Work Performed from March 2004 through February 2005

While the information sources cited above treat haze sources in general, they do not provide explicit direction concerning which emissions are classified as natural emissions. During the past project year, the primary focus of our research for Task 6 was to clearly define the distinction between natural and anthropogenic emissions sources contributing to visibility impairment in the WRAP region. The RMC initiated the 2004 work with a draft memorandum identifying all potential sources of natural emissions in the WRAP region (Tonnesen, 2004). A comprehensive literature review based on this memo identified sources of emission factors published in the primary literature and in technical reports in the past decade (CEP, 2004b). These documents outline potential deficiencies in the current inventories and provide a basis for enhancing the WRAP emissions inventories to explicitly treat natural emissions sources in the future. To prepare for the development of refined WRAP emissions inventories for addressing the issue of natural haze sources, the WRAP Emissions Forum worked on characterizing natural versus anthropogenic emissions for various emissions sectors.

The RMC and several WRAP forums completed work in 2004 to identify the components of emissions sources that contribute to haze. The Fire Emissions Joint Forum worked to define natural versus anthropogenic fires in their existing inventories (Randall, 2004b), and in September 2004 the RMC received a revised set of 2002 WRAP fire inventories applying this distinction for prescribed-fire emissions. (Wildfire emissions are defined as natural, and agricultural burning emissions are defined as manmade; prescribed-fire emissions can be either.) After modeling these new fire inventories in SMOKE, we conducted a CMAQ sensitivity to evaluate the impact of the natural fires on modeled visibility. We discuss the emissions preparation for these simulations in Section 5.4. The Dust Emissions Joint Forum is currently working on characterizing natural versus anthropogenic dust sources and will provide guidance during the next project year on how to develop refined fugitive and windblown dust inventories that make this distinction. Exploratory work by the RMC has looked at adding sea salt emissions, geogenic and volcanic emissions, and lightning NO_x emissions to the WRAP 2002 modeling. In addition to emissions inventory refinements, we have included boundary conditions derived from a global model (GEOS-CHEM) to better capture the temporal and spatial variation in the pollutants transported to the boundary of the WRAP modeling domain.

To enhance the representation of the background sources of haze, we integrated seasonally averaged 1° x 1° grid cell GEOS-CHEM (Park et al., 2003) modeled boundary conditions representing calendar year 2001 into the preliminary 2002 simulations. We used 2001 GEOS-CHEM results because they were readily available during the time frame in which we performed this modeling; we anticipate replacing them with 2002 data when they become available. These temporally and spatially resolved boundary conditions better capture seasonal variations in pollutant transport impacting the United States.

8.3 Next Steps

Upcoming work will focus on finalizing the definition of what sources constitute natural emissions sources and on integrating refinements to the WRAP inventories for distinguishing between natural and anthropogenic sources. During the next project year we anticipate receiving

fugitive and windblown dust inventories that are split to identify the natural components of these emissions. We will also work on integrating missing natural emissions sources into the 2002 modeling, such as lightning NO_x, sea salt, and geogenic emissions. With the creation of these refined and new emissions inventories, the RMC will continue the simulation and analysis of air quality model sensitivities to assess the contribution of natural emissions to visibility impairment.

8.4 Status of Task 6 Deliverables

Table 8-1 gives the status of each Task 6 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 8-1. Status of the Task 6 deliverables.

Deliverable	Status
Natural emissions inventory	Partially complete. Natural versus manmade fire inventories became available in September 2004; still need emissions for other categories (e.g., dust, marine, geogenic).
CMAQ simulation with natural emissions	Partially complete. Simulations are underway to study the effects of the natural versus manmade fires; will complete when other natural emissions sources are modeled (see above).
Report describing natural emissions research and CMAQ simulations	A literature review of natural emissions sources was completed in August 2004; will complete this deliverable in 2005.

9. Task 7: Evaluation and Comparison of Alternative Models

Under this task, the RMC was directed to apply an alternative air quality model and compare its results to those from CMAQ. The Comprehensive Air quality Model with extensions (CAMx) (ENVIRON, 2004) was selected as the alternative model. CAMx is currently being applied as the primary model by MRPO and is also being used by VISTAS as a secondary model to corroborate and serve as a diagnostic tool for the CMAQ results. CENRAP is currently applying the CMAQ and CAMx models in parallel and has not yet decided whether one will be a primary and the other a secondary model. Thus, it may be important for WRAP to familiarize themselves with CAMx in order to interpret other RPOs' modeling procedures and results.

Under Task 7 the RMC applied CAMx for February and July 2002 on the 36-km grid, and compared CAMx's performance with that of CMAQ. In addition, the CAMx PM Source Apportionment Technology (PSAT) was configured in a way that is similar to CMAQ's TSSA source attribution algorithm (see Section 7) and the two PM source attribution schemes were compared for February and July 2002.

9.1 Advantages in Operating Multiple Models

Although CMAQ is the primary air quality modeling system being used by WRAP, there are many advantages in applying and evaluating alternative models. All models have uncertainties and limitations. By applying multiple models, we obtain more confidence in the results and also obtain an estimate of the uncertainties in the modeling. During the CY02 work efforts, WRAP applied and evaluated the CMAQ, REMSAD, and CAMx models for 1996. The three models generally exhibited similar performance, both good and bad. CAMx was operated in both a two-section mode and a multisection mode whereby secondary PM (e.g., sulfate and nitrate) was allowed to grow into the coarse (i.e., PM_{2.5-10}) mode; CMAQ, on the other hand, assumes that all of the secondary PM is in the fine mode. The CAMx model estimated that a vast majority of the secondary PM was in the fine mode, a finding that strengthened the credibility of CMAQ's assumption and therefore the confidence in its results. Thus, WRAP has already received some benefits from applying multiple models.

EPA's guidance on model selection for PM_{2.5} SIPs/TIPs and regional haze reasonable progress demonstrations does not identify a preferred photochemical grid modeling system, recognizing that at present there is "no single model which has been extensively tested and shown to be clearly superior or easier to use than several alternatives" (U.S. EPA, 2001, pg. 169). The agency recommends that models used for PM_{2.5} SIPs/TIPs or regional haze reasonable progress demonstrations should meet the requirements for alternative models. The CMAQ, CMAQ-MADRID (Model of Aerosol Dynamics, Reaction, Ionization, and Dissolution), CMAQ-AIM (Aerosol Inorganic Module), and CAMx modeling systems all meet these requirements.

We believe that there may be significant value in including multiple modeling systems in the WRAP modeling analysis. Our testing and comparisons of the CMAQ and CAMx models for

WRAP, VISTAS, and other recent PM_{2.5}/regional haze applications demonstrate that the models are capable of producing results of comparable accuracy and reliability, and having results from CAMx as well as CMAQ has many benefits. For example:

- *Diagnosis:* To serve as an efficient diagnostic tool for addressing model performance issues that may arise in the establishment of the annual 2002 base case. CMAQ and CAMx both include process analysis that can help diagnose model performance. CAMx's suite of diagnostic probing tools and its flexi-nesting algorithms make it an attractive tool for assisting in the diagnosis of model performance.
- *Model Evaluation Corroboration:* To provide corroboration of the base case model performance evaluation exercises to be performed with the two models, and help identify any compensatory errors in the modeling systems.
- *Emission Control Response Corroboration:* To provide corroboration of the response of a modeling system to generic and specific future-year emissions changes on modeled gas-phase and particulate aerosol concentrations and resultant regional haze impacts.
- *Quantification of Model Uncertainty:* To provide one estimate of the range of uncertainty in the annual and episodic base case simulations, and in the estimates of PM_{2.5} and visibility reductions associated with future emissions-change scenarios.
- *Alternative Science:* CAMx and CMAQ contain alternative science algorithms that may elucidate model performance issues with one model or the other or provide an alternative approach for simulating aerosols.
- *Consistency with Other RPOs:* MRPO may end up using CAMx for their regional haze modeling. The CENRAP states are currently using both CMAQ and CAMx. As sources in the MRPO and CENRAP regions likely influence visibility at Class I areas in the WRAP region, and vice versa, having results from both models would be useful for reconciling any differences.
- *Backup Contingency:* To provide a "backstop" model in the event that unforeseen difficulties with the primary model occur.

The benefits of employing a pair of complementary state-of-the-science air quality models are thus quite significant and well worth the extra effort. Note that these two particular models can be applied without performing any additional meteorological or emissions modeling, because the same MM5 output (through MCIP2.3 and MM5CAMx) and SMOKE output and CMAQ IC/BC files (through CMAQ-to-CAMx emissions and IC/BC converters) can be used to operate both CMAQ and CAMx.

9.2 Description of the CAMx Modeling System

9.2.1 Overview

The CAMx modeling system is a publicly available (<http://www.camx.com>), three-dimensional, multiscale photochemical-aerosol grid modeling system that ENVIRON developed and is

maintaining. CAMx was developed with all new code during the late 1990s using modern and modular coding practices. This has made the model an ideal platform for extension to treat a variety of air quality issues, including ozone, PM, visibility, acid deposition, and mercury and other air toxics. The flexible CAMx framework has also made it a convenient and robust host model for the implementation of a variety of mass balance and sensitivity analysis techniques, including process analysis (Integrated Reaction Rates [IRR] and Integrated Process Rates [IPR]), the decoupled direct method (DDM), and the Ozone Source Apportionment Technology (OSAT). Designed originally to address multiscale ozone issues from urban to regional scales, CAMx has been widely used in recent years by a variety of regulatory agencies for 1-h and 8-h ozone and PM₁₀ SIP/TIP modeling studies, as well as by several RPOs for regional haze modeling. Key attributes of the CAMx system include the following:

- Two-way grid nesting that supports multiple levels of fully interactive grid nesting (e.g., 36/12/4/1.33 km);
- Carbon Bond IV (CB-IV) or Statewide Air Pollution Research Center (SAPRC-99) chemical mechanisms;
- Two chemical solvers, the CAMx Chemical Mechanism Compiler (CMC) Fast Solver or the highly accurate Implicit-Explicit Hybrid (IEH) solver;
- Multiple numerical algorithms for horizontal transport, including the Piecewise Parabolic Method (PPM), Bott, and Smolarkiewicz advection solvers;
- A sub-grid-scale plume-in-grid algorithm to treat the near-source plume dynamics and chemistry from large NO_x point-source plumes;
- The ability to interface with a variety of meteorological models, including the MM5 and RAMS prognostic hydrostatic meteorological models and the CALMET diagnostic meteorological model (others are also compatible);
- The OSAT ozone attribution technique, which identifies the ozone contribution due to geographic source regions and source categories (e.g., mobile, point, biogenic);
- The DDM sensitivity method, which is implemented for emissions and ICs/BCs to obtain first-order sensitivity coefficients for all gas-phase species; and
- Treatment of PM using an empirical aerosol thermodynamics algorithm.

Culminating extensive model development efforts at ENVIRON and other participating groups, the CAMx (ver 4.11s) code was released in autumn 2004 as a truly “one-atmosphere” model that rigorously integrates the gas-phase ozone chemistry with the simulation of primary and secondary fine and coarse particulate aerosols. This extension of CAMx to treat PM involved the addition of several science modules to represent important physical processes for aerosols. Noteworthy among these are the following:

- Two separate treatments of PM. The Mechanism 4 (M4) “one-atmosphere” treatment uses two size sections and science modules comparable to CMAQ’s (e.g., the Regional Acid Deposition Model [RADM] aqueous-phase chemistry and ISORROPIA equili-

brium). The multisection “full-science” approach uses aerosol modules developed at Carnegie Mellon University (CMU).

- Size distribution is represented using the Multicomponent Aerosol Dynamics Model (MADM), which uses a sectional approach to represent the aerosol particle size distribution (Pilinís et al., 2000). MADM treats the effects of condensation/evaporation, coagulation, and nucleation upon the particle size distribution.
- Inorganic aerosol thermodynamics can be represented using the ISORROPIA (Nenes et al., 1998, 1999) equilibrium approach within MADM, or a fully dynamic or hybrid approach can be used.
- Secondary organic aerosol thermodynamics are represented using the semivolatile scheme of Strader and coworkers (1999).
- Aqueous-phase chemical reactions are modeled using either the RADM module (as CMAQ does) or the Variable Size-Resolution Model (VRSIM) of Fahey and Pandis (2001), which automatically determines whether water droplets can be represented by a single “bulk” droplet-size mode or whether it is necessary to use fine and coarse droplet-size modes to account for the different pH effects on sulfate formation.

CAMx (ver 4.11s) provides two key options to users interested in simulating PM. For CPU-efficient annual PM modeling applications, CAMx can be run using M4 with only two size sections (fine and coarse) and the efficient RADM bulk aqueous-phase module (as is used in CMAQ). Alternatively, more rigorous aerosol simulations (perhaps for shorter episodes) can be addressed using the version that treats N size sections (N is typically 10) and the rigorous, but computationally intensive, CMU multisection aqueous-phase chemistry module.

9.2.2 PM Source Apportionment Technology (PSAT)

PSAT has been developed for CAMx to provide geographic and source-category-specific PM source attribution (Yarwood et al., 2004). PM source attribution information from PSAT is useful for:

1. understanding model performance and thereby improving model inputs/formulation,
2. performing culpability assessments to identify sources that contribute significantly to PM pollution, and
3. designing the most effective and cost-effective PM control strategies.

Source attribution for primary PM is relatively simple to obtain from any air pollution model, because source-receptor relationships are essentially linear for primary pollutants. Gaussian steady-state models and Lagrangian puff models have been used extensively to model primary PM pollution from specific sources, which provides source attribution. The Gaussian and Lagrangian approaches work for primary PM because the models can assume that emissions from separate sources do not interact. This assumption breaks down for secondary PM pollutants (e.g., sulfate, nitrate, ammonium, secondary organic aerosol), so puff models may dramatically simplify the chemistry (to eliminate interactions between sources) when they are applied to

secondary PM. Eulerian photochemical grid models are better suited to modeling secondary pollutants because they account for chemical interactions between sources. However, these models do not naturally provide source attribution because the impact of all sources has been combined in the total pollutant concentration. PSAT has been developed to retain the advantage of using a grid model to describe the chemistry of secondary PM formation and also provide source attribution.

Like the CMAQ TSSA algorithm discussed in Section 7, the CAMx PSAT source attribution uses reactive tracers (or tagged species), which are extra species added to a grid model to track pollutants from specific sources. For example, a standard grid model calculates concentrations for a species X that has many sources, and the concentration of X is the total concentration due to all sources. A reactive tracer (x_i) is assigned to each source (i) with the intention that the sum of the reactive tracers will equal total concentration ($X = \sum x_i$). The challenge is to develop numerical algorithms for solving the reactive tracer concentrations that ensure this equality is maintained. Depending upon the formulation of the tracer algorithms, it may be possible to model tracers for a single source of interest and omit tracers for all other sources, or it may be necessary to include tracers for all sources (as is the case for PSAT). Reactive tracers can potentially provide true source attribution ($X = \sum x_i$); however, the numerical value of the source attribution will depend upon assumptions within the reactive tracer formulation. In particular, for any process that is nonlinear in species concentrations (e.g., chemistry), there is no unique way to assign the total concentration change to the reactive tracers. The researchers at ENVIRON and UCR have separately and independently implemented the PSAT and TSSA PM source attribution approaches into CAMx and CMAQ, respectively. A comparison and evaluation of these two PM source attribution methods is warranted.

MRPO is using the CAMx PSAT to address their requirements to identify whether Best Available Retrofit Technology (BART)-eligible sources contribute to visibility impairment at Class I areas (see <http://www.ladco.org/tech/photo/photochemical.html>). The MRPO BART PSAT application demonstrates the usefulness of these techniques for satisfying regulatory modeling requirements.

9.3 Approach for Testing and Evaluation of Alternative Models

CAMx was set up on the same RPO Unified Continental 36-km Modeling Grid domain used for CMAQ modeling. The CAMx modeling was conducted for February and July 2002 using the latest 2002 MM5 simulations that are discussed in Section 4. We used the MM5CAMx processor to generate the CAMx-ready meteorological inputs from the WRAP final 2002 36-km MM5 simulation. The CAMx ICs/BCs and emissions were generated from the CMAQ inputs using the CMAQ-to-CAMx IC/BC and emissions processors. The CAMx model simulations used a 15-day spin-up period that started on January 16 and June 15 for the February and July 2002 runs, respectively. Although approximately 45 days were simulated for each of the monthly applications, only the last ~30 days were analyzed in the model performance evaluation. CAMx was applied using the 2002 pre02d Base D base case emissions and evaluated against measurements; the model performance was compared with CMAQ's. Since one of the objectives of this work was comparison of the CAMx PSAT and CMAQ TSSA PM source attribution approaches, a beta version of the CAMx Version 4.20 (V4.20beta) that includes the PSAT

algorithm was used in the analysis. This version of the model is going through its final testing and evaluation and will soon be made available on the CAMx website (www.camx.com), and is currently publicly available on request.

9.4 Comparative Evaluation of the CAMx and CMAQ Models

The CMAQ and CAMx models were evaluated using speciated PM measurements from four separate air quality monitoring networks:

- IMPROVE
- CASTNet;
- STN
- SEARCH

Because some of these networks use different averaging times (IMPROVE and STN collect 24-hour samples, whereas CASTNet collects weekly samples) and measurement technologies, the two models were evaluated separately for each network. Note that differences in measurement technologies can result in differences in measured speciated concentrations comparable to model performance objectives. For example, a comparison of the IMPROVE and STN measurement technologies using collocated samples found differences in sulfate (SO_4) and organic carbon (OC) as high as 20% and 50%, respectively (Solomon et al., 2004).

The comparative evaluation of the CMAQ and CAMx models for February and July 2002 was conducted for all monitors in the United States (U.S.) and for five subregions:

- Monitors in the WRAP Western states
- Monitors in the CENRAP Central states
- Monitors in the MRPO Midwestern states
- Monitors in the VISTAS Southeastern states
- Monitors in the MANE-VU Northeastern states

In the discussion below we present results for the entire United States.

9.4.1 Evaluation for Sulfate (SO_4)

Figure 9-1 compares the CMAQ and CAMx sulfate (SO_4) model performance at sites across the U.S. from the IMPROVE, CASTNet, STN, and SEARCH monitoring networks. Sulfate model performance for July 2002 for the two models (Figure 9-1a) is generally quite good, with fractional bias $\leq \pm 10\%$ and fractional error of 30-40%. The exception to this is the SEARCH network in the Southeastern U.S., where both models exhibit a slight overestimation tendency of 17% (CMAQ) and 25% (CAMx) and errors of approximately 50%.

For February 2002 (Figure 9-1b), both models generally exhibit a slight SO₄ overestimation tendency, with the CAMx overestimation tendency being greater than CMAQ's. For example, for the IMPROVE monitors in February 2002, CMAQ and CAMx produce fractional bias values of 26% and 41% and fraction error values of 49% and 56%, respectively.

9.4.2 Evaluation for Nitrate (NO₃)

Comparisons of the CMAQ and CAMx nitrate (NO₃) model performance for February and July 2002 are shown in Figure 9-2. NO₃ model performance for both models is fairly poor, exhibiting summer underestimation and winter overestimation tendencies. The summer NO₃ underestimation is more severe in CMAQ than in CAMx, whereas the winter NO₃ overestimation is more severe with CAMx than CMAQ. The winter overestimation tendency is of more concern, given that NO₃ can be is a higher fraction of the fine particulate in the winter on some days.

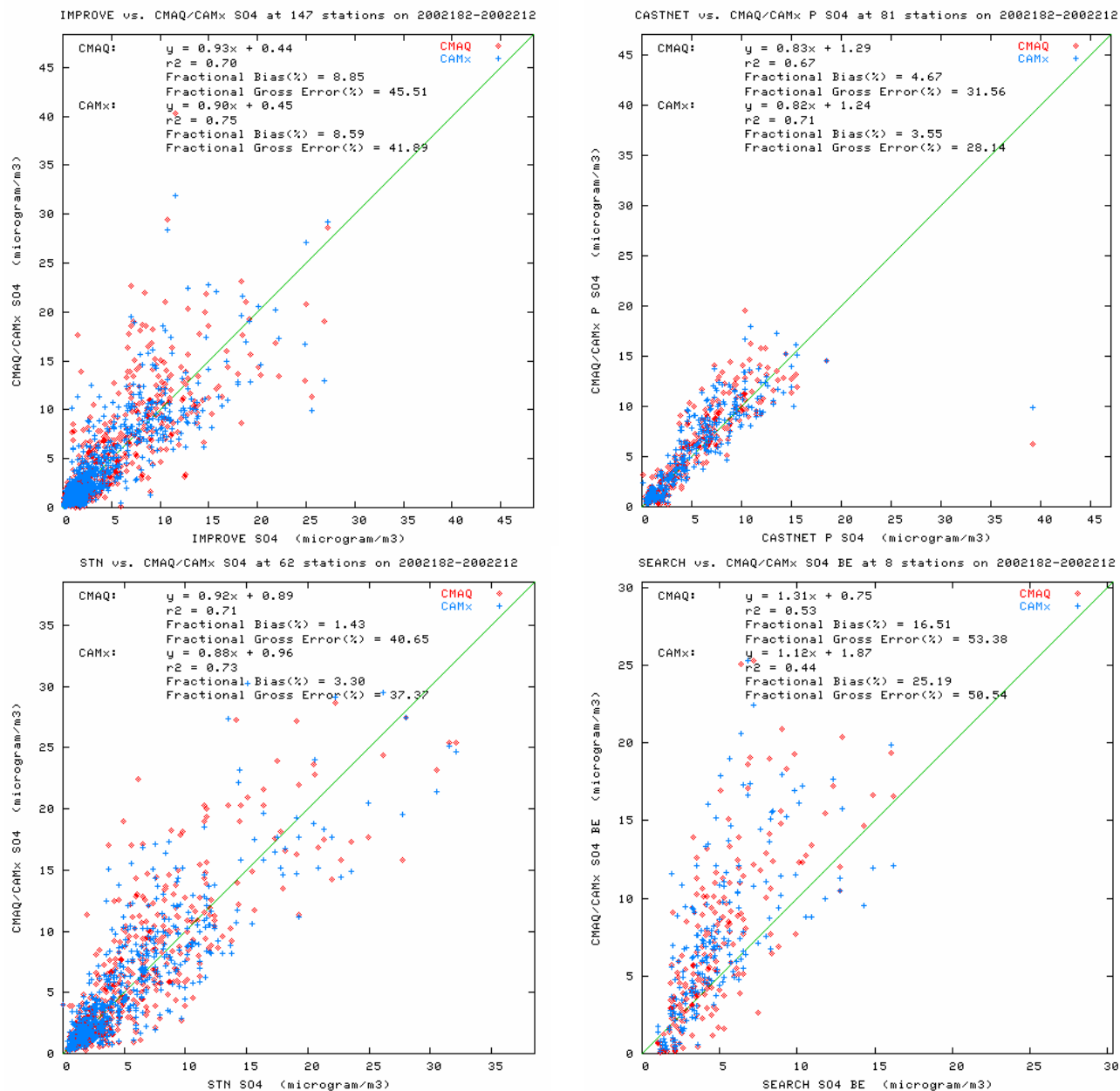


Figure 9-1a. Comparison of CMAQ (red) and CAMx (blue) SO₄ model performance at sites across the U.S. for July 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and SEARCH (bottom right) monitoring networks.

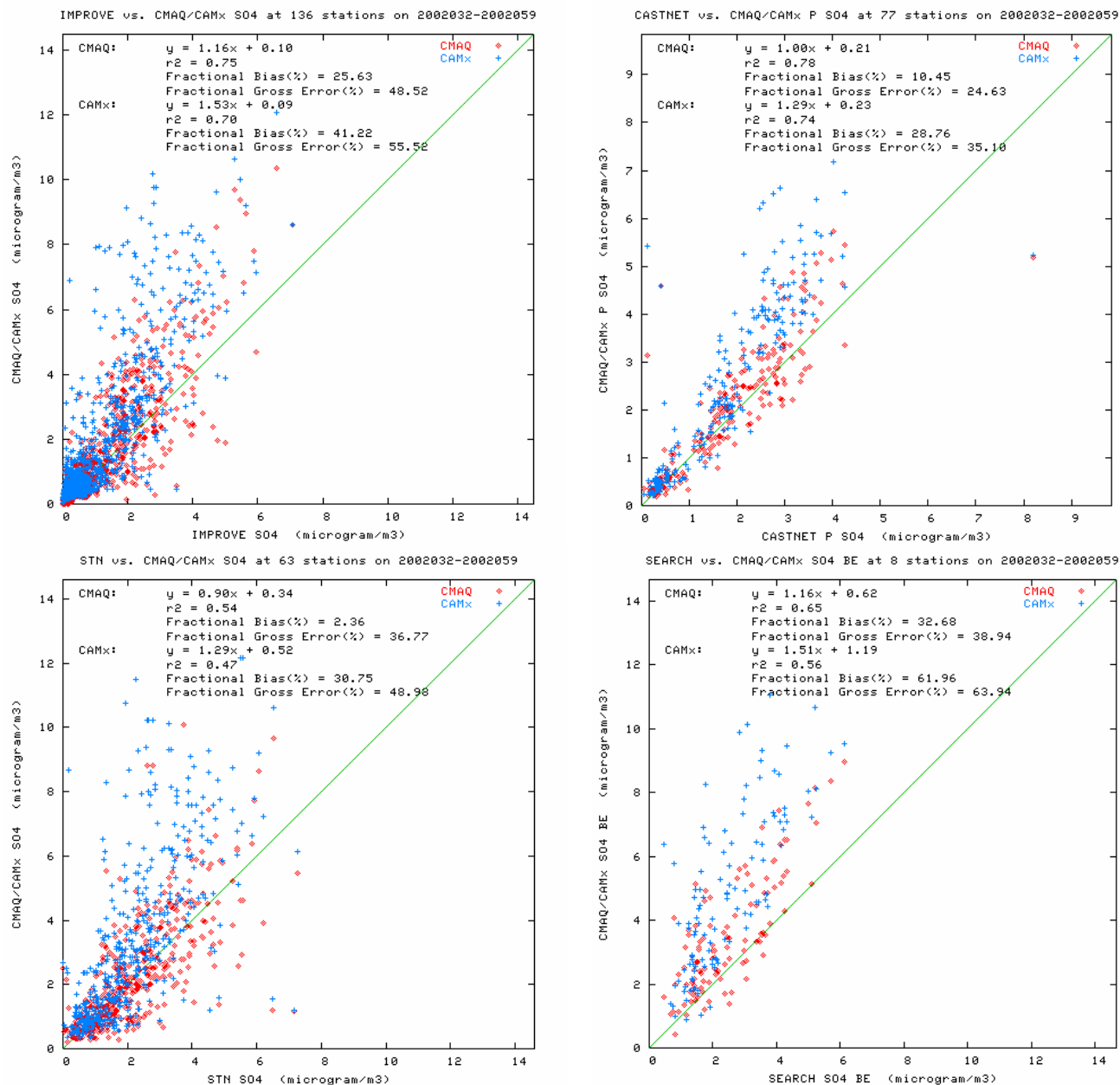


Figure 9-1b. Comparison of CMAQ (red) and CAMx (blue) SO₄ model performance at sites across the U.S. for February 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and SEARCH (bottom right) monitoring networks.

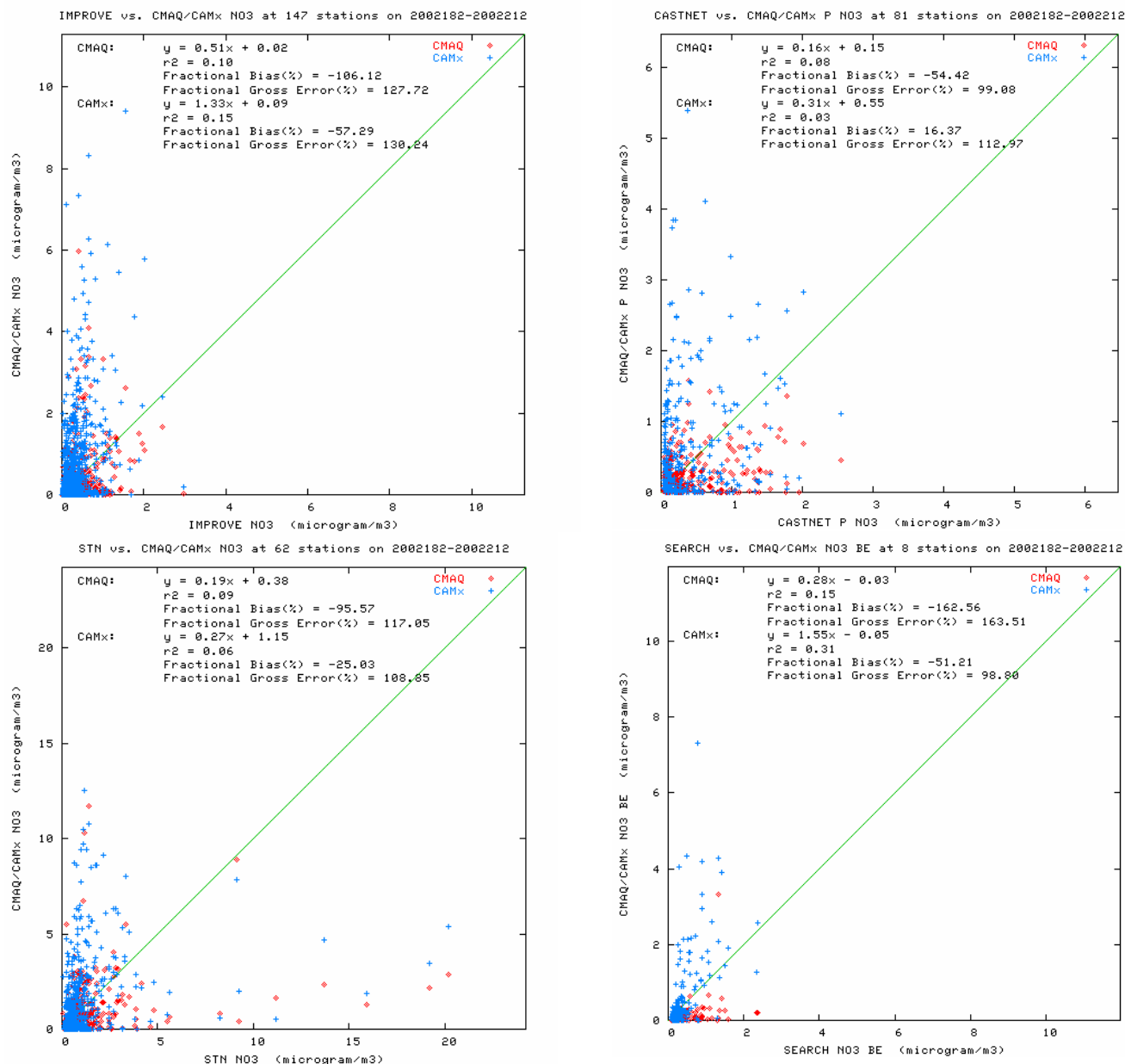


Figure 9-2a. Comparison of CMAQ (red) and CAMx (blue) NO₃ model performance at sites across the U.S. for July 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and SEARCH (bottom right) monitoring networks.

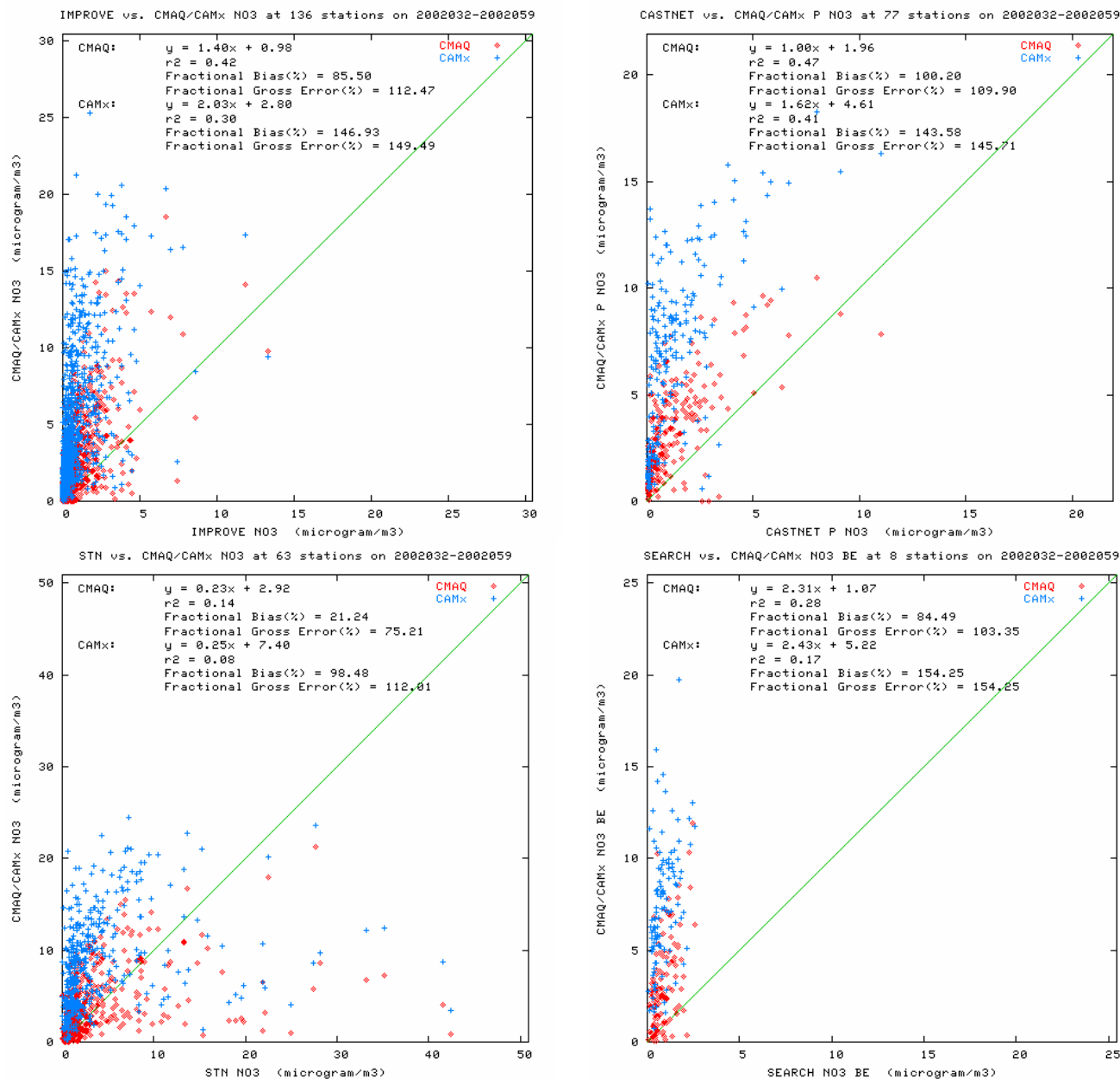


Figure 9-2b. Comparison of CMAQ (red) and CAMx (blue) NO₃ model performance at sites across the U.S. for February 2002 using the IMPROVE (top left), CASTNet (top right), STN (bottom left), and SEARCH (bottom right) monitoring networks.

9.4.3 Evaluation for organic carbon (OC) and elemental carbon (EC)

Figure 9-3 compares the CMAQ and CAMx OC and EC model performance at IMPROVE sites across the U.S. for February and July 2002. Both models exhibit a similar fractional bias underestimation for OC for July 2002 of -34% and -39% and fractional errors of 83% and 63% for CMAQ and CAMx, respectively. OC performance for the two models in February 2002 is also very similar except the bias is toward overestimation, with fractional bias values of 30% and 33% and fraction errors of 63% and 65% for CMAQ and CAMx, respectively. EC model performance for July 2002 differs between the two models, with CMAQ exhibiting a -16% underestimation and CAMx exhibiting a +16% overestimation fractional bias, and the CAMx fractional error (57%) being slightly lower than that for CMAQ (68%). For February 2002, however, CMAQ exhibits a lower EC fractional bias of -4% whereas the CAMx value is 47%, and the CMAQ fractional error (60%) is slightly lower than is seen for CAMx (69%).

9.4.4 Evaluation for other PM_{2.5} (soil) and coarse mass (CM)

The soil and CM model performance across the U.S. IMPROVE monitors for CMAQ and CAMx for February and July 2002 are shown in Figure 9-4. The soil species is overestimated by both CMAQ and CAMx for July (17% and 62%) and for February (102% and 136%). This overestimation is expected, as the modeled species mapped to the IMPROVE soil measurement contains other unidentified compounds, whereas the IMPROVE soil measurement is built up from the elements. In fact, the usual application of the CAMx model is to model the fine and coarse crustal PM separately from the other unidentified PM components so that the crustal PM can be compared directly against the IMPROVE soil measurement. When CAMx treats dust emissions as separate crustal species, much better soil performance is seen. However, since the CAMx emissions for this application were generated from the CMAQ emissions using the CMAQ-to-CAMx processor and CMAQ does not separately treat the soil species, CAMx could not be configured with the separate fine and coarse crustal species.

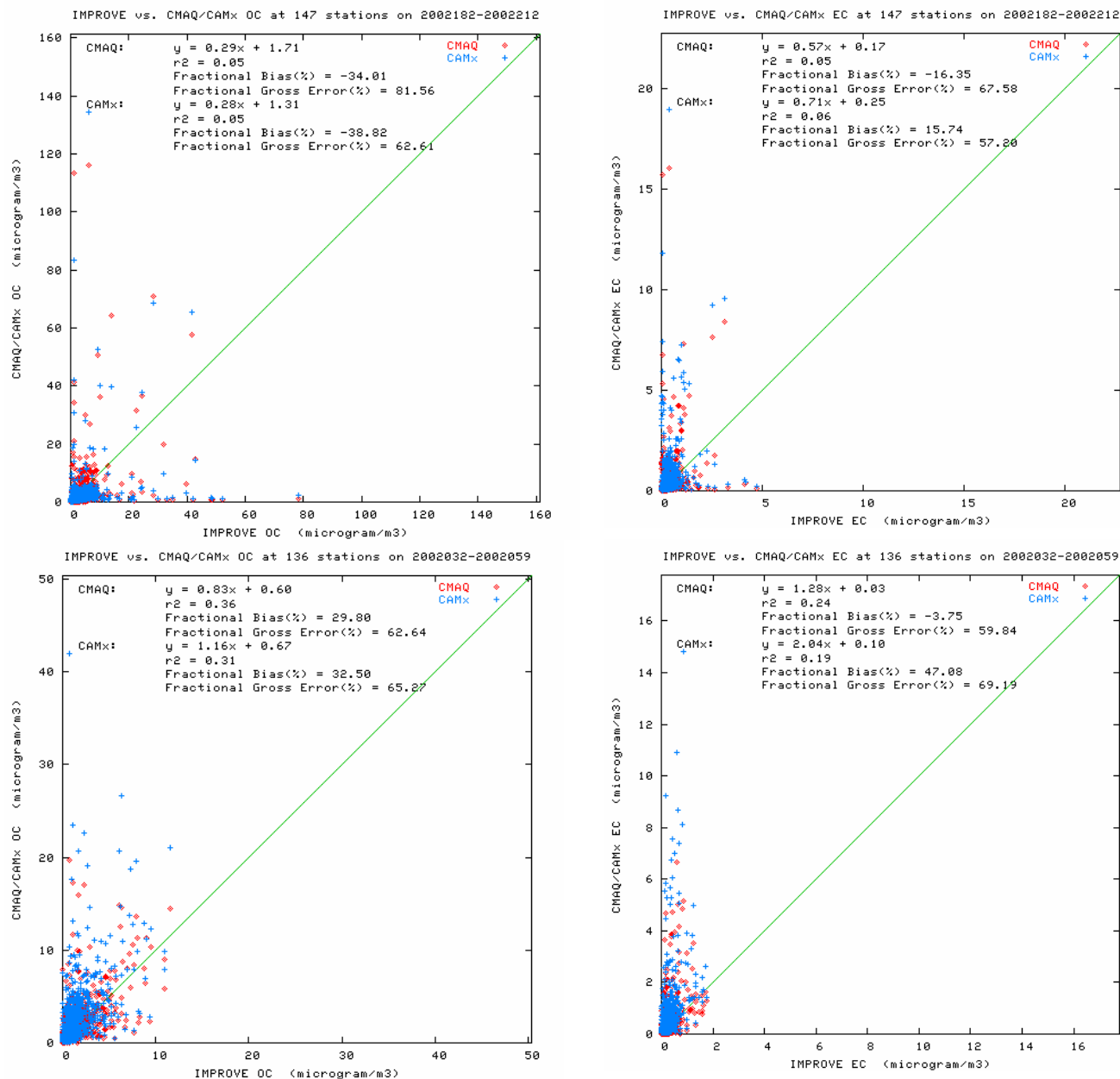


Figure 9-3. Comparison of CMAQ (red) and CAMx (blue) OC (left) and EC (right) model performance at sites across the U.S. for July 2002 (top) and February 2002 (bottom) using the IMPROVE monitoring network.

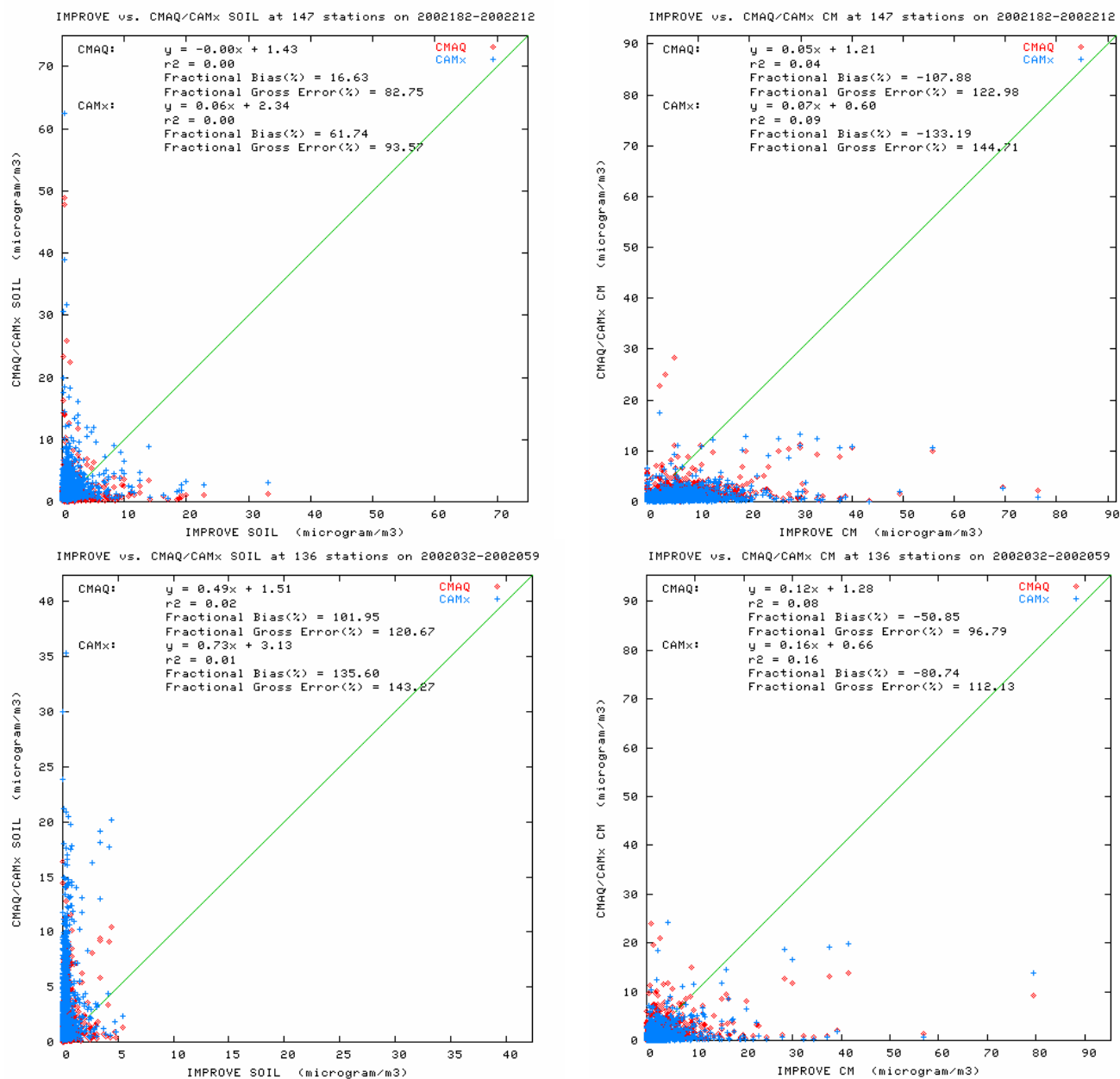


Figure 9-4. Comparison of CMAQ (red) and CAMx (blue) soil (left) and CM (right) model performance at sites across the U.S. for July 2002 (top) and February 2002 (bottom) using the IMPROVE monitoring network.

9.5 Comparison of the PSAT and TSSA PM Source Attribution

In Section 7, results from the TSSA PM source attribution algorithm implemented in CMAQ were described and presented. In this section we compare those source attribution results with results from the CAMx PSAT scheme.

Currently CMAQ TSSA is capable of providing source attribution for SO₄, NO₃, and primary PM particle species and related gaseous compounds (e.g., SO₂ and NO_x). The CAMx PSAT is capable of providing PM source attribution for the following families of species:

- SO₄
- NO₃
- NH₄
- Primary PM, which includes EC, primary organic carbon (POC), PMFINE, and PMc
- SOA (secondary organic aerosols)
- Hg (mercury)

For the WRAP February and July 2002 PSAT application, only the SO₄ family of PM source attribution was specified.

9.5.1 CAMx PSAT PM Source Attribution Configuration

CAMx PSAT was applied for February and July 2002 using a configuration similar to the one used in the CMAQ TSSA source attribution modeling.

Both TSSA and PSAT obtain PM source attribution for user-defined source groups. Source groups typically consist of geographic source regions combined with source categories—for example, elevated-point-source emissions in Arizona. Figure 9-5 displays the geographic source regions used in the TSSA and PSAT source attribution modeling. These regions are defined in Table 9-1.

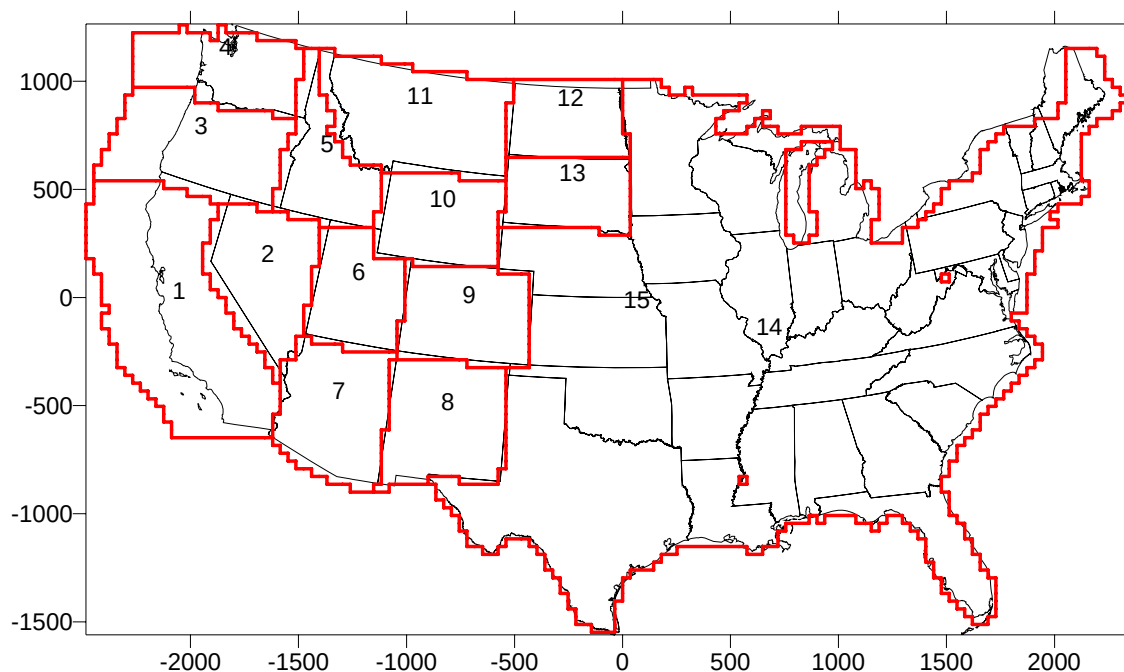


Figure 9-5. Geographic source regions used in the PSAT and TSSA PM source attribution modeling.

Table 9-1. Definitions of the geographic source regions used in the TSSA and PSAT source attribution modeling.

Region	Definition	Region	Definition	Region	Definition
1	California (CA)	6	Utah (UT)	11	Montana (MT)
2	Nevada (NV)	7	Arizona (AZ)	12	North Dakota (ND)
3	Oregon (OR)	8	New Mexico (NM)	13	South Dakota (SD)
4	Washington (WA)	9	Colorado (CO)	14	Eastern States (East)
5	Idaho (ID)	10	Wyoming (WY)	15	Mexico/Canada/Ocean (Mex)

For the CAMx PSAT source attribution modeling, the emissions inventory was split into the following major source categories:

- Biogenic sources (Bio)
- On-road mobile sources (Mob)
- Point sources (Pts)
- Fires (Fir)
- Area plus nonroad mobile sources (ANR)

Thus, the CAMx PSAT application was configured with 15 geographic regions and five source categories. Adding in the initial conditions (ICs) and boundary conditions (BCs) that are always included in the CAMx PSAT source attribution, this results in a total of 77 source groups that tracked PM source attribution in PSAT ($15 \times 5 + 2 = 77$).

9.5.2 Differences in TSSA and PSAT Configurations

The PM source attribution algorithms in PSAT and TSSA were developed independently from one other, so they would be expected to produce similar, but not exactly the same, results. In addition, there were some differences in the way the two schemes were configured that will also produce results differences.

One of the biggest differences between the PSAT and TSSA source attribution schemes is that in PSAT all emissions in the domain must be accounted for by the source groups. In TSSA, on the other hand, only a portion of the emissions inventory can be tagged, emission sources that are not tagged are collected in an “Other” category. This “Other” category also includes mass conservation errors and mass adjustments designed to ensure mass consistency in the CMAQ model. After the completion of the CMAQ TSSA modeling using CMAQ Version 4.4beta in 2004, a mass conservation error was discovered in the CMAQ vertical transport algorithm; it was subsequently corrected in the final version of CMAQ Version 4.4. The mass conservation error, along with the CMAQ mass adjustment, can accumulate in the TSSA “Other” category, resulting in its being a large contributor to PM source attribution. As CAMx does not have similar mass conservation errors or the mass adjustment operator, all PM is accounted for and allocated to the source groups.

Two differences in the way the TSSA and PSAT source attribution schemes were configured for the source attribution tests were as follows:

- TSSA modeled on-road and nonroad mobile sources as one source group (mv), whereas PSAT modeled on-road mobile sources (mob) and area plus nonroad sources (ANR) as separate source groups.
- TSSA did not track separate source attribution for fires (fir) and ICs/BCs, whereas CAMx did. Thus, TSSA accumulated any SO₄ source attribution due to fires and BC in the “Other” category.

9.5.3 Source Attribution Modeling Results

We present TSSA and PSAT source attribution modeling results for a few IMPROVE sites/Class I areas and days from the February and July 2002 modeling periods. These Class I areas and days were selected to illustrate the similarities and differences between the TSSA and PSAT PM source attribution approaches. Figure 9-6 shows the locations of the Class I areas (actually, IMPROVE and IMPROVE protocol sites) where PM source attribution was obtained. Example results are presented below for the following sites:

- GRCA – Grand Canyon National Park in northwestern Arizona

- FOPE – Fort Peck in northeastern Montana
- RMHQ – Rocky Mountain National Park in central Colorado
- SALM – Salmon in eastern-central Idaho

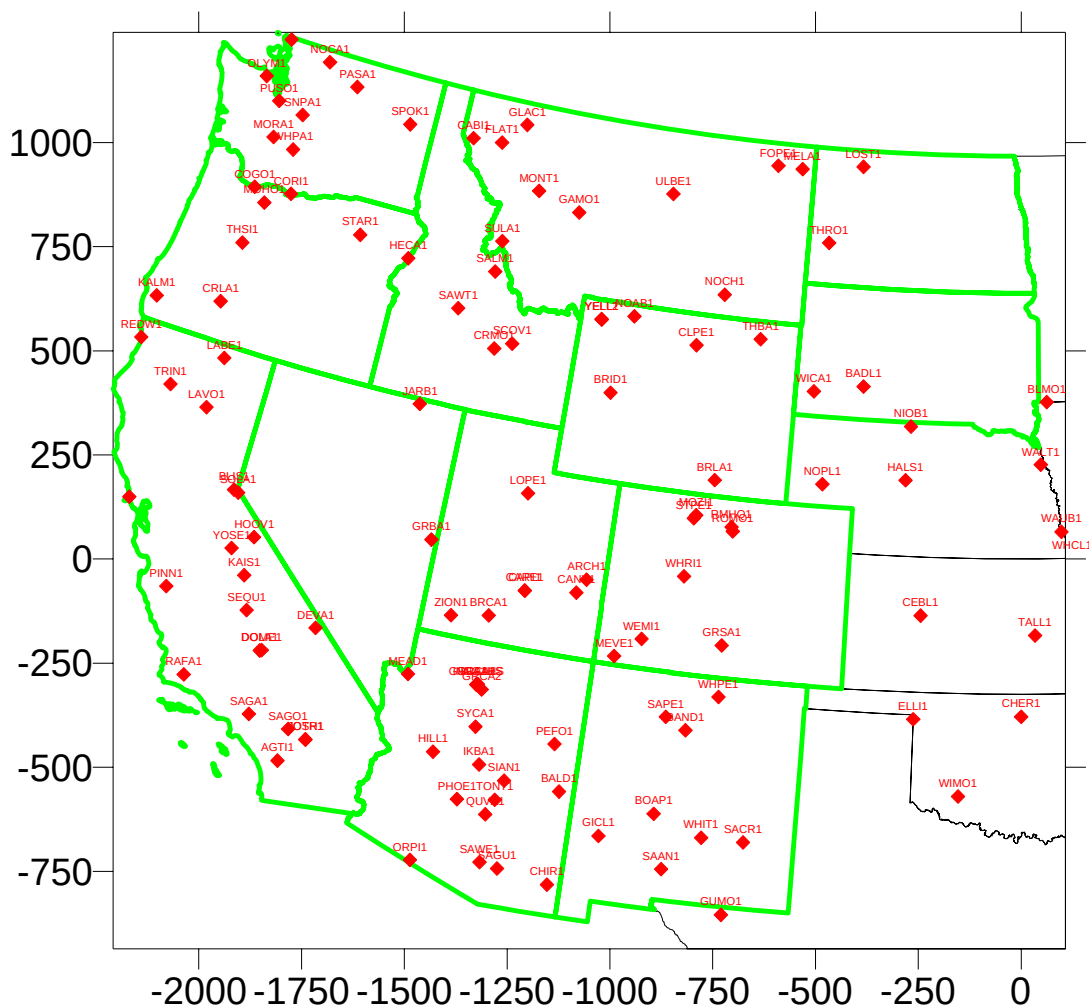


Figure 9-6. Locations of IMPROVE monitoring sites in the western U.S. where the TSSA and PSAT PM source attribution approaches were compared.

Figures 9-7 through 9-9 display three example comparisons of TSSA and PSAT SO₄ source contributions to sulfate at GRCA for July 1, July 7, and February 1, 2002. July 1, 2002 (Figure 9-7) was the worst visibility day at GRCA during 2002. Both TSSA and PSAT agree that point sources from Nevada (Pts_NV) are the largest contributor to SO₄ at GRCA on this day, although the PSAT Pts_NV SO₄ contribution is over twice that of TSSA. The TSSA second largest contributing category is “Other” (described in Section 9.5.2). TSSA and PSAT agree that point sources from Arizona and “Mexico” (i.e., Mexico, Canada, and Ocean) are the next most important contributors, but then the rankings of the source contributions begin to deviate from

each other. PSAT estimates that fires from Arizona and boundary conditions (BC) are the next most important categories, whereas in TSSA these contributions are assumed to reside in the “Other” category. Both source attribution schemes estimate that mobile sources from NV, AZ, and CA make contributions in the TSSA mv category (on-road plus nonroad mobile sources) and the PSAT ANR category (area plus nonroad mobile); because on-road mobile sources use low-sulfur gasoline, most of the SO₂ emissions in the TSSA mobile sources mv category come from the nonroad mobile-source sector, suggesting that the TSSA mv and PSAT ANR contributions are being driven by the same source category and so are consistent.

July 7, 2002, was the 15th worst visibility day at the Grand Canyon in 2002. The SO₄ contributions from TSSA and PSAT (Figure 9-8) exhibit more differences than were seen for July 1. Whereas PSAT estimates that point sources from Nevada (Pts_NV) are the largest contributors to SO₄ at GRCA on this day, the TSSA “Other” category is by far the largest contributor (over 3 times larger than the Pts_NV contribution). This “Other” category consists of untagged sources, such as BCs and possibly fires, and mass errors/corrections in CMAQ. Based on this category’s dominant contribution, the mass conservation errors in CMAQ must have accumulated to a large amount on this day. Although the rankings are a little different between the two source attribution methods, they agree that point sources and nonroad sources from AZ, NV, CA, and Mex are the major contributors to SO₄ at GRCA on July 7, 2002.

February 1, 2002, was the cleanest visibility day at the Grand Canyon during 2002. The TSSA and PSAT SO₄ contributions are shown in Figure 9-9. Both source attribution techniques agree that point sources from Utah are the largest contributor to SO₄ at GRCA on this clean day. Whereas PSAT estimates that BCs are the next largest contributor, TSSA estimates that the “Other” category is next largest. In fact, looking at the cleanest days at other Class I areas across the western U.S., TSSA almost always estimates that the “Other” category is one of the largest contributors. This likely occurs because the BC contribution is included in the “Other” category and because the mass conservation and adjustment terms are a relatively larger share of the total SO₄ mass under cleaner conditions. Although the two source attribution methods differ on the rankings of the remainder of the sources, they both agree that point sources from more distant states to the northwest of GRCA (such as OR, ID, and WA) contribute to SO₄ at GRCA on this cleanest day of 2002. This is consistent with the Clean Air Corridor concept that the cleanest days at GRCA occur when winds are out of the northwest.

Up at the Fort Peck, MT (FOPE) site, July 4 was the 6th worst visibility day at FOPE during 2002. TSSA and PSAT both estimate that different source groups contribute to the SO₄ concentrations than is the case at GRCA (Figure 9-10); this is expected, given their different geographic locations. Both source attribution methods agree that point sources from North Dakota (Pts_ND) contribute the most to SO₄ at FOPE on this day, although the PSAT Pts_ND contribution is almost twice that of TSSA. The two methods also agree that the next three source groups contributing to SO₄ at FOPE on July 4 are much smaller and are due to nonroad emissions from ND and MT and point sources east of the WRAP states. Again the TSSA “Other” category is the second largest contributor to SO₄ at FOPE on this day. Since PSAT suggests that most of the significant contributions at FOPE are due to identified sources that are tagged in the TSSA run (i.e., not fires or BCs), this suggests that the “Other” category at FOPE on this day is due primarily to mass conservation errors and the mass adjustment terms.

The SO₄ contributions at Rocky Mountains National Park (RMNP) on July 1, 2002, estimated by TSSA and PSAT are shown in Figure 9-11. This was the worst visibility day at RMNP during 2002. If fires are included in the TSSA “Other” category, then TSSA and PSAT exhibit good agreement in the source contributions to SO₄ at RMNP on this day, with fires from Utah and Colorado having significant contributions along with point sources in CO, NV, and UT and nonroad sources in CO and CA.

The TSSA and PSAT SO₄ contributions at the Salmon, Idaho (SALM) site in eastern ID are shown in Figure 9-12. With the exception of the large “Other” contribution in TSSA and the BC contribution in PSAT, the two source attribution methods agree on the top contribution sources groups (i.e., point sources in OR and WA and nonroad sources in OR, WA, ID, and MT). Examining the BC and fire contributions to SO₄ at SALM estimated by PSAT does not explain the TSSA highest “Other” contribution, suggesting that the mass conservation errors and mass adjustment terms in PSAT have a large influence on the SO₄ predictions at SALM on July 1.

9.5.4 Conclusions on PM Source Attribution

The comparisons of the CMAQ TSSA and CAMx PSAT PM source attribution modeling results for SO₄ for February and July 2002 were confounded due to the presence of the TSSA “Other” category, which includes untagged source terms, such as BCs and fires, and the accumulation of mass conservation errors and the CMAQ mass adjustment term designed to insure mass consistency. The PSAT SO₄ source attribution accounts for all sources in the region, so there are no untagged sources and the CAMx model is formulated without a mass adjustment step. It is unfortunate that the WRAP CMAQ TSSA modeling used Version 4.4beta of CMAQ that was later found to have mass conservation errors in the vertical transport algorithm; this has been fixed in the final Version 4.4 of CMAQ. Even with the confounding influence of the TSSA “Other” category, the SO₄ contributions from TSSA and PSAT were generally consistent in identifying the same top contributors to SO₄ across the western U.S.

Until the relative magnitudes of the contributions of untagged sources, mass conservation errors, and mass adjustment terms in the CMAQ TSSA “Other” category can be resolved, the TSSA PM source attribution should be viewed qualitatively. As the CAMx PSAT PM source attribution does not suffer these limitations, it can be viewed in more quantitative terms.

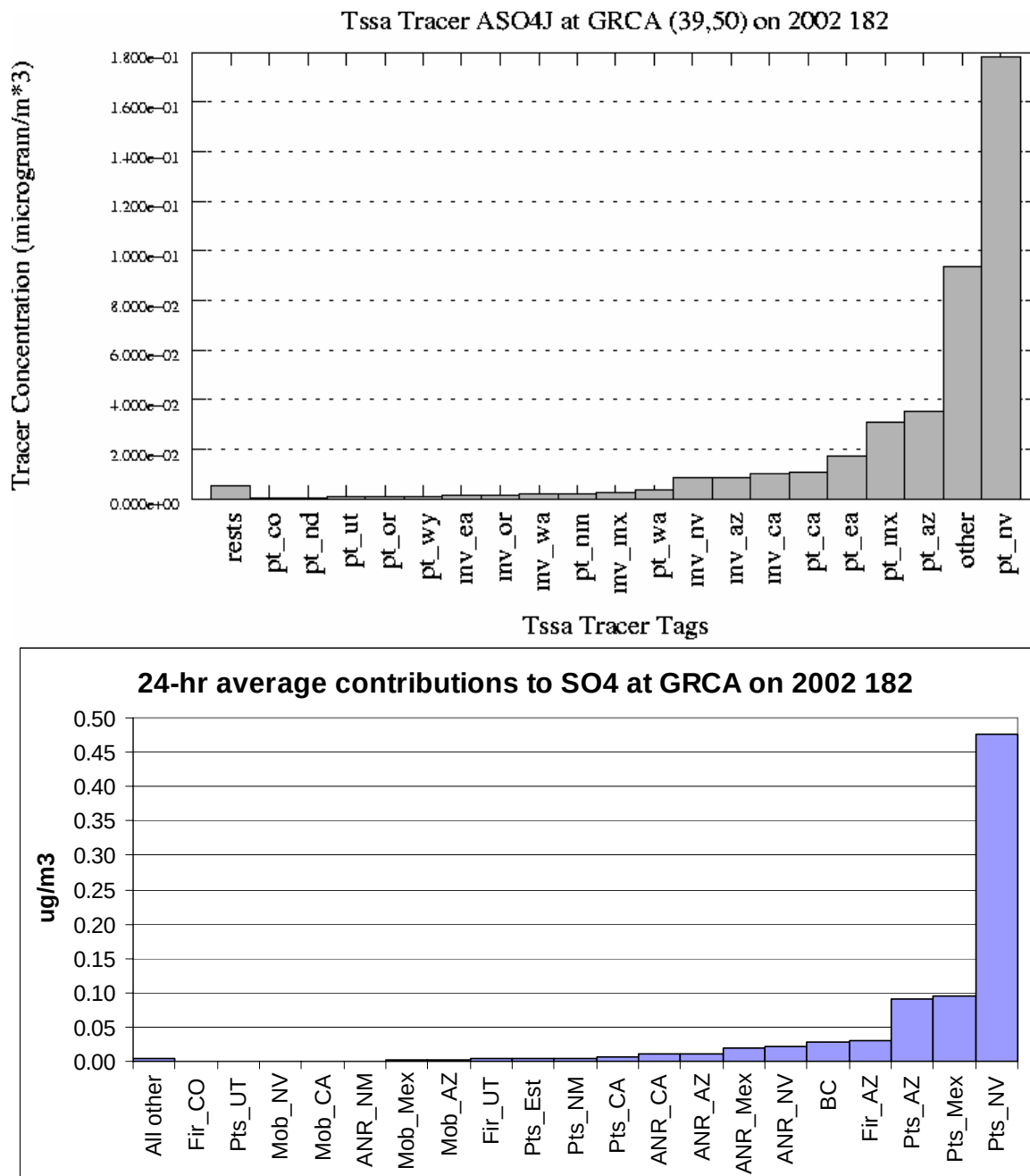


Figure 9-7. Comparison of TSSA (top) and PSAT (bottom) sulfate source attribution at Grand Canyon National Park on July 1, 2002 (day 182).

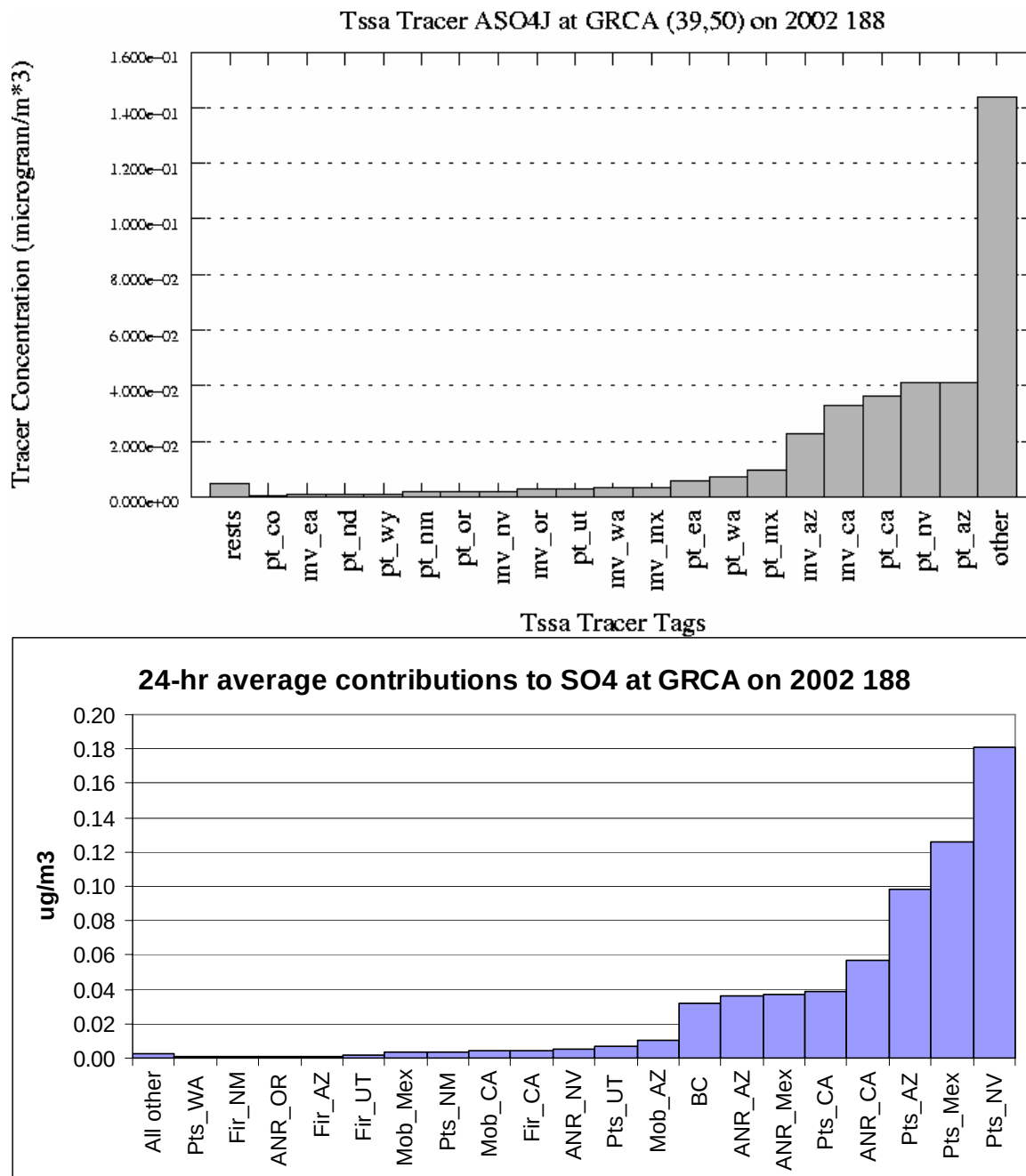


Figure 9-8. Comparison of TSSA (top) and PSAT (bottom) sulfate source attribution at Grand Canyon National Park on July 7, 2002 (day 188).

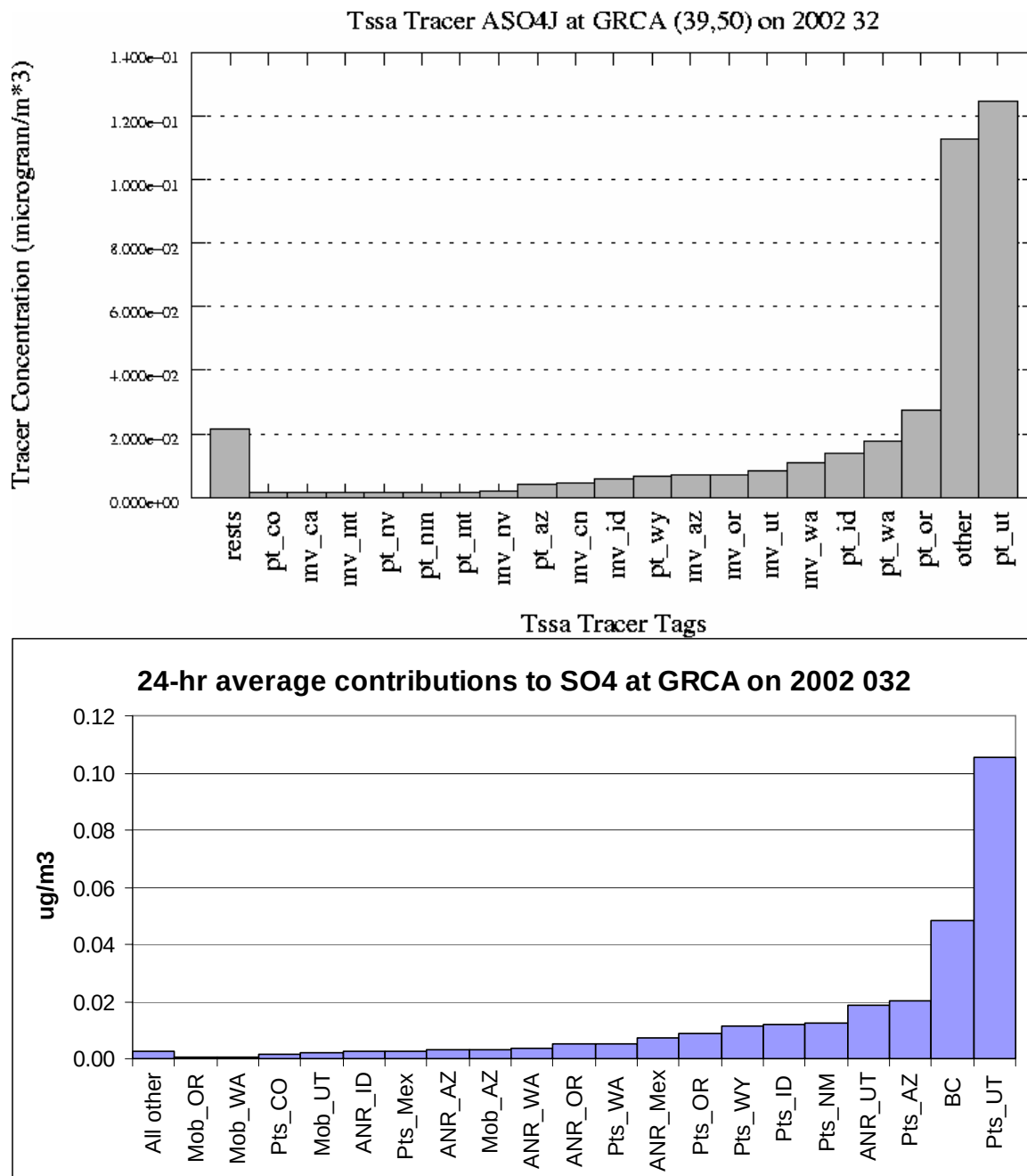


Figure 9-9. Comparison of TSSA (top) and PSAT (bottom) sulfate source attribution at Grand Canyon National Park on February 1, 2002 (day 32).

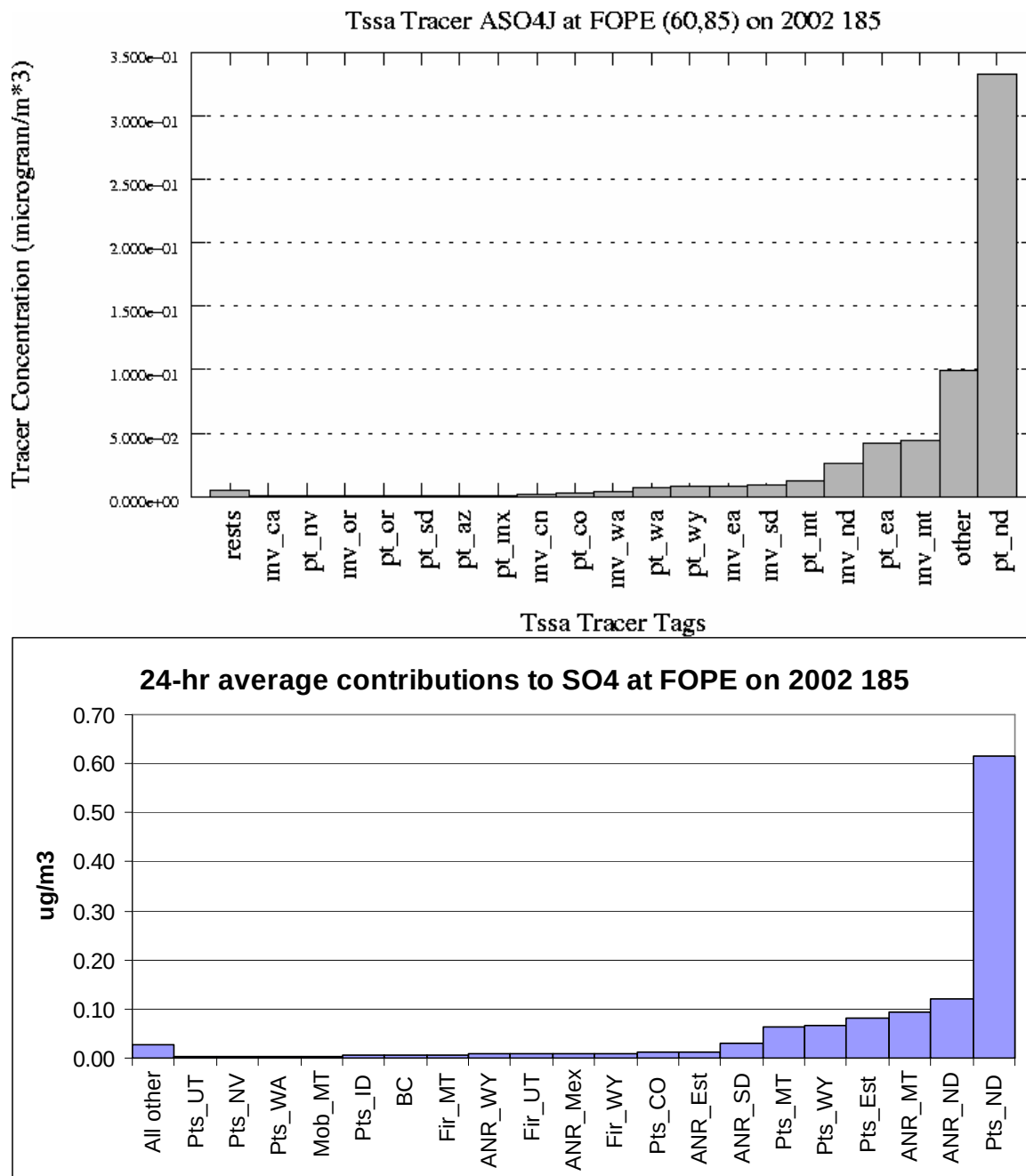


Figure 9-10. Comparison of TSSA (top) and PSAT (bottom) sulfate source attribution at Fort Peck, Montana on July 4, 2002 (day 185).

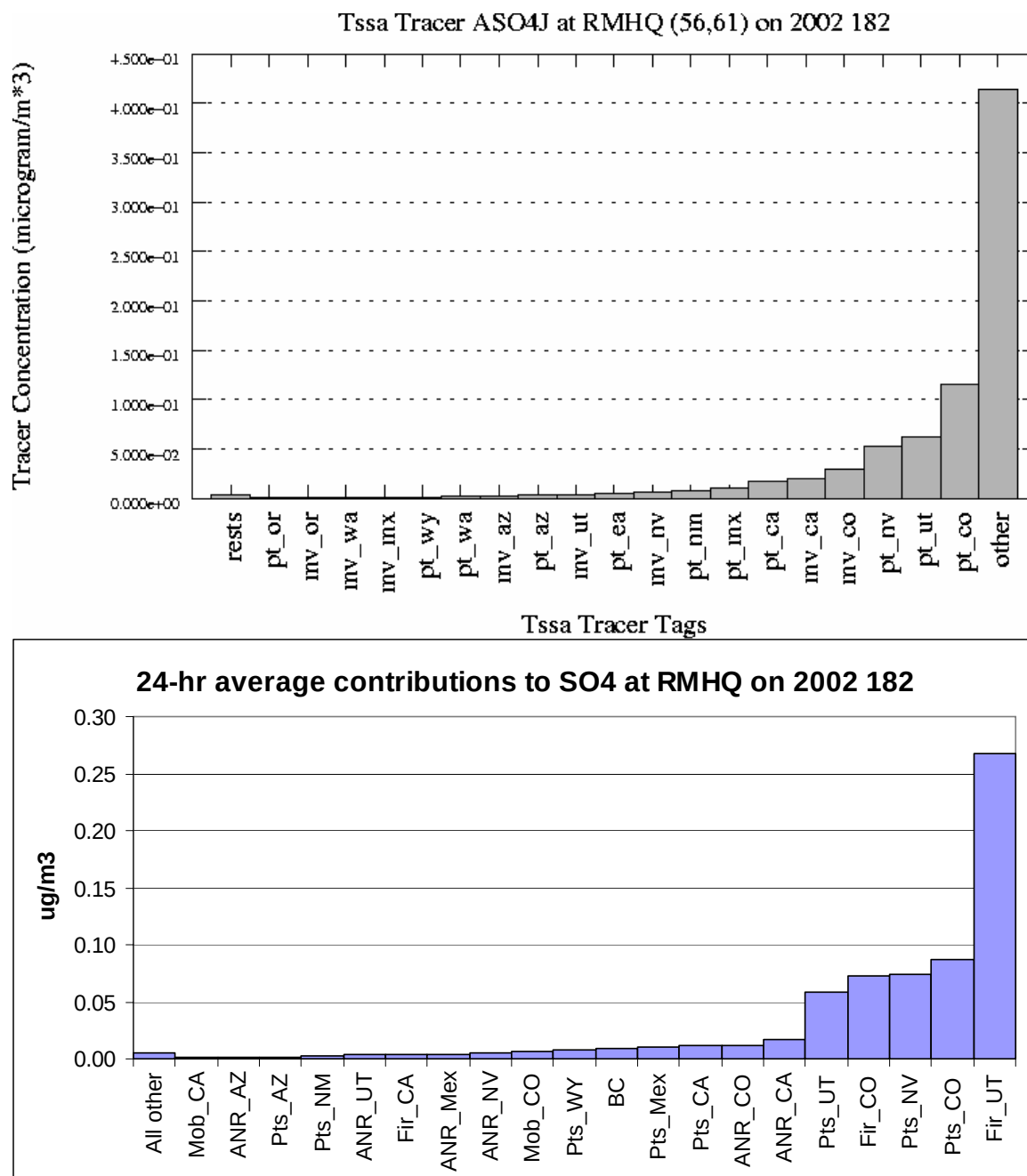


Figure 9-11. Comparison of TSSA (top) and PSAT (bottom) sulfate source attribution at Rocky Mountain National Park, CO, on July 1, 2002 (day 182).

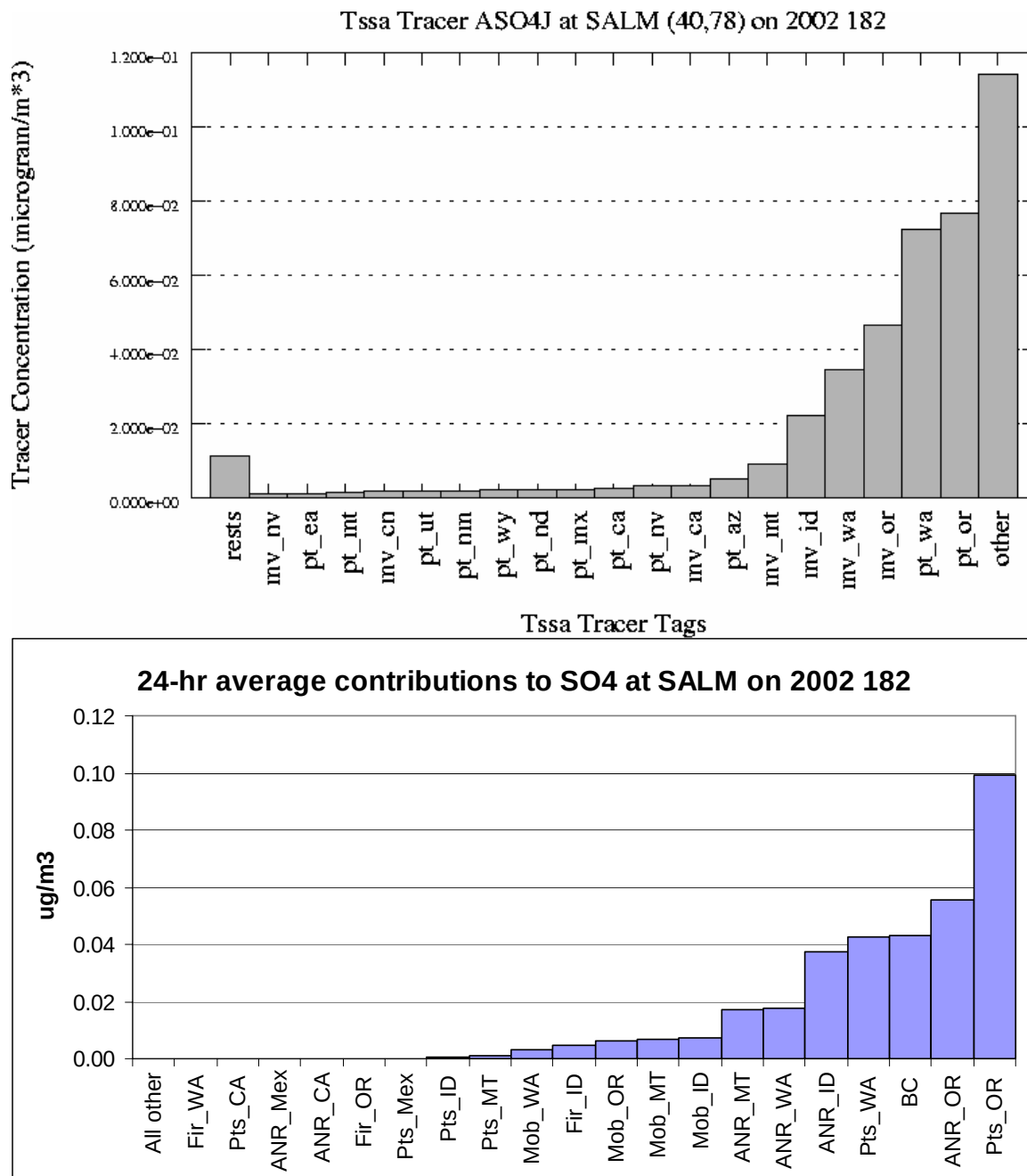


Figure 9-12. Comparison of TSSA (top) and PSAT (bottom) sulfate source attribution at Salmon, ID, on July 1, 2002 (day 182).

9.6 Status of Task 7 Deliverables

Table 9-2 gives the status of each Task 7 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 9-2. Status of the Task 7 deliverables.

Deliverable	Status
Acquisition of the CMAQ TSSA results, latest 2002 MM5 data, and Pre02d emissions	Completed January 2005
Initial testing and evaluation of CAMx and comparison of the CAMx PSAT and CMAQ TSSA PM source attribution techniques	To be completed March 2005
PowerPoint presentation at WRAP Modeling Forum meeting (available at http://pah.cert.ucr.edu/aqm/308/meetings/March_2005/03-08_09-05.SF_CA/Alternative_Model_Mar8-9_2005_MF_Meeting.ppt)	To be completed March 2005

10. Task 9: Testing and Further Improvements to the Windblown Dust Emissions Modeling Methodology

10.1 Introduction

The WRAP area-source emissions inventory currently does not include fugitive windblown dust because of strong concern that the methodology previously used to calculate these particulate emissions yielded inaccurate and misleading results. WRAP has funded a task under which the RMC is addressing this lack of windblown dust emissions. The task objective is to develop a model and inventory of PM dust emissions from wind erosion. We documented our fugitive windblown dust methodology and results from Phase I of this task in a final report (ENVIRON, 2004a) and technical memoranda (Mansell, 2003a,b). Many of the assumptions employed in the Phase I methodology were related to a lack of detail in the underlying data used to characterize vacant land use types and soil conditions. In addition, the Phase I methodology relied on arbitrarily assigned threshold friction velocities and dust reservoir characteristics. The results of the initial model runs and subsequent sensitivity simulations demonstrated a need to revise and/or update various assumptions associated with the development of the emissions inventory.

We are currently in Phase II of the task, during which we have developed a general Phase II estimation methodology for PM dust emissions from wind erosion. Various approaches for refining and enhancing the existing version of the windblown dust model were presented and discussed in Mansell et al. (2004b). These refinements focus primarily on improving the determination of surface friction velocities and threshold friction velocities, as well as the calculation of dust emission fluxes. We also considered the characterization of the disturbance level of vacant land parcels. Land use datasets to more accurately characterize vacant lands were identified for use in the revised dust emission estimation methodology. In addition, we identified a number of studies for review, and incorporated algorithms and methodologies from these studies, as appropriate, into the revised windblown dust model.

Section 10.2 briefly summarizes the Phase I methodology, assumptions, and shortcomings, and discusses the literature review conducted for Phase II. The methodologies, assumptions, and data sources for the Phase II revised windblown dust model are documented in Section 10.3. Results for calendar year 2002 are presented and discussed (Section 10.4), as are preliminary results of an initial model performance evaluation (Section 10.5).

10.2 Summary of Phase I Methodology and Phase II Literature Review

10.2.1 Summary of Phase I methodology

The development and implementation of the Phase I windblown dust model, including various assumptions incorporated in the estimation methodology, have been documented previously

(ENVIRON, 2004a, 2003a,b; Mansell, 2003a,b). The estimation method that was ultimately implemented in Phase I is referred to as the MacDougall method (see ENVIRON [2004] for more details). In summary, it relies on the characterization of vacant land use types and soil conditions, and numerous assumptions regarding dust reservoir characteristics. Wind erosion is initiated in the model based on an arbitrary wind speed assignment, independent of surface conditions. Emission factors, or dust fluxes, were derived from limited wind tunnel study results as a function of wind speed and soil texture. Adjustments were applied to the resulting emission rates based on the vegetation density of vacant land parcels. Surface disturbance levels were based on land use types. In addition, adjustments were applied for agricultural lands based on nonclimatic factors. Land use characterization was based on BELD3; soil texture was derived from the STATSGO database.

The relative lack of detail in the datasets used for characterizing the physical conditions of land parcels and soils required a number of assumptions to be employed in the methodology. These assumptions are presented and discussed in detail in Mansell (2003b) and Mansell et al. (2004a). The primary assumptions affecting the model results can be summarized as follows:

- *Threshold Wind Velocity:* The threshold wind velocity is assumed to be 20 mph, independent of land use and soil texture.
- *Vacant Land Stability:* The methodology relies on specification of the stability of vacant land parcels. The stability characteristics are based solely on the land use type.
- *Dust Reservoirs:* The amount of erodible soil available for suspension into the atmosphere for a given vacant land parcel is referred to as the reservoir. Reservoir properties are based on the stability characteristics of land parcels, and determine the duration of dust events. Limited reservoirs emit dust for a shorter time than unlimited reservoirs. Assumptions are made concerning the amount of time a reservoir will emit windblown dust. Also assumed are the reservoir recharge intervals.
- *Rain, Snow, and Freeze Events:* Assumptions are included that determine the time intervals after which land parcels will emit dust following precipitation, snow, and freeze events. These assumptions greatly affect the number of wind events treated in the methodology as well as the total dust emissions generated.
- *Vegetation Density:* The percentage of vegetative, or canopy, cover is determined by the general land use category of vacant land parcels. These percentages are constant for a given land use type. Estimated emission factors, or emission rates, are attenuated based on the assumed canopy cover percentage.

The above assumptions have a number of implications with respect to the estimation of fugitive dust from wind erosion. However, in many cases the data necessary to address these issues for a regional-scale domain are lacking. These issues and their implications are discussed in Mansell et al. (2004a). Phase II of the windblown dust task, documented in this section, seeks to address these assumptions and limitations and improve the overall estimation methodology and dust model implementation.

10.2.2 Review of recent literature

A number of windblown dust studies have been identified in the literature and are summarized below with respect to the algorithms and physical parameters considered. These studies are compared with each other and summarized in regard to improving the model application for the Phase II dust study. A more detailed comparison of the salient features of each of the windblown dust emission estimation methodologies is presented in Mansell et al. (2004a).

10.2.2.1 Recent dust emission models

Draxler et al. (2001) constructed a regional model for estimating PM_{10} from windblown dust using the concept of threshold friction velocity, which is dependent on the aerodynamic roughness length of the surface, z_0 . PM_{10} vertical mass flux was calculated using the Marticorena et al. (1997) algorithm. The flux is a function of wind velocity, threshold wind velocity, and a coefficient that relates the surface soil texture to PM_{10} emissions. Emissions start when the friction velocity is greater than the threshold friction velocity at that height. Friction velocity was calculated as a function of z_0 .

Threshold friction velocity is calculated as the ratio of the threshold velocity for a smooth surface (u_{*ts}) to the effective friction velocity (f_{eff}). Marticorena and Bergamette (1995) define f_{eff} as the ratio of friction velocity for a smooth surface to actual friction velocity. To determine this ratio, the aerodynamic roughness length for a smooth surface (z_{0s})—which is defined as the mean soil particle diameter (D_p) divided by 30 (Greeley and Iversen, 1985)—is divided by the actual aerodynamic roughness length. Soil samples were collected from the modeled area to determine D_p . The value for z_{0s} was calculated using the measured D_p . Using a mean value of 22 cm/s for u_{*ts} , the actual threshold friction velocity was calculated for different values of aerodynamic roughness length.

Using images of the area, a map of surface conditions and geomorphology, and the u_{*t} data from the Mojave Desert (Gillette et al., 1980, 1982), the authors estimated the threshold friction velocity and surface roughness length for each surface classification. The coefficient that relates the surface soil texture to PM_{10} emissions was estimated using data for several soils from semi-arid areas (Gillette et al., 1997) showing the ratio of vertical flux of PM_{10} to total horizontal mass flux as a function of friction velocity.

In their work, Draxler et al. (2001) considered a special case of windblown dust. Land with vegetative cover has a relatively high threshold velocity and was not considered as an emission source. Two types of soil surface conditions were considered: loose undisturbed soil and disturbed soil. All the area was considered dry and therefore the effect of rain and snow was not considered.

Zender et al. (2003) developed a Dust Entrainment and Deposition (DEAD) model for studying dust-related processes at both local and global scales. They considered three major factors that affect the dust flux: wind friction velocity, vegetation cover, and surface soil moisture content. The approach developed by Marticorena and Bergamette (1995) was used to develop the model. For computing the threshold friction velocity they used a semi-empirical equation developed by Iversen and White (1982). In this equation, the friction velocity is a function of soil density and

particle size, and air density and kinematic viscosity. A constant surface roughness length of 0.01 cm was assumed for the entire domain.

The change in threshold friction velocity was calculated using the equation developed by Marticorena and Bergamette (1995), similar to what Draxler et al. (2001) used in their model. Zender et al. used one global value of 0.0033 cm for the roughness length for a smooth surface. The effect of moisture content of the surface soil was considered in the Zender et al. model. A threshold moisture content was calculated as a function of the mass fraction of clay, as adopted from Fécan et al. (1999). Land covered by vegetation was not considered as a dust-emitting source.

The vertical mass flux was calculated as a function of the horizontal mass flux, a global tuning factor, a source erodibility factor, the fraction of bare soil, and the fraction of clay mass. The horizontal mass flux was calculated as a function of friction velocity and threshold friction velocity.

Shao (2001) developed an emission flux model as a function of the horizontal mass flux, threshold friction velocity, and an empirical function of the diameters of saltating and emitted particles. In his work, Shao emphasized the microscale forces working on saltating particles and the impact of these particles on dust emissions. In this model, a particle size distribution of the soil is required.

10.2.2.2 ENVIRON/RMC model

The “ENVIRON/RMC model” refers to the estimation methodology proposed by the RMC’s Phase I fugitive windblown dust task team and documented in ENVIRON (2003a). Based on a review of wind tunnel studies, we noted that the two important components for characterizing dust emission process from an erodible surface are (1) the threshold friction velocity, which defines the inception of the emission process as a function of the wind speed and as influenced by the surface characteristics; and (2) the strength of the emissions that follow the commencement of particle movement. The two critical factors affecting emission strength are the wind speed (wind friction velocity), which drives the saltation system, and the soil characteristics.

10.2.2.2.1 Threshold friction velocities

The methodology relies on the determination of threshold surface friction velocities, u_{*t} , as a function of aerodynamic surface roughness length, z_0 . In addition to aerodynamic roughness, the degree of disturbance of the surface also plays a key role in estimating threshold friction velocities. Based on the work of Marticorena et al. (1997), relationships between u_{*t} and z_0 were identified and compared with wind tunnel data from Gillette et al. (1980, 1982), Gillette (1988), and Nickling and Gillies (1989). This comparison is presented in Figure 10-1.

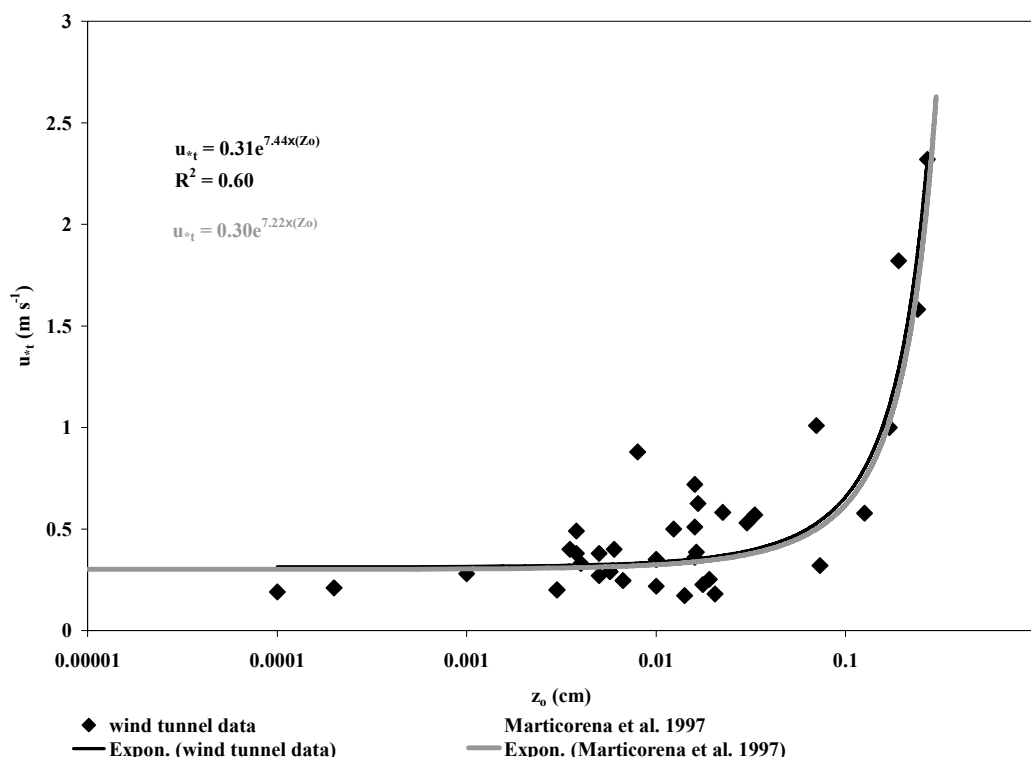


Figure 10-1. Comparison between (1) the Marticorena et al. (1997) modeled relationship of threshold friction velocity and aerodynamic roughness length and (2) wind tunnel data from Gillette et al. (1980, 1982), Gillette (1988), and Nickling and Gillies (1989).]

Several general relationships can be described for threshold friction velocity data. Two major factors have the greatest influence on the threshold of wind-erodible soils: the degree of disturbance and the aerodynamic roughness. For loose or disturbed soils, the most important factor controlling the threshold friction velocity is aerodynamic roughness. The effect of surface disturbance on threshold friction velocity has been evaluated and documented by others (Gillette et al., 1980, 1982; Gillette, 1988; Nickling and Gillies, 1989). For a given surface type, the effect of disturbance is to lower the threshold to between ~90% and ~20% of the undisturbed value.

Applying the relationship shown in Figure 10-1 to assign a threshold friction velocity to a surface requires information on a surface's aerodynamic roughness length. This type of information is not generally available in land use databases, because they were not specifically developed to quantify aerodynamic properties of surfaces. Based on the designation of land use type, the aerodynamic roughness can be assigned using previously reported values for similar surfaces.

10.2.2.2 Emission factors

Field and wind tunnel experiments suggest that the dust emissions are proportional to wind friction speed and approximate theoretical model predictions, but the considerable scatter in the available data makes it impossible to clearly define this dependence (Nickling and Gillies, 1993).

Different surfaces appear to have different constants of proportionality for the flux versus wind friction velocity relationship, implying that the flux is predictable, but that surface and soil properties affect the magnitude of the flux. A detailed discussion of wind tunnel studies, including various limitations and measured data, is provided in ENVIRON (2003a,b). The findings of the various wind tunnel studies are briefly summarized here.

Alfaro et al. (2003) re-analyzed the Nickling and Gillies (1989) data and found that the tendency of a surface to emit dust does not depend primarily on its textural qualities, but instead on the size distribution of the loose soil aggregates available for saltation, and the aerodynamic roughness length that conditions the emission threshold. The re-analysis was based in part on the work of Chatenet et al. (1996) in which they found that desert soils could be broadly divided into four populations based upon their soil aggregate populations. The differences between the four groups are based upon the estimated geometric mean diameter of the soil particles. The four size classes are 125 μ m, 210 μ m, 520 μ m, and 690 μ m, which they label FSS (silt), FS (sandy silt), MS (silty sand), and CS (sand). The emission flux relationships are displayed in Figure 10-2.

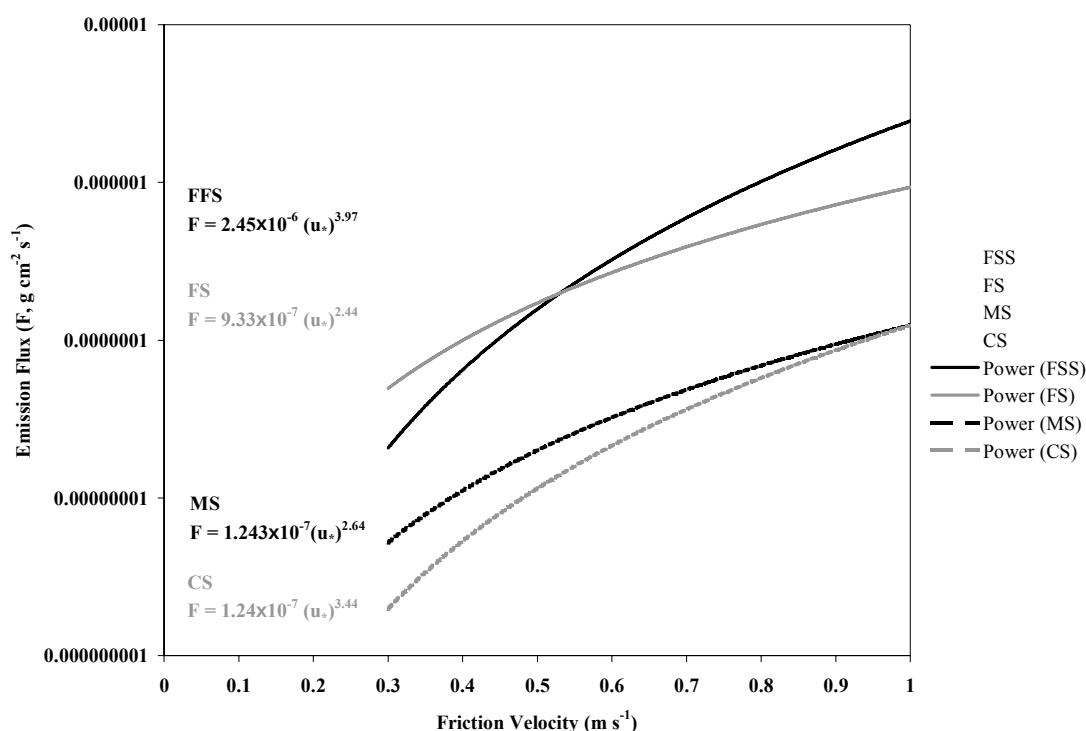


Figure 10-2. The emission flux as a function of friction velocity predicted by the Alfaro and Gomes (2001) model constrained by the four geometric-mean-diameter soil classes of Alfaro et al. (2003).

Using the Alfaro et al. (2003) approach, emissions of dust for soils can be confined to four different emission factors, depending on the geometric mean grain size, as determined by the

methods of Chatenet et al. (1996). The model predictions were tested against the wind tunnel dataset of Nickling and Gillies (1989) and found to fit the measured data satisfactorily. Of key importance is that Chatenet et al. (1996) established relationships between the 12 soil types that are defined in the classical soil texture triangle and their four dry soil types (FSS, FS, MS, and CS). The soil texture categorization and the relationships among texture assignments and soil groupings are discussed in Section 10.3.7.2.

10.3 Phase II Windblown Dust Emission Estimation Methodology

We found that all of the dust model applications we reviewed (Section 10.2.2), including the ENVIRON/RMC methodology, utilize a similar approach for determining threshold friction velocities and dust emission flux rates. With each particular application, certain simplifying assumptions are incorporated. These assumptions are generally required because there is not enough detailed information to fully characterize physical conditions and parameters of erodible surfaces.

The Phase II dust model implementation follows the same general approach as the ENVIRON/RMC methodology originally proposed by the RMC team during the Phase I work effort and the other models discussed above, but with improvements. The approach for determining and applying each of the required elements of the model is presented below.

10.3.1 Friction velocities

Surface friction velocities are determined from the aerodynamic surface roughness lengths and the 10-m wind speeds from the MM5 model simulations. Friction velocity, u_* , is related to the slope of the velocity versus the natural logarithm of height through this relationship:

$$\frac{u_z}{u_*} = \frac{1}{\kappa} \ln \frac{z}{z_0}$$

where

u_z = wind velocity at height z (m s^{-1})

u_* = friction velocity (m s^{-1})

κ = von Karman's constant (0.4)

z_0 = aerodynamic roughness length (m)

10.3.2 Threshold friction velocities

The threshold friction velocities, u_{*t} , are determined from the relationships developed by Marticorena as a function of the aerodynamic surface roughness length, z_0 . This relationship was presented in Figure 10-1.

10.3.3 Surface roughness lengths

Surface friction velocities, including the threshold friction velocity, are a function of the aerodynamic surface roughness lengths. The surface roughness lengths are in turn dependent on surface characteristics, particularly land use/land cover. While these values can vary considerably for a given type of land, published data are available that provide a range of surface roughness lengths for various land use types and vegetation covers. Table 10-1 summarizes the assignments of surface roughness for each land cover type considered for wind erosion. Other land cover types were not considered erodible due to the large assumed surface roughness lengths.

Table 10-1. Summary of surface characteristics for application of the Phase II dust model.

Parameter	Dust Code 3	Dust Code 4	Dust Code 6	Dust Code 7
Land use category	Agricultural	Grassland	Shrubland	Barren
Surface roughness length (cm)	0.031	0.1	0.05	0.002
Threshold friction velocity (mi/h)	8.33	13.81	9.62	6.81
Threshold wind velocity at 38 m height (mi/h)	29.5	44.3	32.8	28.5

10.3.4 Emission fluxes

Emission fluxes, or emission rates, are determined as a function of surface friction velocity and soil texture. The relationships developed by Alfaro and Gomes (2001) for each of the soil texture groups of Alfaro et al. (2003) is applied for estimating dust emission fluxes. These relationships were presented in Figure 10-2 above.

10.3.5 Reservoir characteristics

Dust emissions from vacant lands are limited by the amount of erodible soil available for suspension into the atmosphere. In addition to the amount of soil present, the condition of the soil (including texture and stability) and climatological factors influence the total windblown dust emission potential of a given parcel of vacant land. The amount of soil available for a given land parcel is referred to as the reservoir and can be classified as limited or unlimited. The classification chosen has implications with respect to the duration of time over which the dust emissions are generated. In general, the reservoirs should be classified in terms of the type of soils, the depth of the soil layer, soil moisture content, and meteorological parameters. Finally, the time required for a reservoir to recharge following a wind event is influenced by a number of factors, including precipitation and snow events and freezing conditions of the soils.

Given that the soils database for use in this task does not provide information concerning the moisture content or the depth of the soil layer, we made certain assumptions regarding the determination and classification of soil reservoirs. These assumptions are based primarily on the land

use type and stability of the vacant land parcel. Reservoirs are classified as limited for stable land parcels and unlimited for unstable land parcels.

The duration and amount of precipitation and snow and freeze events also affect the dust emissions from wind erosion. In the Phase I application, these parameters were somewhat arbitrarily assigned. Barnard (2003) has compiled a set of conditions for treating these events based on season, soil characteristics, and the amounts of rainfall and snow cover. These conditions were based on limited information found in the literature and additional assumptions. The results of the analysis of Barnard are summarized in Tables 10-2 and 10-3.

Table 10-2. Number of days after precipitation event to re-initiate wind erosion for rainfall amounts (constant) ≥ 2 in.

Soil type	Spring/Fall	Summer	Winter
Sand	3	2.1	4.2
Sandy loam	3	2.1	4.2
Fine sand loam	3	2.1	4.2
Loam	4	2.9	3.8
Silt loam	4	2.9	3.8
Sandy clay loam	4	2.9	3.8
Clay loam	5	3.6	7.2
Silty clay loam	6	4.3	8.6
Clay	7	5.0	10.0

Table 10-3. Number of days after precipitation event to re-initiate wind erosion for rainfall amounts (constant) < 2 in.

Soil type	Spring/Fall	Summer	Winter
Sand	1	0.7	1.4
Sandy loam	1	0.7	1.4
Fine sand loam	1	0.7	1.4
Loam	2	1.4	2.8
Silt loam	2	1.4	2.8
Sandy clay loam	2	1.4	2.8
Clay loam	3	2.0	4.0
Silty clay loam	4	2.8	5.6
Clay	5	3.6	7.2

10.3.6 Soil disturbance

The level of disturbance of an erodible surface is an important parameter in estimating wind-blown dust emissions. Disturbed surfaces tend to generate more dust than undisturbed ones. In the application of the Phase I model, different emission rates were applied for disturbed versus undisturbed surfaces. The disturbance level of surfaces was assumed to be determined by the land use type and to be invariant in time and across the modeling domain. Thus, assumptions were required to assign surface disturbance based on land cover type. As noted previously, the disturbance level of a surface more appropriately has the effect of altering the threshold surface friction velocity; disturbed surfaces have lower thresholds while undisturbed surfaces exhibit higher threshold friction velocities.

The disturbance level of various surfaces across a regional-scale simulation is difficult to determine, given the lack of detail in both the LULC and soils data available for use in the model. Except for agricultural lands, which are treated separately in the model (see Section 10.3.8), vacant land parcels are typically undisturbed unless some activity is present that causes a disturbance—for example, off-road vehicle activity in desert lands, or animal grazing on rangelands.

For the Phase II model application, we chose to consider all nonagricultural land use types as undisturbed surfaces, since there is no a priori information to indicate otherwise for the regional-scale modeling domain being considered. The effects of assumed disturbance levels were evaluated with sensitivity simulations (discussed in Section 10.4). For the sensitivity simulations, threshold surface friction velocities for the assumed disturbed land use types were based on limited experimental data.

10.3.7 Data sources

The various datasets required for implementing the Phase II approach to windblown dust estimation are summarized below.

10.3.7.1 Land use/land cover

The land use/land cover data used for Phase II were based on the National Land Cover Database (NLCD). These are the same datasets used in developing the ammonia emissions inventory, and are documented in Section 2. A summary of land use types for the U.S. portion of the RPO Unified domain is given in Table 10-4.

Table 10-4. Percentage of each land use type for the U.S. portion of the modeling domain.

Land Use Type	Total Area (Acres)	% of Total When Water Included	% of Total When Water Excluded
Water	98,484,739	5.0%	—
Urban	35,629,865	1.8%	1.9%
Barren	37,204,176	1.9%	2.0%
Forest	556,424,387	28.1%	29.6%

Land Use Type	Total Area (Acres)	% of Total When Water Included	% of Total When Water Excluded
Shrubland	355,796,082	18.0%	18.9%
Grassland	302,601,621	15.3%	16.1%
Agricultural	515,624,831	26.0%	27.4%
Wetlands	78,127,135	3.9%	4.2%
Total when water included	1,979,892,836	100.0%	—
Total when water excluded	1,881,408,097	—	100.0%

10.3.7.2 Soil characteristics

Application of the emission factor relationships described above requires the characterization of soil texture in terms of the four soil groups considered by the model. The type (characteristics) of soil is one of the parameters of primary importance when applying the emission estimation relationships derived from wind tunnel study results. We used the STATSGO database to determine the types of soils present in the modeling domain. These data were developed from the same databases as the soils data for the ammonia emissions inventory (see Section 2).

The classification of soil textures and soil group codes is based on the standard soil triangle that classifies soil texture in terms of percent sand, silt, and clay. Combining the soil groups defined by the work of Alfaro et al. (2003) and Chatenet et al. (1996) and the standard soil triangle provides the mapping of the 12 soil textures to the four soil groups considered in their study (see Section 10.2.2.2.2). This soil texture/soil group mapping (Table 10-5) allows the application of emission factor data.

Table 10-5. STATSGO soil texture and soil group codes.

STATSGO Soil Texture	Soil Group	STATSGO Soil Texture	Soil Group
No data	N/A	Sandy clay loam	MS
Sand	CS	Silty clay loam	FFS
Loamy sand	CS	Clay loam	MS
Sandy loam	MS	Sandy clay	MS
Silt loam	FS	Silty clay	FFS
Silt	FFS	Clay	FS
Loam	MS		

10.3.7.3 Meteorology

As with the Phase I model implementation, gridded hourly meteorological data are required for the dust estimation methodology. The meteorological data for Phase II are based on MM5 model simulation results. Data fields required include wind speeds, precipitation rates, soil temperatures, and ice/snow cover. The 2002 MM5 model results on the RPO Unified domain (see Section 4), at both 12- and 36-km resolutions, are processed as in Phase I and used in the application of the Phase II windblown dust model.

10.3.8 Agricultural land adjustments

Unlike other types of vacant land, windblown dust emissions from agricultural land are subject to a number of nonclimatic influences, including irrigation and seasonal crop growth. We therefore developed several nonclimatic correction or adjustment factors to apply in calculating the agricultural wind erosion emissions. These factors address:

- long-term effects of irrigation (i.e., soil “cloddiness”);
- crop canopy cover;
- post-harvest vegetative cover (i.e., residue);
- bare soil (e.g., barren areas within an agriculture field that do not develop crop canopy for various reasons); and
- field borders (i.e., bare areas surrounding and adjacent to agricultural fields).

The methodology used to develop individual nonclimatic correction factors for the Phase I study was described in ENVIRON (2004a). Most of these methods were based upon previous similar work performed by CARB in their development of California-specific adjustment factors for USDA’s Wind Erosion Equation (WEQ) (CARB, 1997). We developed these correction factors for specific soil textures, crop types, and geographic locations and then applied them to the wind erosion estimates developed from the wind tunnel studies. Correction factors were developed only for the 17 field crops specifically identified in the BELD3.1 dataset (i.e., alfalfa, barley, corn, cotton, grass, hay, oats, pasture, peanuts, potatoes, rice, rye, sorghum, soybeans, tobacco, wheat, and miscellaneous crops). Due to the insufficient characterization of the wind erosion emission processes for orchards and vineyards, correction factors for this type of agricultural land were not developed.

For the Phase II dust model implementation, we applied these same nonclimatic adjustments. However, because the BELD3 database was not used, these factors were instead related to the agricultural land use types available in the NLCD LULC data. The existing county-level crop percentages from the BELD3 database were linked to the aggregated agricultural land parcels from the NLCD data. Note that for all states outside of the WRAP and CENRAP regions, no agricultural data were collected. Therefore, for those states no agricultural adjustments were applied.

10.4 Model Results for 2002

This section discusses the results obtained from running the Phase II revised windblown dust emission model using the estimation methodologies and data described above. However, note that after this set of model runs was performed, a minor error was discovered in the meteorological data processor. The effect of the error was to shift the wind fields a fixed number of grid cells to the west. The model is therefore being rerun to correct this error and to utilize the latest MM5 simulation results. The revised windblown dust emission estimates, as well as the emission estimates based on the 12-km resolution meteorological data, will be documented in the draft final report for this task, which is scheduled for completion in March 2005. Nevertheless, the results from the four sensitivity scenarios described below are still relevant because in each case the wind field shift is the same. The results of these scenarios can still be compared with each other to provide some insight into the sensitivity of the model and the estimation methodology to various assumptions.

Four scenarios were conducted to evaluate the sensitivity of the model to the various assumptions incorporated in the methodology. These scenarios were designed to consider the effects of soil disturbance and reservoir characteristics. The scenarios were as follows:

- a. No limitation on dust event duration; all soils loose and undisturbed
- b. Dust event duration limited to 10 hours per day; all soils loose and undisturbed
- c. No limitation on dust event duration for disturbed or undisturbed soils; 10% of grassland, shrubland, and barren land area assumed disturbed; threshold friction velocity for disturbed grass and shrubland = $0.5 \cdot (\text{undisturbed value})$; threshold friction velocity for barren land = $0.27 \cdot (\text{undisturbed value})$
- d. Dust event duration limited to 10 hours per day for undisturbed soils; no limitation on dust event duration for disturbed soils; 10% of grassland, shrubland, and barren land area assumed disturbed; threshold friction velocity for disturbed grass and shrubland = $0.5 \cdot (\text{undisturbed value})$; threshold friction velocity for barren land = $0.27 \cdot (\text{undisturbed value})$

Sections 10.4.1 through 10.4.4 present plots of coarse PM (PM_c) and PM₁₀ for each scenario. Section 10.4.5 discusses the results for the scenarios, and recommends the scenario to use for further evaluation and air quality modeling. Displays of the spatial distribution of dust emissions are presented in terms of PM_c, while state-level and domainwide results (bar charts) are presented in terms of PM₁₀. The spatial displays are generated from the gridded model-ready emission files, which represent PM_c as required by the air quality models. PM₁₀ emission estimates are available as text files output directly from the dust model and are summarized by land type and/or state for presentation.

10.4.1 Scenario a

Scenario a considered all soils to be loose and undisturbed. In addition, no limit on the duration of dust events was imposed. The spatial distribution of PM_c emissions is displayed in Figure

10-3. Figure 10-4 shows the distribution of predicted PM_{10} dust emissions by land use type for each of the WRAP states.

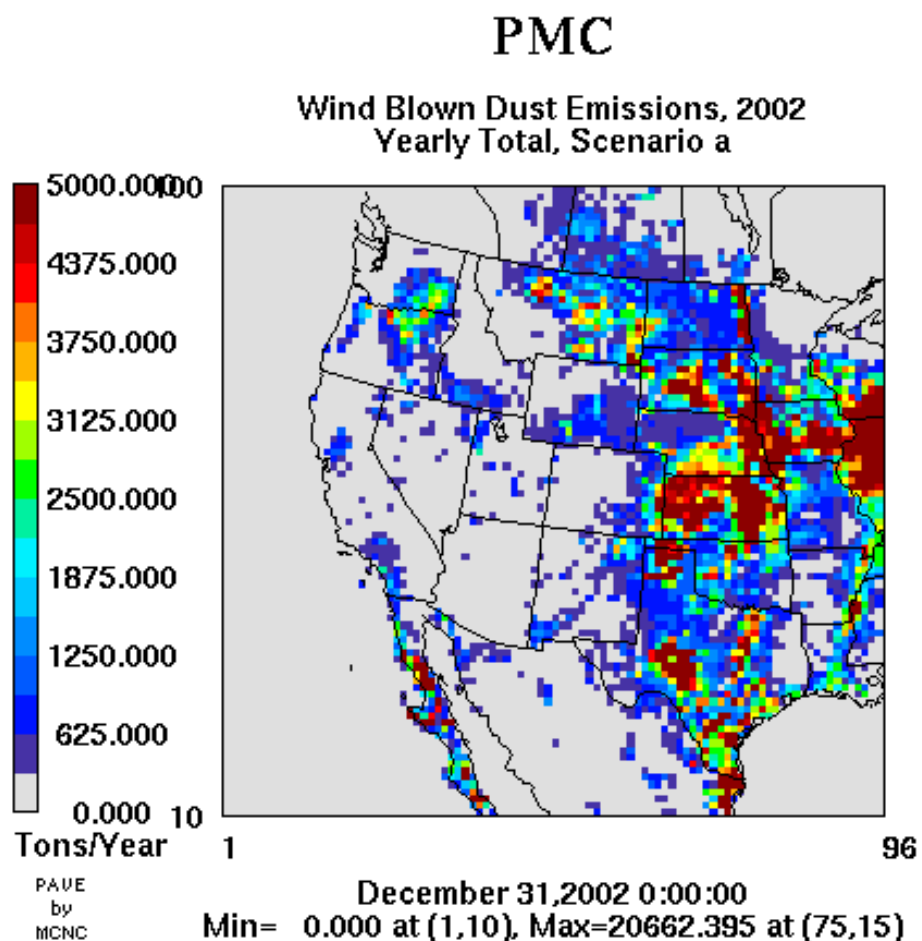


Figure 10-3. Spatial distribution of total 2002 annual PMc dust emissions for Scenario a.

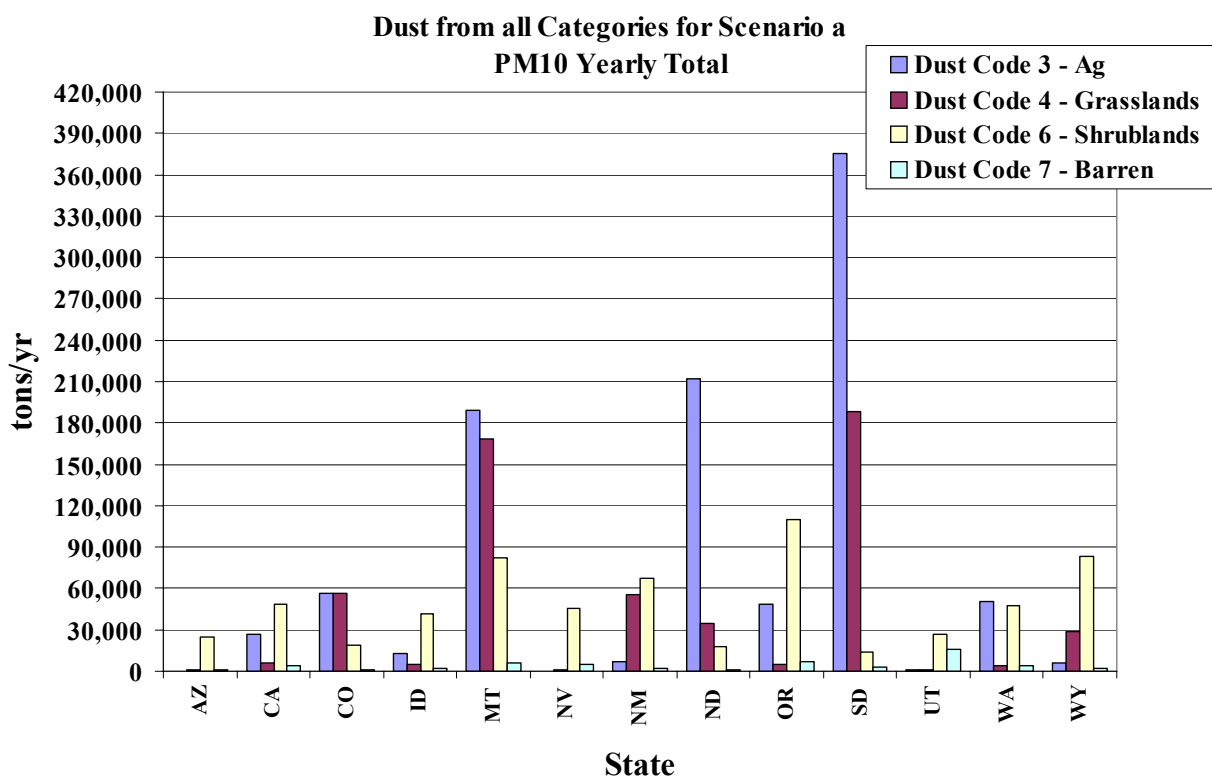


Figure 10-4. Distribution of total annual 2002 PM₁₀ dust emissions by land use type and state for Scenario a.

10.4.2 Scenario b

As in Scenario a, Scenario b considered all soils to be loose and undisturbed. In contrast to Scenario a, however, the duration of dust events was limited to 10 hours per day. Figure 10-5 shows the spatial distribution of PM_c emissions. The distribution of predicted PM₁₀ dust emissions by land use type for each of the WRAP states is displayed in Figure 10-6.

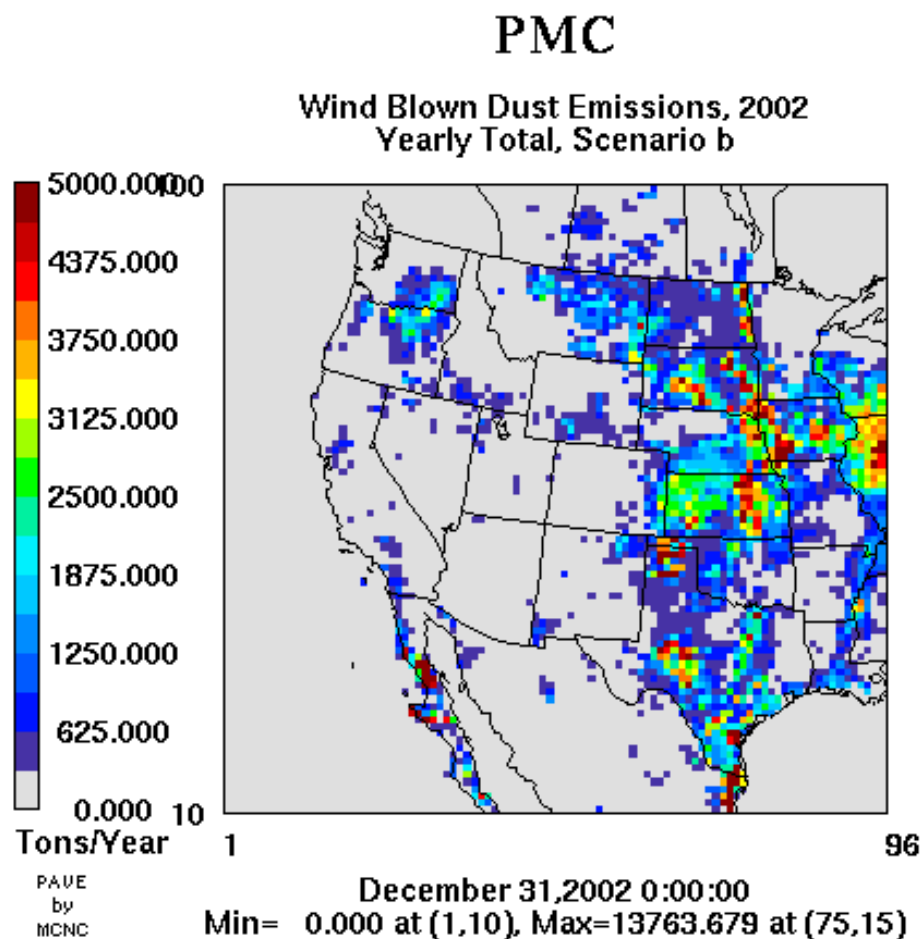


Figure 10-5. Spatial distribution of total 2002 annual PM_c dust emissions for Scenario b.

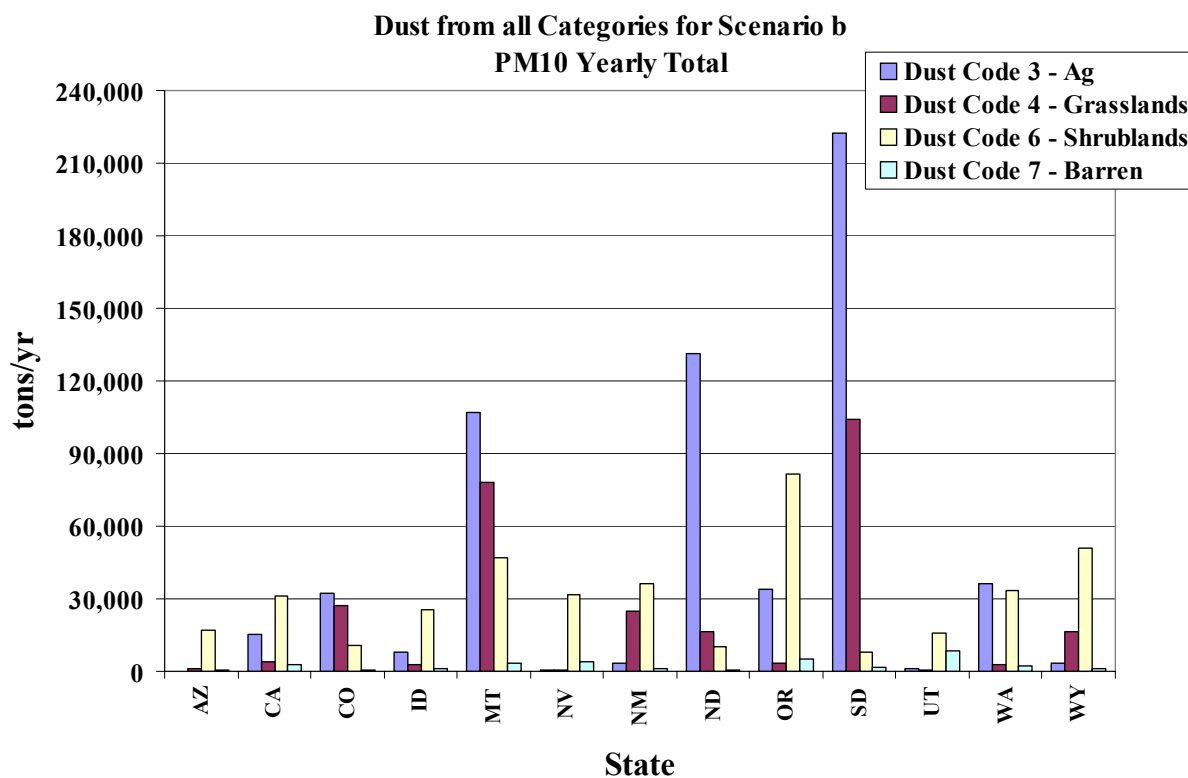


Figure 10-6. Distribution of total annual 2002 PM₁₀ dust emissions by land use type and state for Scenario b.

10.4.3 Scenario c

Scenario c assumed that 10% of the grassland, shrubland, and barren land area was disturbed. For the disturbed areas, threshold friction velocities were reduced, resulting in the initiation of wind erosion at lower wind speeds. For disturbed grassland and shrubland the threshold friction velocity was assumed equal to 0.5 times the undisturbed value; for disturbed barren land the threshold friction velocity was assumed equal to 0.27 times the undisturbed value. In addition, no limit on the duration of dust events was imposed for either disturbed or undisturbed soils. The spatial distribution of PM_c emissions is displayed in Figure 10-7, while Figure 10-8 shows the distribution of predicted PM₁₀ dust emissions by land use type for each WRAP state.

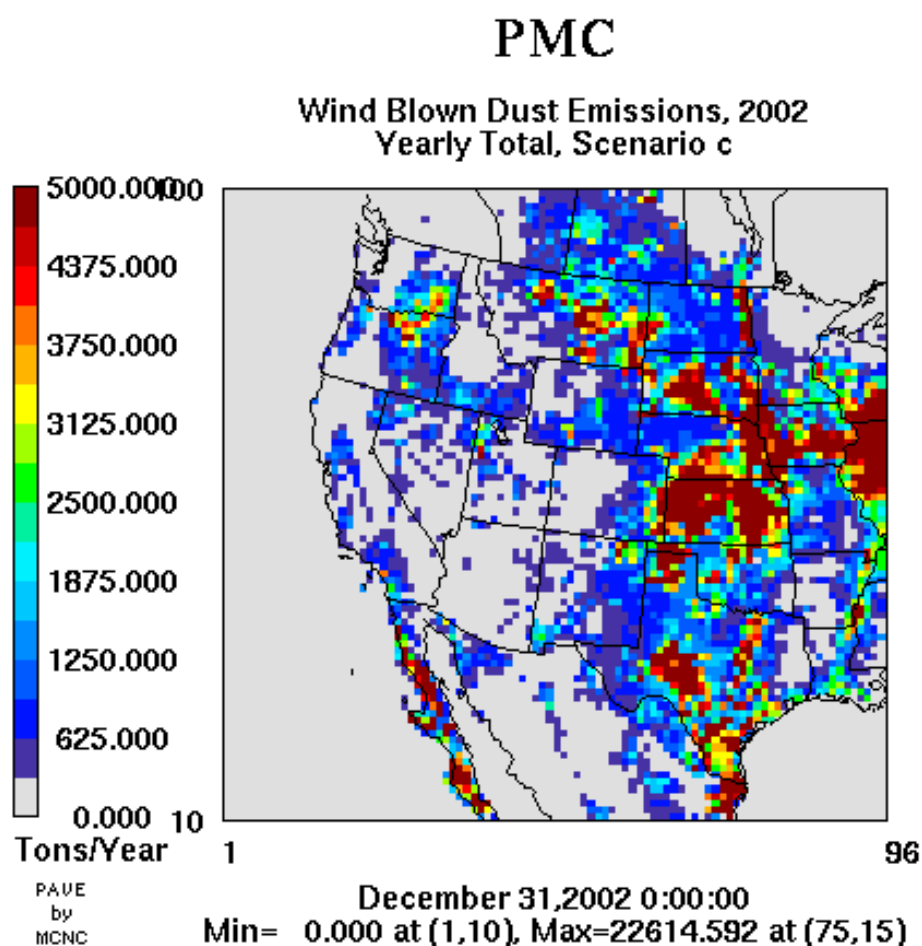


Figure 10-7. Spatial distribution of total 2002 annual PM_c dust emissions for Scenario c.

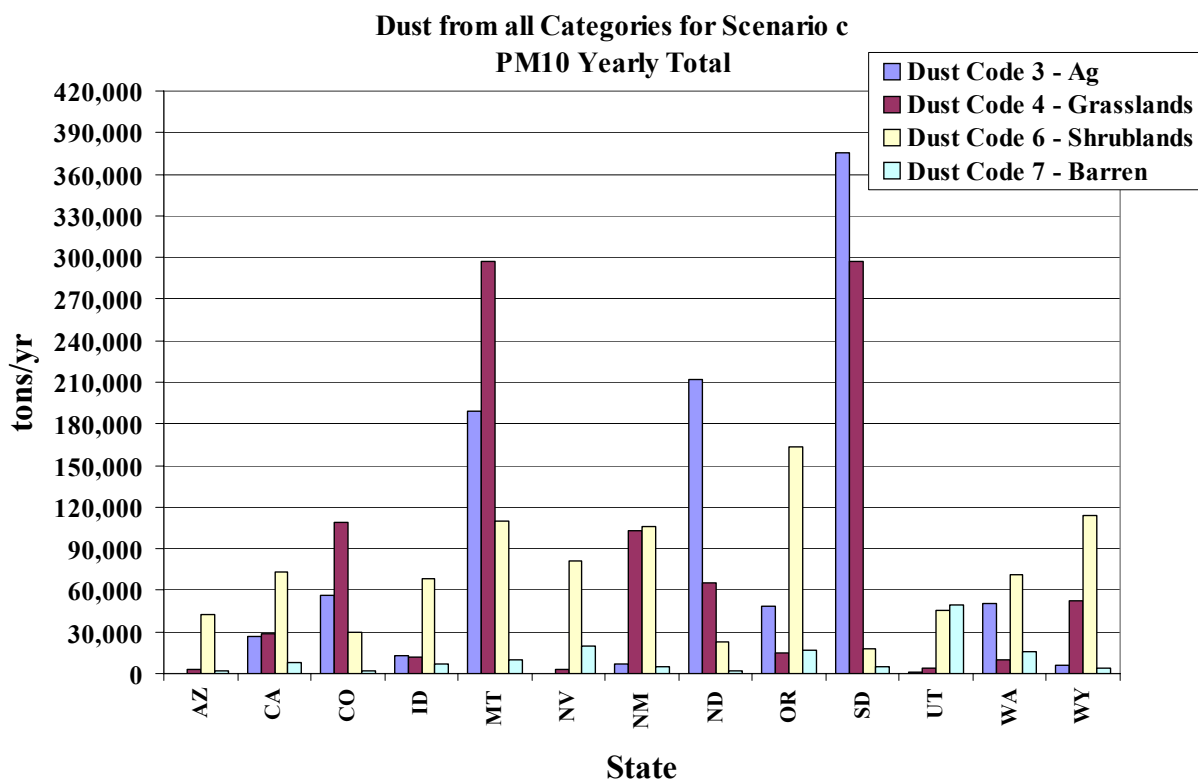


Figure 10-8. Distribution of total annual 2002 PM₁₀ dust emissions by land use type and state for Scenario c.

10.4.4 Scenario d

Scenario d made the same assumption as Scenario c concerning the disturbance of grassland, shrubland, and barren land. However, a 10-hour-per-day limit on dust event duration was imposed for all undisturbed soils, while no limit on the dust event duration was imposed for disturbed soils. This scenario differs from the previous scenario in that Scenario c has no limit on the event duration imposed for either disturbed or undisturbed soils. Figure 10-9 shows the spatial distribution of PM_c emissions. The distribution of predicted PM₁₀ dust emissions by land use type and WRAP state is displayed in Figure 10-10.

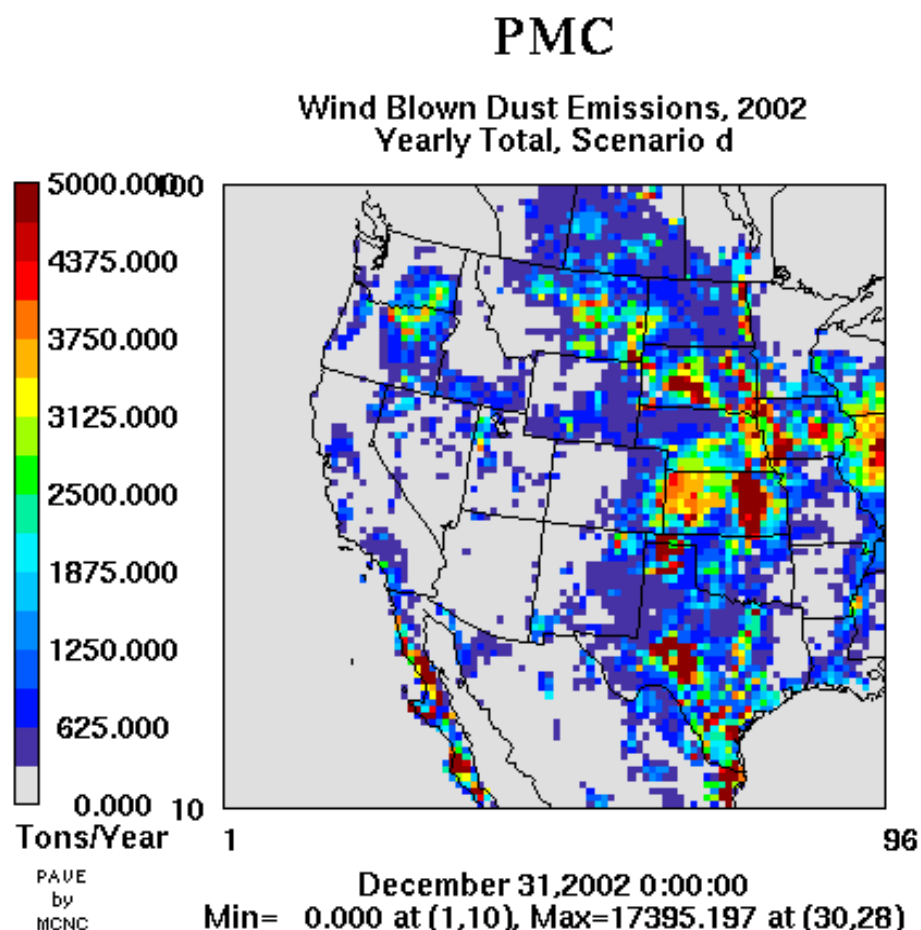


Figure 10-9. Spatial distribution of total 2002 annual PM_c dust emissions for Scenario d.

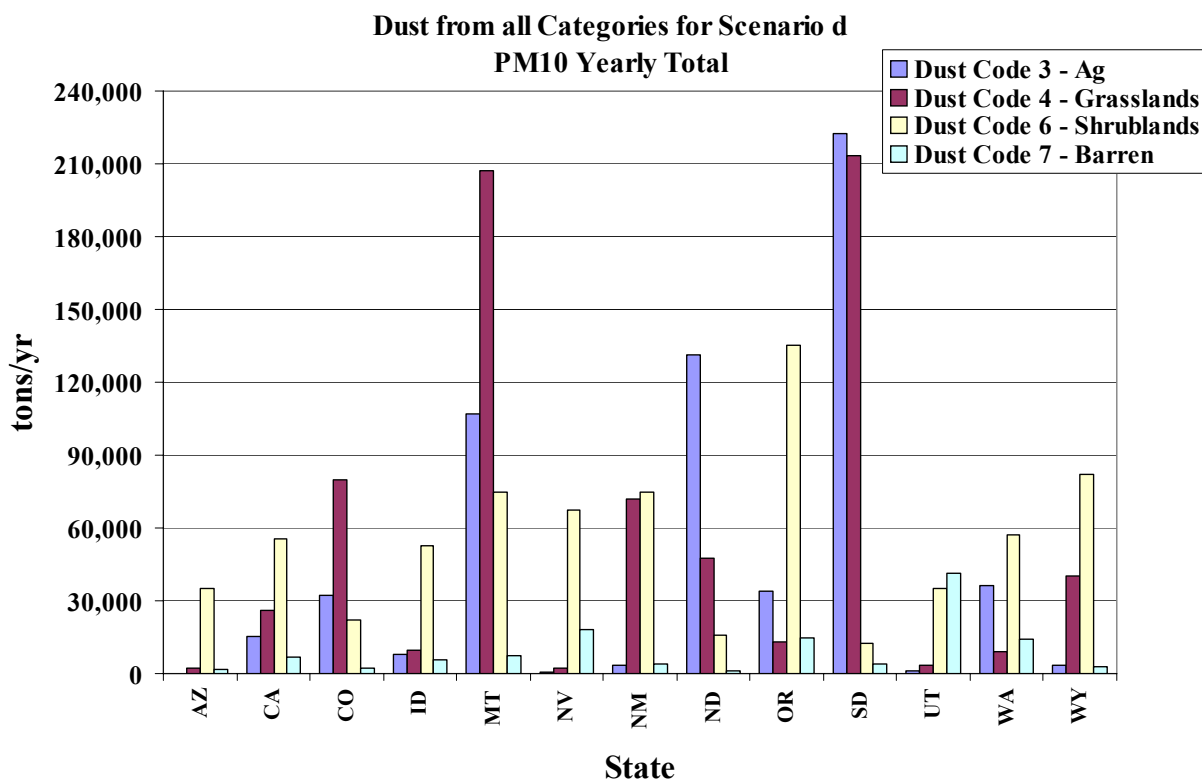


Figure 10-10. Distribution of total annual 2002 PM₁₀ dust emissions by land use type and state for Scenario d.

10.4.5 Summary of results and recommendations

The results of the four sensitivity simulations are compared below. Figure 10-11 is a state-by-state comparison of the total annual 2002 PM₁₀ dust emissions for the four scenarios. Also displayed in this figure are the total annual PM₁₀ dust emissions for 1996 estimated as part of Phase I of this task. Figure 10-12 shows the distribution by month of total PM₁₀ for the entire domain for the four scenarios. The emissions for Scenarios a and c (no limitation on dust event duration) are consistently higher than those from their counterparts, Scenarios b and d (dust event duration limited to 10 hours a day). This result is expected, since the lack of limitation on dust events causes higher emissions to be generated in regions where winds exceed the land-use-dependent threshold surface velocities for longer time periods. Also as expected, the cases with assumed disturbance of grassland, shrubland, and barren land (Scenarios c and d) show consistently higher emissions than those with no assumed soil disturbance (Scenarios a and b).

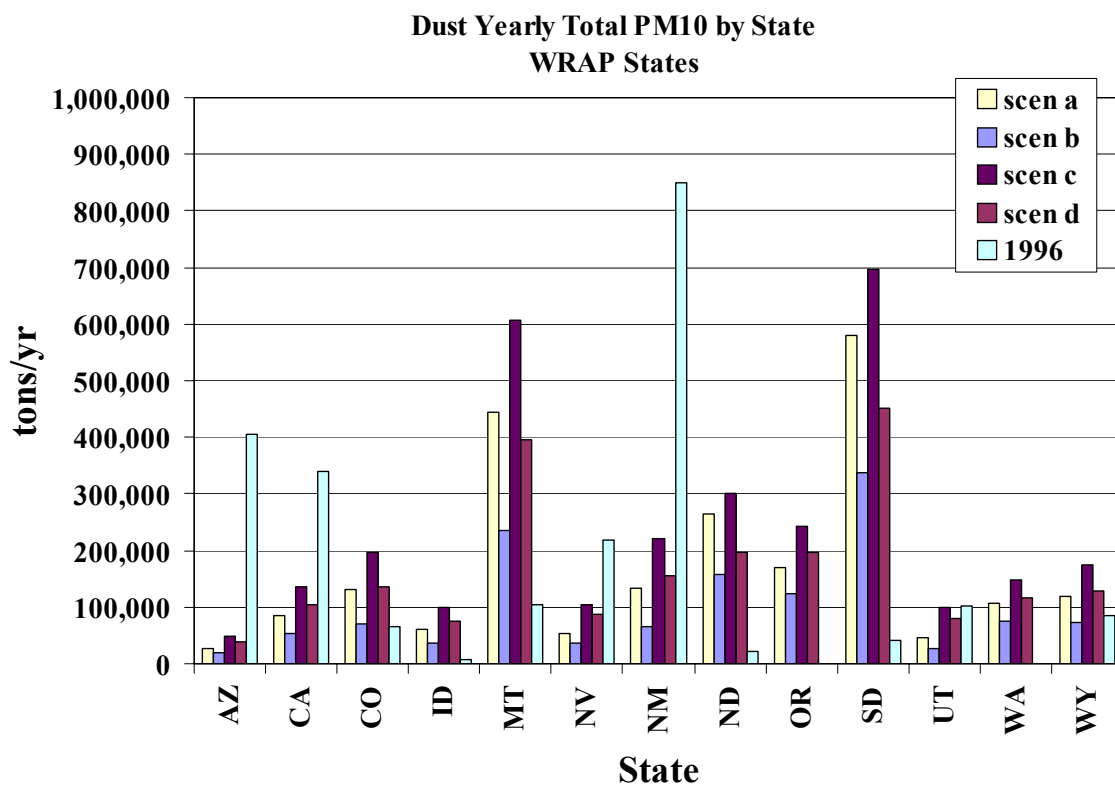


Figure 10-11. Distribution of total annual 2002 PM₁₀ dust emissions by scenario and state.

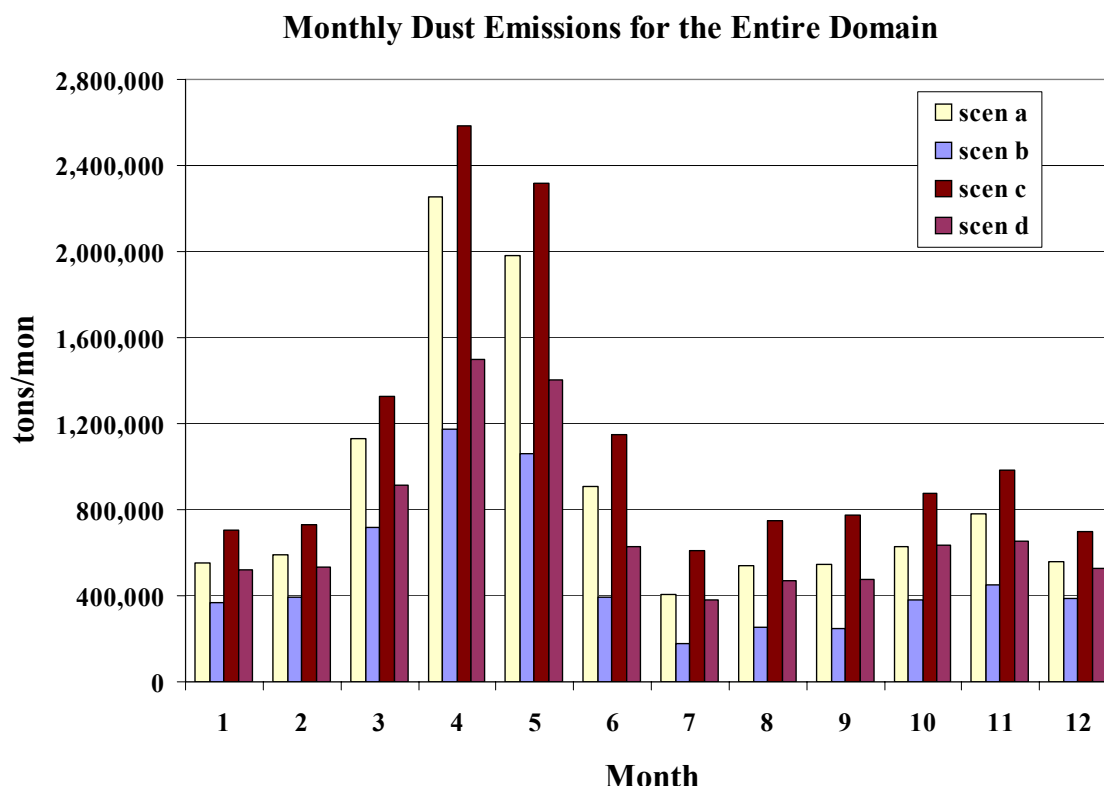


Figure 10-12. Monthly distribution of total 2002 PM₁₀ dust emissions for each scenario across the entire WRAP domain.

The seasonal variation of predicted dust emissions can also be discerned from Figure 10-12. The dust emissions tend to peak in the spring months due to generally higher winds throughout most of the domain. In addition, for agricultural areas this time period corresponds to the spring planting when the crop canopy is relative small or absent. A second, smaller peak occurs in the fall for similar reasons.

Figure 10-13 displays the percentage of dust by land use type across the WRAP domain for each scenario. In all cases, the dust emissions are dominated by those from agricultural lands. Shrubland and grassland make up the majority of the remaining dust emissions, while barren land contributes only a minor portion. Although barren lands have the lowest surface threshold velocity based on the assumed surface roughness length, there are only limited areas across the domain characterized as barren lands based on the NLCD used for the project. The impact of the various assumed disturbance levels of the soils and reservoir characteristics are reflected in the differences between the four pie charts and are seen to be consistent with expectations. For example, a comparison of Scenario a and Scenario c shows the expected increase in estimated dust emissions for the assumed disturbed lands. A comparison of Scenario b and Scenario d shows similar results.

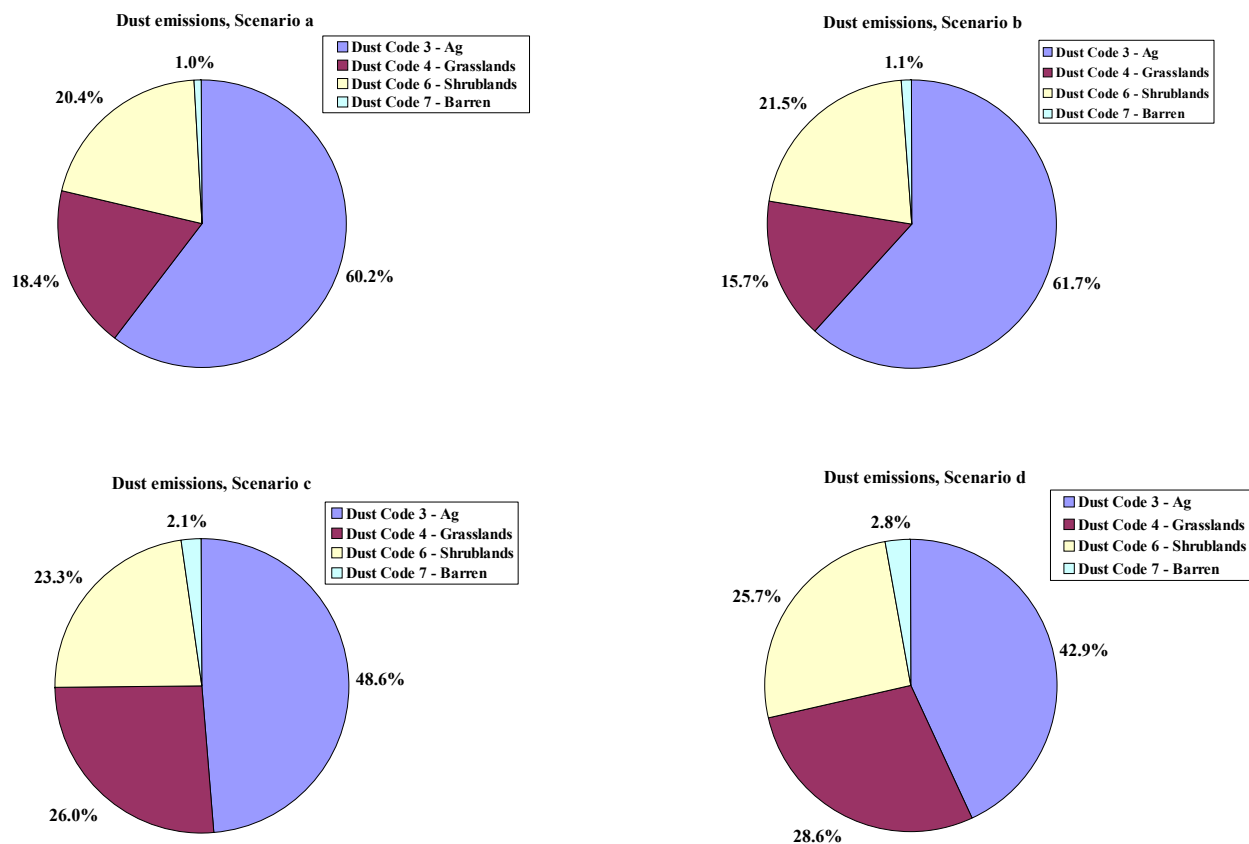


Figure 10-13. Distribution of total 2002 PM₁₀ dust emissions by land use type for each scenario for all WRAP states combined.

Based on review and comparison of the results of the sensitivity simulations, we recommend that the results of Scenario b be used for further evaluation and air quality modeling. Scenario b assumes that all soils are loose and undisturbed, and imposes a 10-hour-per-day limit on the duration of dust events. Given the limitations of the data used for this task, this scenario appears to be the most appropriate, for the following reasons:

- Dust Event Duration:** It is reasonable to expect that a limit on the dust event duration is related to the type and amount of soil available for erosion due to winds. Therefore, the assumed limit of 10 hours per day, although only an assumption, is more appropriate than imposing no limit at all on the dust reservoirs.
- Soil Disturbance:** Although clearly not all soils are undisturbed, there is no information available to assign disturbance levels to various areas throughout the region. Scenarios c and d assumed a 10% level of disturbance, but that was only for conducting sensitivity simulations. Clearly the percent disturbance will vary by region, soil type, and season. In addition, the threshold surface velocities for the disturbed soil cases are based on only very limited test results and are therefore not likely to apply regionwide.

Given the lack of supporting data for the dust reservoir and soil disturbance characteristics, we feel that the results of Scenario b would be more universally applicable on a regional scale for the WRAP's air quality modeling purposes.

The spatial distributions of modeled coarse PM dust from Scenario b are presented in Figures 10-14 (annual total)^{*} and 10-15 (seasonal totals).[†] The dust emissions are highest in agricultural areas in the central portion of the U.S. and in parts of the West that are dominated by shrub- and grassland. Echoing the results shown in Figure 10-12, the seasonal plots in Figure 10-15 indicate that the highest predicted dust emission occur during the spring, when winds are typically stronger throughout the region and agricultural crops have recently been planted. Lower overall dust emissions are predicted in the summer months, corresponding to the higher level of crop canopy cover and, in the Southwest, to increased periods of precipitation.

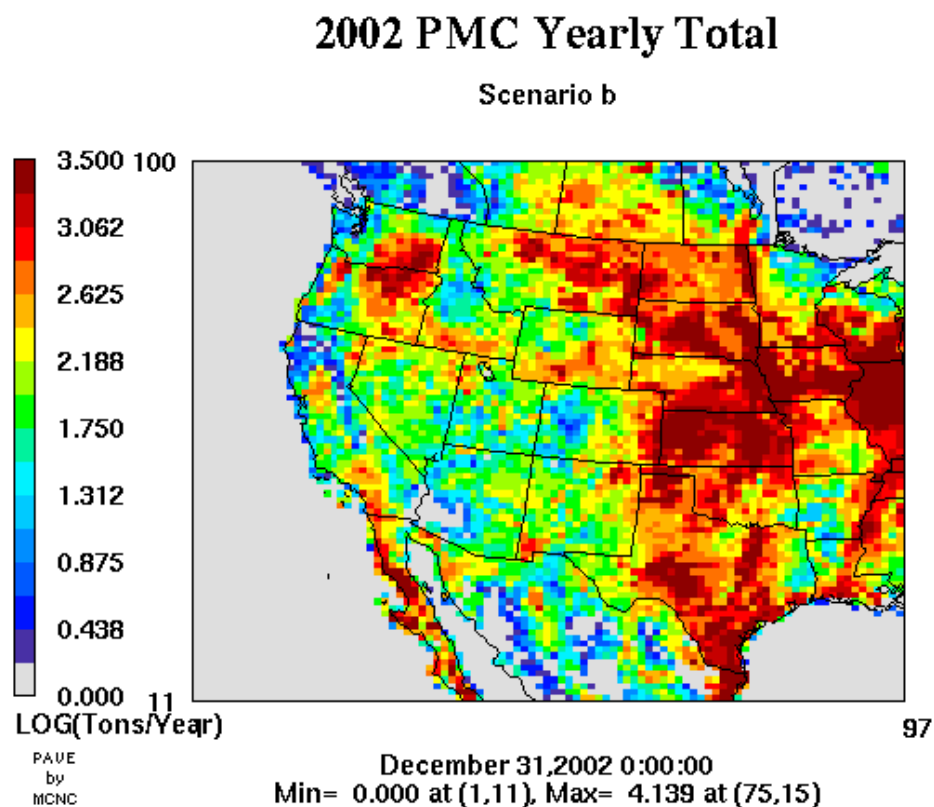


Figure 10-14. Spatial distribution of annual 2002 PMc dust emissions for Scenario b.

^{*} This figure looks different from Figure 10-5 because Figure 10-5 uses tons/yr while Figure 10-14 uses log(tons/yr).

[†] Note that these figures show only the western portion of the domain. Due to the lack of detailed agricultural information for states outside the WRAP and CENRAP regions, we could not apply the nonclimatic agricultural adjustments described above outside those two regions. Because the assumed surface roughness for agricultural lands is representative of a bare field, these areas have a greater potential for wind erosion. Therefore, since no agricultural adjustment could be applied to the eastern portion of the domain, results for that region are overestimated and are therefore neither realistic nor applicable. The displays were prepared for the western region only in order to highlight spatial details not apparent when the entire domain is displayed.

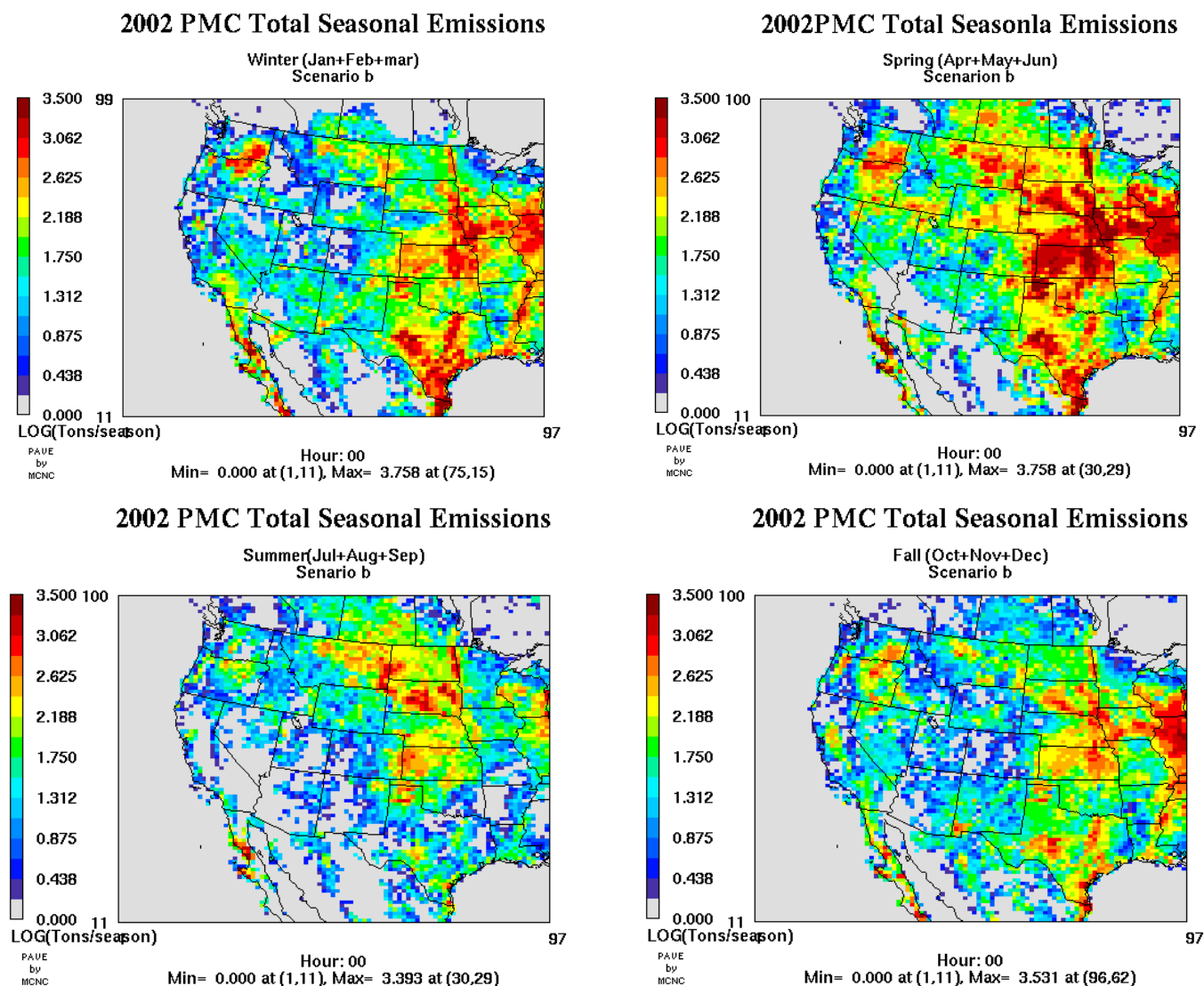


Figure 10-15. Spatial distribution of 2002 PMc dust emissions by season for Scenario b.

10.5 Model Performance Evaluation

As part of Phase II of this task, the RMC is to conduct a model performance evaluation of the revised windblown dust emission model. We have initiated this evaluation, but at this time only preliminary information has been collected and analyzed, so there are no results to discuss yet. The model performance evaluation has been delayed due to the need to rerun the windblown dust emissions model with the latest MM5 meteorological data for the WRAP 12-km modeling domain. These results will be fully documented in this task's Phase II final report, to be completed in early March 2005. In this section we summarize the model performance evaluation approach and procedures.

The 2002 windblown dust emissions model will be evaluated several ways for the reasonableness and accuracy of its output. One of the challenges in this evaluation is that measurements generally do not distinguish between windblown dust and other forms of dust (e.g., from paved and unpaved roads). Moreover, measurements of coarse mass, which is typically assumed to be dust, can contain other nondust compounds (e.g., sulfate and nitrate compounds).

The IMPROVE monitoring network measures a fine soil species and a CM species that are generally assumed to be due to dust emissions. The fine soil species consists of mineral elements, so in the absence of interference by fires it is probably a fairly good estimate of the fine dust contribution. The CM measurement, on the other hand, is the difference between the PM_{10} and $PM_{2.5}$ mass measurements, so it can contain compounds other than dust.

WRAP is performing a study titled “Assessment of the Major Causes of Dust-Resultant Haze in the WRAP” (Etyemezian et al., 2004) that will characterize dust events at IMPROVE monitors for 2001-2003. This study is using visibility extinction due to fine soil (FS) and CM to define extinction due to dust:

$$B_{\text{dust}} = [\text{FS}] + 0.6 [\text{CM}]$$

Dust events at the WRAP IMPROVE monitors are being characterized as follows:

- Transcontinental events
- Regional windblown dust events
- Wildfire-related events
- Local windblown dust
- Other events
- Unknown source

This analysis will be very valuable as we evaluate the windblown and other dust emissions. However, results from this study are not yet available.

We initially intended to conduct the model performance evaluation in three parts: (1) an initial comparison of modeled dust emissions with measured dust at IMPROVE monitors; (2) an evaluation of the CMAQ model results with and without the windblown dust emissions; and (3) a refined evaluation using the results of the Causes of Dust project. However, due to the delays in the Causes of Dust project and the desire to complete the windblown dust emissions inventory in a reasonable time frame, the enhanced model performance evaluation was dropped from the scope of work for this task. The remaining two parts of the model performance evaluation are described in Sections 10.5.1 and 10.5.2.

10.5.1 Evaluation, Part 1: Comparisons of windblown dust emissions with the occurrence of enhanced “dust” at IMPROVE monitors

For each 24-hour IMPROVE sample during 2002, we will match the IMPROVE dust extinction (B_{dust}) with modeled windblown dust emissions for the concurrent day in the nine (3 x 3) and 25

(5 x 5) grid cells centered on the IMPROVE monitor. Statistics will be generated to identify the occurrence of four different situations:

1. near-zero B_{dust} and zero modeled windblown dust (nonoccurrence of both measured and modeled dust);
2. near-zero B_{dust} and enhanced (i.e., exceeding background levels) modeled windblown dust (no measured dust, but modeled windblown dust in vicinity of monitor);
3. enhanced B_{dust} and no windblown dust (occurrence of measured dust, but no modeled windblown dust); and
4. enhanced B_{dust} and modeled windblown dust emissions (occurrence of both enhanced measured and enhanced modeled dust).

These classifications allow a qualitative evaluation of the windblown dust emissions. It is expected that type 1 would occur most frequently, especially at more northerly sites and during the winter months, and there should be a lot of agreement between the modeled values and the measurements. Type 2 does not necessarily indicate a problem with the windblown dust model, as the dust cloud may be real but may not have impacted the monitor. Likewise, the elevated B_{dust} in type 3 may be due to sources other than windblown dust, so type 3 also does not necessarily indicate a problem. Type 4 may provide the most information, especially if a positive correlation can be established between windblown dust emissions and B_{dust} . If the above analysis provides useful information, it would be repeated for the fine and coarse components of the measured (FS and CM) dust and modeled windblown dust emissions.

10.5.2 Evaluation, Part 2: Enhancements to CMAQ to separately track dust

CMAQ currently tracks all fine PM that is not SO_4 , NO_3 , EC, or OC as a single species (A25). Similarly, all coarse PM is typically tracked as one species (ACORS).^{*} We will modify CMAQ by adding two additional fine and coarse PM species, one set to track fine and coarse windblown dust emissions and the other set to track fine and coarse “other dust” emissions. This will allow the separate accounting of CMAQ’s fine and coarse PM species into windblown dust, other dust, and other primary fine and coarse PM emissions species.

We will run the modified CMAQ and compare the model estimates against the IMPROVE measures for fine soil and CM. The evaluation will be performed for dust (windblown and other) species alone and with and without windblown dust to determine whether adding the windblown dust emissions improves model performance. The performance of CMAQ using all other fine and coarse emissions would also be evaluated, as has been done in the past.

10.6 Summary

This section summarizes the major findings so far of Phase II of the windblown dust model task. It also lists recommendations with regard to improvements in data quality, and suggests enhancements and refinements of the estimation methodology. As noted at the beginning of

^{*}Note that there are other coarse species for sea salt and soil, but they are not typically used.

Section 10.4, we are currently revising the windblown dust emissions estimates due to a minor error that occurred in processing the wind fields used in the estimation methodology. However, the general qualitative discussion of the results presented here is not expected to change significantly. The revised emission estimates will be presented in the draft final task report. Several of the recommendations provided below also will be addressed in that report.

10.6.1 Results

Based on a review of recent studies concerning dust emission from wind erosion, we developed a general Phase II estimation methodology for PM dust emissions from wind erosion. Emission rates were developed by soil type and stability class. Land use/land cover data were based on the NLCD database and used to determine the surface roughness lengths necessary for estimating threshold surface friction velocities. Wind speed, precipitation rates, and soil temperatures were based on MM5 model simulation results at a spatial resolution of 36 km. Although the overall estimation methodology was updated and improved upon from the Phase I methodology, a number of assumptions were still required to implement the methodology, primarily related to limitations in the input data used in the model (see Section 10.3).

We implemented the Phase II estimation methodology for calendar year 2002 on the RPO Unified domain. A number of sensitivity simulations were performed to investigate the effects of the various assumptions regarding dust reservoir characteristics and the disturbance levels of the soils across the domain. The results were presented and discussed in Section 10.4. Qualitatively, the results appear to be consistent with what would be expected based on the various assumptions made.

A more detailed analysis of the model results and a comparison with ambient data are currently underway and will be documented in the task final report.

10.6.2 Recommendations

As the results of the task are still under review and a more detailed model performance evaluation is underway, it is too early to present a full set of recommendations. However, based on a preliminary assessment of the results from the Phase II fugitive windblown emission estimation methodology, we can make the following initial set of recommendations:

- An attempt should be made to identify more detailed data on land use types and soil characteristics for the regional domain.
- The lack of information needed to apply agricultural adjustments to the eastern U.S. should be addressed.
- The dust model should be rerun using the latest 36-km annual MM5 modeling results from Task 2.
- The model should be applied using the 12-km-resolution MM5 meteorology data when they become available from Task 2.

- To validate the methodology, the model should be applied to a smaller local domain for which detailed data are available.
- The transport fractions developed by the EPA should be applied. This should be implemented from within the dust model to make use of the higher resolution of the land use data, as opposed to application at the county level.

10.7 Status of Task 9 Deliverables

Table 10-6 below gives the status of each Task 9 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 10-6. Status of the Task 9 deliverables.

Deliverable	Status
Draft final task report	Expected completion in early March 2005.
Final task report	To be completed after receiving comments on draft final task report.
Updated model results	To be included in the draft final task report.

11. Task 10: Continued Improvement to Model Evaluation Software

11.1 Work Performed from March 2004 through February 2005

During this project year, the RMC continued to use and improve the UCR model performance evaluation (MPE) software that was developed earlier in the project and that has been supported primarily by WRAP. We note that funding from VISTAS was also used to improve the MPE software during 2003; in return, VISTAS realized substantial benefits from applying the MPE software. This example represents one of many benefits of this project to multiple RPOs.

Only minor changes in the MPE software were planned for 2004. The original work plan included tasks to process Photochemical Assessment Monitoring Station (PAMS) and PM Supersite data, and to develop software for creating contour plots of error and bias. In consultation with the WRAP Air Quality Modeling Forum, however, it was agreed that these were low priority tasks, so instead those resources were reallocated for the acquisition of additional disk storage that was needed for the project. Because there is relatively minimal benefit in evaluating the small amount of PAMS (primarily located in urban areas) and Supersite data for the WRAP region, we do not recommend continuing those tasks in the 2005 work plan.

We continued to revise and improve the MPE software during 2004. For a snapshot of the MPE software as of January 2005, please refer to Appendix F, which is MPE draft documentation titled “User’s Guide, Air Quality Model Evaluation Software, Version 2.0.1.” Because model performance guidance does not yet exist for visibility modeling, we continue to explore new evaluation methods, and sometimes discover improved methods for presenting model results that necessitate changes in the MPE software. In particular, during 2004 we experimented with various types of plots for summarizing and effectively presenting the results of the model-to-ambient-data comparisons, including soccer plots and bugle plots. Beginning in January 2005 we also adapted a Microsoft Access Database program originally developed by Air Resource Specialists (Cassie Archuleta, Air Resource Specialists, Inc., personal communication) to produce stacked-bar time-series plots.

While there is not yet official EPA guidance on which model performance metrics or which type of evaluation products should be used, we have found that the stacked-bar time-series plots and the bugle plots are most effective for conveying both qualitative and quantitative information about model performance. Although we continue to compute a wide variety of model performance metrics, we typically use mean fractional bias (MFB) and mean fractional error (MFE) when presenting evaluation results because these metrics provide the most balanced and symmetrical approach for characterizing model underpredictions and overpredictions.

Figures 11-1 through 11-4 present examples of the newer model evaluation products. We present these to illustrate the types of model evaluation results that can be produced using the MPE.

An advantage of our traditional MPE products (i.e., time-series plots and scatterplots) was that they were produced automatically by the MPE software with minimal staff time. The new evaluation products (soccer plots, bugle plots, stacked-bar time-series plots) have been very resource intensive to produce because we have prepared them “manually” by importing error and bias metrics into Excel spreadsheets or Access and then preparing the plots. Therefore, we spent additional effort in 2004 to begin automating development of the stacked-bar time-series plots.

We plan to release a public version of the MPE software after completing revisions to the MPE user’s guide given in Appendix F. This documentation will also be posted to the RMC web site.

During this project year, we also invested substantial effort in attempting to identify updated site information for IMPROVE sites that can be used in the MPE software. There are at least three different versions of site classifications that are referenced in policy guidance from EPA, so we made an effort to determine the most correct list of IMPROVE sites for use in the MPE software. We have implemented additional sets of site lists into the routine model evaluation. These include some sites that are in Class I areas but for which there are no monitoring data. These sites can be used for evaluating the results of different model sensitivity experiments and emissions reductions or for producing source attribution products. However, these sites cannot be used in model performance evaluations for which ambient monitoring data are required.

11.2 Status of Task 10 Deliverables

Table 11-1 gives the status of each Task 10 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 11-1. Status of the Task 10 deliverables.

Deliverable	Status
Visualization tools for source attribution	Completed in March 2004, with periodic updates afterward. Source code available to WRAP members on request.
GUI for using model evaluation tools and visualization tools	We developed GUI tools for using the model performance evaluation software, as described in the MPE documentation. However, we believe that the script version of the MPE software is easier to use and maintain, and we recommended continuing with only a script version of the software. Therefore, per agreement with the WRAP Air Quality Modeling Forum, we agreed to drop this deliverable to focus resources in other areas.
Revised version of MPE package	Periodic updates were made throughout the project year. List of sites used in evaluation in October 2004 was revised to accommodate vague EPA guidance on identification of site definitions. Source code is available to WRAP members on request. We plan to release a public, open-source version for wider distribution when the MPE documentation is completed in March 2005.
Documentation of model software	To be completed in March 2005.

12. Task 11: Sensitivity Studies Designed to Evaluate Uncertainties in Fire Emissions

With the Fire Emissions Joint Forum and Air Sciences Inc., the RMC developed several emission scenario combinations to study the effect of fires on air quality in general, and on visibility in particular. Some of these scenarios include 2018 emissions and fires; others include 2002 emissions and fires. In general, we compared CMAQ results created using emissions with no fires in the WRAP domain against CMAQ results created after adding either one type of fire or all types of fires to the emissions. Development of fire emissions data was completed by Air Sciences Inc. under contract from WRAP. Processing of fire emissions is described in Section 3 of this report. Figure 12-1a, discussed in more detail in Section 3.1, shows the locations and magnitudes of total fire emissions for July 2002.

Sections 12.1 through 12.6 describe the results of the fire sensitivity modeling scenarios. We have completed emissions processing and CMAQ simulations and analysis for all of the fire sensitivity model simulations that were included in the revised 2004 work plan. The primary analysis products include the following:

- Monthly-average spatial visibility plots using both deciview (dV, or dcV) and the extinction coefficient (B_{ext}) and concentrations of selected PM species and ozone. These include plots showing spatial distributions of concentration for a model base case simulation, and difference plots that show the spatial change in concentration for a sensitivity scenario compared to the base case simulation. The base case spatial plots are included in the analysis and evaluation of the Pre02b, Pre02c and Pre02d base case simulations at the RMC web page <http://pah.cert.ucr.edu/aqm/308/cmaq.shtml>. Therefore, our analysis here focuses on the difference plots for the fire sensitivity simulations. Key results are discussed below; for complete results, see <http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#fire>.
- Stacked-bar time-series plots showing the summed contribution to B_{ext} at each selected sites. Example plots are shown in Figure 12-2, for the anthropogenic and natural fire emissions at the Grand Canyon IMPROVE site. At sites for which monitoring data are available, these time-series plots can also be compared to a stacked-bar time-series plot of the ambient monitoring data. Alternatively, model-versus-model results can be compared at sites for which ambient data are not available. Stacked bar plots for the Pre02d base case are available at <http://pah.cert.ucr.edu/aqm/308/cmaq.shtml>, so here we focus on the stacked-bar difference plots comparing the fire sensitivity runs to a base case run. Note that in some instances we may compare the differences between two different fire sensitivity cases rather than a sensitivity case and base case. These plots have been used primarily as a qualitative approach for assessing source attribution to fire emissions.

Table 12-1 lists the new model simulations completed, including a short name used to identify each modeled fire sensitivity case. Each of the sensitivity scenarios is also summarized below. In addition to these new model simulations, we also completed further analysis for some fire

model simulations carried out using the 1996 and 2018 scenarios that were developed during the Section 309 modeling effort.

Table 12-1. Summary of new air quality model simulations used to evaluate effects of fire emissions.

Model Case	Motivation	Case ID
Base case (no fire)	Base case to compare with modeled fire sensitivity simulations	Pre02b
Base + ag vertical sens (Scenario 4)	Evaluate model sensitivity to uncertainty in plume rise of emissions from agricultural burning.	Pre02b_agmod
Base + wildfires	Evaluate effect of all wildfires on model-simulated visibility	Pre02b_wf02
Base + “natural” fires (Scenario 5a)	Evaluate effect of natural fires on model-simulated visibility (includes all wildfires and some prescribed burning).	Pre02e
Base + ag burning	Evaluate effect of agricultural burning emissions on model-simulated visibility	Pre02b_ag18
Base + Rx burning	Evaluate effect of prescribed burning on model-simulated visibility	Pre02b_rx02
Base + all fire emis (Scenario 1a)	Reference case with all fires to compare with Pre02b (base case) and with other fire sensitivity cases.	Pre02c
Base + anthro + natural fires	Uses new fire emissions classes. The total of the anthro plus natural fire emissions is identical to the total Pre02c fire emissions in scenario 1a.	Pre02f

12.1 Scenario 1(a)

This scenario was designed to investigate the combined effects of all fire types on air quality. It compares the 2002 CMAQ results that were based on the preliminary Pre02b base case emissions scenario against the 2002 CMAQ results that were based on emissions scenario Pre02c, which includes Pre02b emissions plus the **combined** emissions of three fire types:

- (1) 2002 wildfires (wf02)
- (2) 2018 typical agricultural fires (agbase.073102, also referred to below as ag18)
- (3) 2002 prescribed fires (rx02)

The fire emissions are described in 5.2.10. A detailed description of the other (i.e., nonfire) emissions sources used in these model simulations is also available at http://www.cert.ucr.edu/rmc/2002/emissions/WRAP_2004_Emissions_Workplan_v1-2.xls.

Figure 12-1 shows results of this analysis averaged for the month of July. The July average is shown here as illustrative of the relation between emissions and visibility impact because it is one of the months with large total fire emissions, and total fire emissions of carbon monoxide (CO), shown in Figure 12-1a, are used here as an indicator of fire size and location. Plots of emissions of other gas and particulate species, which are included on the RMC web site, have the same relative intensity and distribution as the CO emissions. Figure 12-1b shows the effect of combined wild fire, ag burning, and prescribed burning fire emissions on visibility (in deciviews) calculated as the July average. We note that the Pre02f case (Figure 12-1b), which combines natural and anthropogenic fire emissions, is identical to the Pre02d case, which combines wild fire, ag burning, and prescribed burning emissions. Figure 12-1 shows that fire emissions have large effects on visibility throughout the western states. The peak impact of 20.6 dV is in western Colorado; also, large regions show visibility changes greater than 4 dV.

Figures 12-3 and 12-4 show the monthly average effects on visibility as deciviews for all 12 months. The effects of the wildfire emissions in June through August are by far the largest contribution to fire emissions, with the highest modeled deciview values occurring August.

12.2 Scenario 1(b)

This scenario was created to investigate the effect of each **individual** fire type on air quality. It is made up of three subscenarios that compare the CMAQ scenario with no fires (Pre02b) with a CMAQ sensitivity run that includes the Pre02b emissions plus one type of fire:

1. *Scenario Pre02b_wf02*: Pre02b vs. Pre02b + wf02 (wild fires for 2002, as identified by SCC in the SMOKE point file). SMOKE was run to merge Pre02b and wf02 emissions to create the emissions input for CMAQ.
2. *Scenario Pre02b_ag18*: Pre02b vs. Pre02b + agbase.073102. SMOKE was run to merge Pre02b and ag18 emissions to create emissions input to CMAQ.
3. *Scenario Pre02b_rx02*: Pre02b vs. Pre02b + rx02 (prescribed fires for 2002, as identified by SCC in the SMOKE PT file). SMOKE was run to merge Pre02b and rx02 emissions to create emissions input to CMAQ.

Figure 12-5 shows the results of each of these three scenarios as spatial plots in PAVE for the month of July, for which the monthly average was calculated from the model simulation results over all hours in the month. Note that the left panels show CO emissions for each fire category, but that the color scale varies across the three plots, and that wildfire emissions are an order of magnitude larger than emissions from prescribed and agricultural burning. The visibility effects of wildfire emissions in Figure 12-5b are very similar to the effects of the combined fire emissions in Figure 12-1b.

12.3 Scenario 2

This scenario compares CMAQ results based on using the 2018 “All control” Base Smoke Management scenario (Allcntl_bsm) with those using the 2018 “All control” Optimal Smoke

Management scenario (Allentl_ism), where base and optimal smoke management have been defined by the Fire Emissions Joint Forum. The Allentl_bsm emissions include 2018 emissions with controls applied to some point sources and to all three base 2018 typical fire emissions. The Allentl_ism emissions include 2018 emissions with controls applied to some point sources and fire emissions reductions derived from the optimal smoke management strategy for 2018 typical agricultural and prescribed fire emissions, and to the wildfires. No new SMOKE or CMAQ runs were required for this scenario because we used model simulation results that we developed in the §309 modeling effort.

Figures 12-6(a-d) show the seasonal differences in CO emissions as a result of changing from the base smoke management (BSM) scenario to the optimal smoke management (OSM) scenario; blue colors indicate reductions in emissions. As expected, the OSM scenario produced only reduced emissions with no increases relative to BSM. The highest reduction was during the spring and the lowest reductions were during the winter. Figures 12-6(a-d) and 12-7(a-d) show the seasonal change in visibility (in deciviews) for OSM compared to BSM. The pattern of temporal (seasonal) and spatial changes in visibility is similar to changes in emissions. The changes in B_{ext} were as low as -15.69 1/Mm (plots for B_{ext} are not shown here but their spatial pattern is identical to that of the deciview plots); in deciviews they were as low as -1.0 deciview.

Figures 12-8 and 12-9 show the monthly average changes in visibility, as monthly average deciviews, for the OSM case compared to the BSM case. The monthly average results are consistent with the seasonal results; the greatest absolute improvement in visibility occurs in September, with a reduction extinction coefficient of 29.7 1/Mm improvement in visibility (plots of extinction coefficient are not shown here but are included in the September 2004 FEJF meeting presentation (see the PowerPoint file at <http://pah.cert.ucr.edu/aqm/308/meetings.shtml>). In terms of deciviews, the largest improvements were in the spring and fall months, both in magnitude and in spatial extent of the improvement, with the greatest improvement being a 2.3-dV improvement in June. There were small improvements in visibility in the summer and winter months.

12.4 Scenario 3

This scenario will compare CMAQ results using emissions simulation Pre02c with those using a modified Pre02c in which the prescribed fires and wildfires will be replaced with new inputs in which some of the smaller fires will be zeroed out. This activity has been deferred until the FEJF develops these data.

12.5 Scenario 4

This scenario, named Pre02b_agmod, was designed to investigate the effect of a vertical redistribution of fire emissions by removing 50% of the agricultural burning emissions from the model's surface layer and redistributing an equal mass of emissions to higher layers in the model. The total agricultural fire emissions in each grid cell for the Pre02b_agmod scenario were the same as those in Scenario Pre02b_ag18 (see Section 12.2). New PTHOUR files were created in which the emission fractions in the first layer (L1FRAC) were reduced by the ratio 38/80. The rest of the

first-layer emissions (42/80) were placed in the higher layers. SMOKE and CMAQ runs were required to complete this scenario. Results are available on the RMC web site (see <http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#fire>) and in PowerPoint files (see the files from the FEJF meetings at <http://pah.cert.ucr.edu/aqm/308/meetings.shtml>). The results are not shown here because the change in vertical distribution had essentially no effect on visibility.

There are two probable reasons why this sensitivity did not show an effect on visibility. First, the agricultural burning emissions were small compared to wildfire emissions, so changes in the agricultural burning vertical profile should logically have only a small relative effect on visibility (Figure 12-5f). Second, the agricultural burning emissions are generally small fires for which the plume rise does not exceed the height of the planetary boundary layer (PBL). Because the PBL is well mixed during the daytime when most agricultural burning emissions occur, these emissions tend to be well mixed in the PBL regardless of which layer they are injected within the model.

However, we would expect a different result for large wildfires for which the plume rise height may extend into the free troposphere, and which also have much larger emissions than agricultural burning, and therefore a larger effect on visibility in general. Additional sensitivity simulations should still be performed to evaluate the effects of plume rise height for large fires.

12.6 Scenario 5

To evaluate the effects of natural versus anthropogenic fire emissions, we created two new emission scenarios using new fire emissions datasets provided by Air Sciences.

1. *Scenario Pre02e*: Includes Pre02b base emissions and the new natural fire emissions files only (i.e., no new anthropogenic fire emissions), using fire emissions received from Air Sciences on September 10, 2004.
2. *Scenario Pre02f*: Includes Pre02b base emissions, the new natural fire emissions, the new anthropogenic fire emissions, and the old agricultural burning emissions.

The following comparisons using these datasets were performed:

- Compare Pre02e to Pre02b to assess source attribution for natural fire emissions.
- Compare Pre02f to Pre02e to assess source attribution for anthropogenic fire emissions.
- Compare Pre02f to Pre02b to assess source attribution for total fire emissions.
- Compare Pre02f to Pre02c to evaluate the effects of the new fire emissions inventory compared to the older fire emissions data used in earlier 2002 modeling.

Complete results are given on the RMC web site (see <http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#fire>); here, we present summary results. Figure 12-10a shows the July total natural fire emissions of CO. Comparing this with Figure 12-1a, it is apparent that the natural fire emissions are almost identical to the wildfire emissions. Natural fire emissions were defined by the FEJF to include all wildfire emissions and a portion of the prescribed burning emissions, while anthropogenic emissions were defined to include all agricultural burning and the remaining portion of the prescribed burning. Because the wildfire emissions are

much larger than the other two categories, the effects of natural fire emissions on visibility, as shown in Figure 12-10b, were nearly identical to the effects of the wildfire emissions. Moreover, the effects of the anthropogenic emissions on visibility (Figure 12-10c) were small, with peak increases of 1.2 dV in Oregon and increases of less than 0.5 dV in all other regions. Finally, comparing Figure 12-10b to Figure 12-10d shows that the effects of the natural fire emissions were nearly identical to the combined natural and anthropogenic fire emissions in Figure 12-10d.

In retrospect, it is not surprising that the anthropogenic emissions had a relatively small effect on visibility, given the small magnitude of anthropogenic agricultural burning compare to total fire emissions. However, anthropogenic fire emissions might show larger effects in model simulations with finer grid resolutions. For example, results shown here were from model simulations on a 36-km grid. It is possible that on a 4-km grid the emissions intensity could be as much as 81 times greater than the 36-km grid because each 36-km grid cell contains 9x9 of the 4-km grid cells. Thus, it is possible that anthropogenic fire emissions might have more significant effects on visibility in model simulations using higher grid resolutions. This would be a special concern for emissions located in or near a Class I area. Thus, the significance of anthropogenic emissions should not be discounted based on these results, and additional studies should be performed at finer grid resolutions.

12.7 Status of Task 11 Deliverables

Table 12-1 gives the status of each Task 11 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 12-2. Status of the Task 11 deliverables.

Deliverable	Status
Report on analysis of existing results	Results were presented at the Fire Emissions Joint Forum meeting in Idaho on Sept 9, 2004. PowerPoint files are available on the RMC web site: Preliminary Fire Emissions Sensitivity Results in CMAQ
Report results of additional model runs.	Deliverables include the PowerPoint presentations given at the Fire Emissions Joint Forum Meetings, available at http://pah.cert.ucr.edu/aqm/308/meetings.shtml. FEJF Meeting in Las Vegas, NV, December 8, 2004: • Additional Fire Emissions Sensitivity Results in CMAQ • Example Stacked Bar Time-Series Plot FEJF Meeting in Idaho, Sept 9, 2004: • Preliminary Fire Emissions Sensitivity Results in CMAQ Additional results are available on the RMC web site at http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#fire. Results of analyzing the air quality model simulations are available on the RMC web site for the following comparisons: Monthly average spatial difference plots to examine source attribution fire emissions: • Pre02f (natural+anthropogenic fire) vs. Pre02e (natural fire only) • Pre02f (natural+anthropogenic fire) vs. Pre02b (no fire) • Pre02f (natural+anthropogenic fire) vs. Pre02c (old fire) • Pre02e (natural fire) vs. Pre02b (no fire) Daily difference stacked-bar plots for extinction contribution: • Pre02f (natural+anthropogenic fire) vs. Pre02e (natural fire only) • Pre02f (natural+anthropogenic fire) vs. Pre02b (no fire) • Pre02e (natural fire) vs. Pre02b (no fire) Monthly average spatial difference plots for the three fire categories individually compared to no fire emissions: • Pre02b_wf02 (Wild Fires) vs. Pre02b (no fire) • Pre02b_rx02 (Prescribed burning) vs. Pre02b (no fire) • Pre02b_ag18 (Ag Burning) vs. Pre02b (no fire) Sensitivity of model to changes in vertical distribution of ag burning emissions, with half of surface layer emissions redistributed to upper layers in the model: • Pre02b_agmod (Redistributed vertical Ag Burning) vs. Pre02b_ag18 (original Ag Burning)

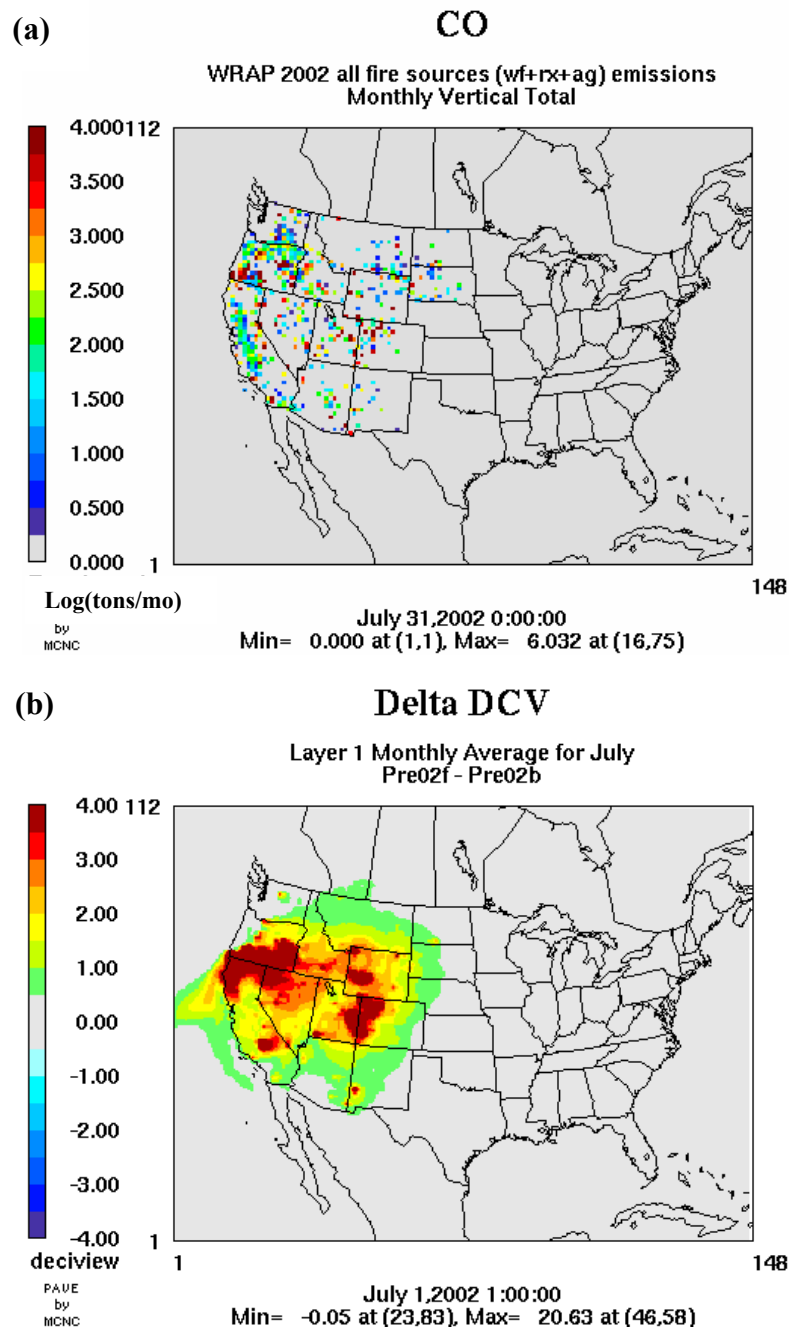


Figure 12-1. (a) The July total fire emissions of carbon monoxide, used as an indicator of fire size and location; (b) the effect of combined wild fire, agricultural burning, and prescribed burning fire emissions on visibility, calculated as the July average.

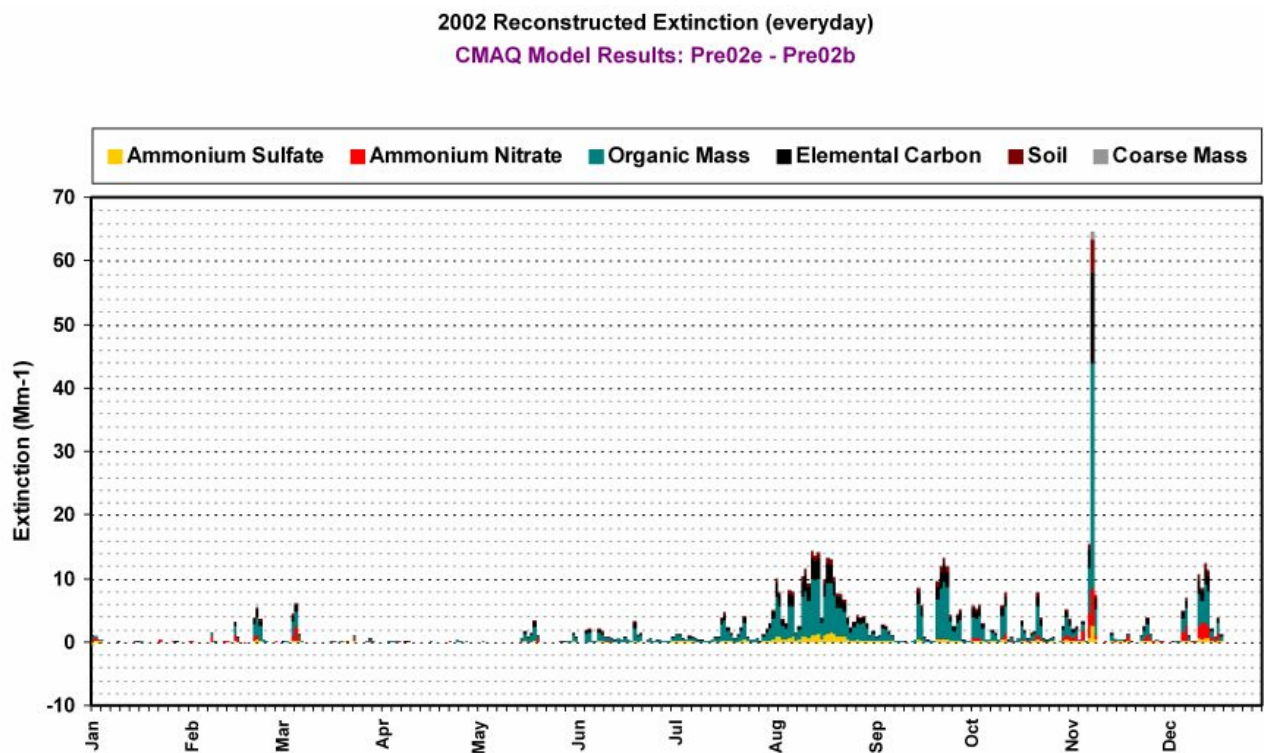
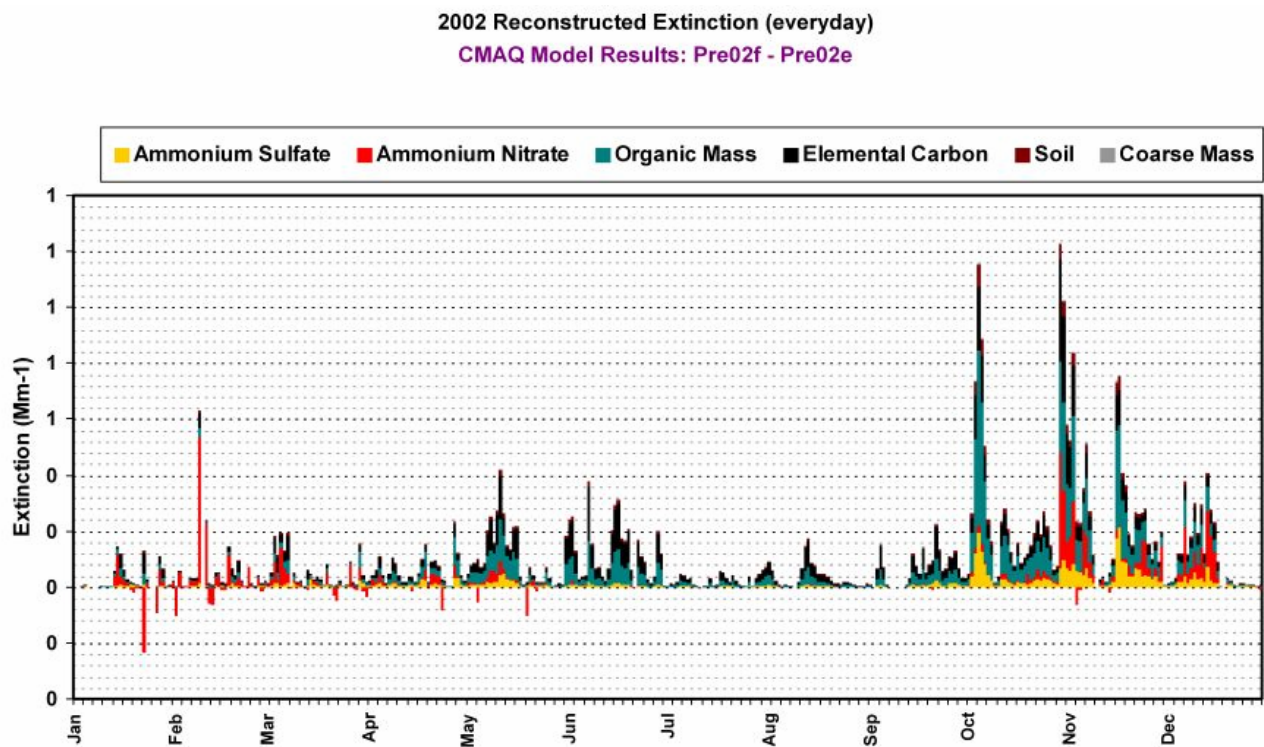


Figure 12-2. Two example plots of results showing effects of fire emissions on extinction coefficient at the Grand Canyon IMPROVE site. Top panel is for anthropogenic emissions; bottom panel is for natural emissions.

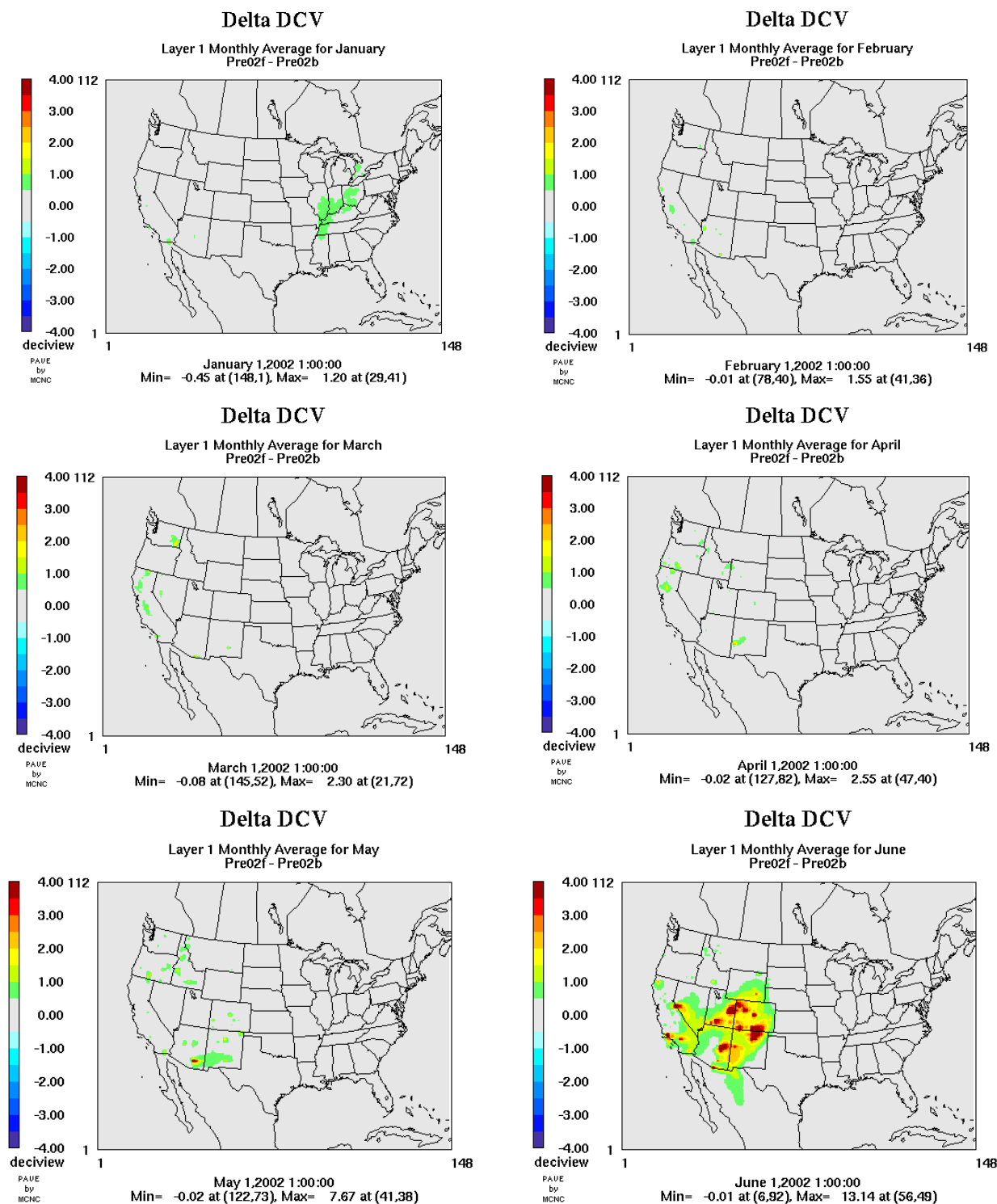


Figure 12-3. Monthly average for January through June (as labeled in each plot) showing effect of total fire emissions calculated as the difference of the Pre02f case with both natural and anthropogenic fire emissions minus the Pre02b case with no fire emissions.

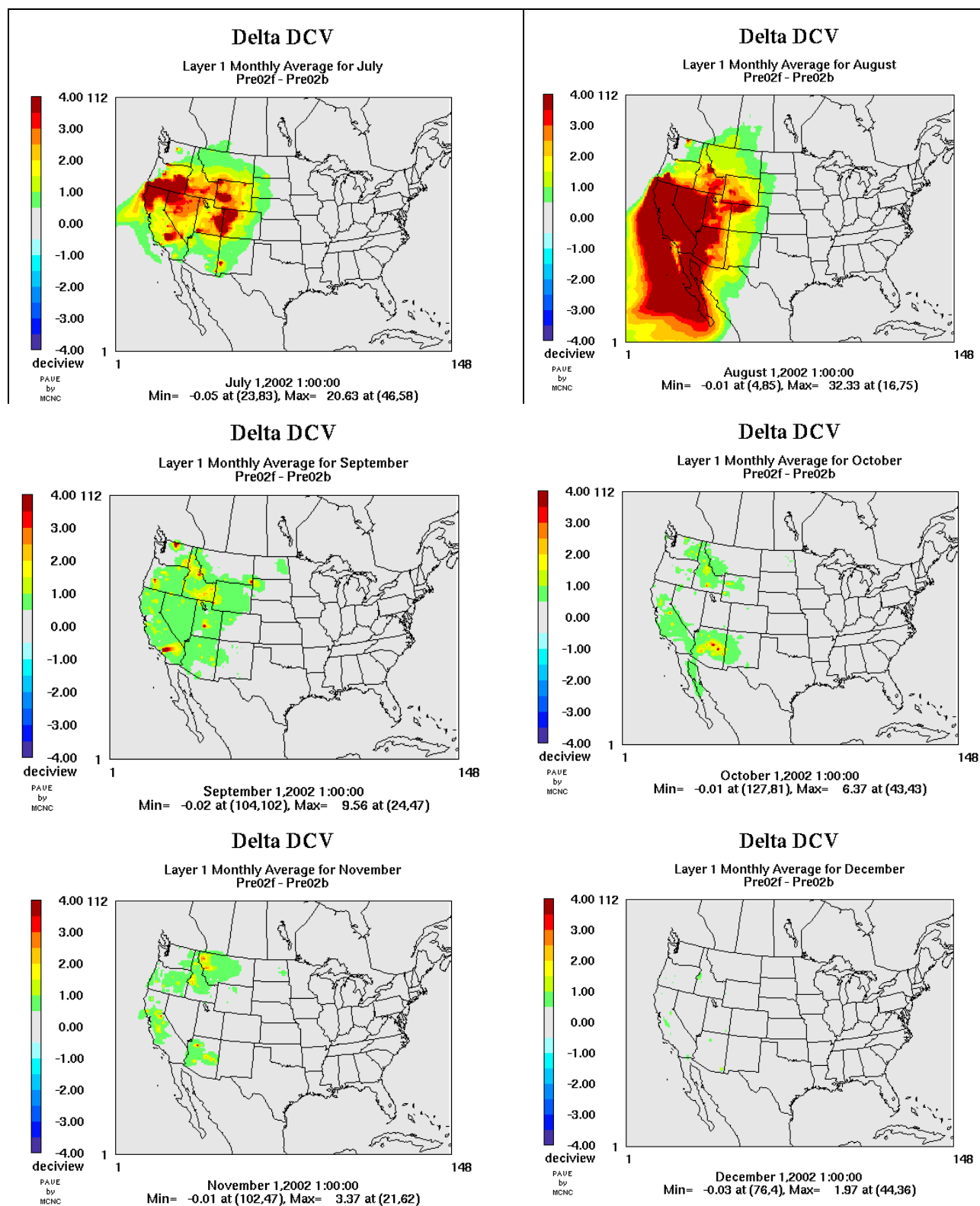


Figure 12-4. Monthly averages for July through December (as labeled in each plot) showing effect of total fire emissions calculated as the difference of the Pre02f case with both natural and anthropogenic fire emissions minus the Pre02 case with no fire emissions.

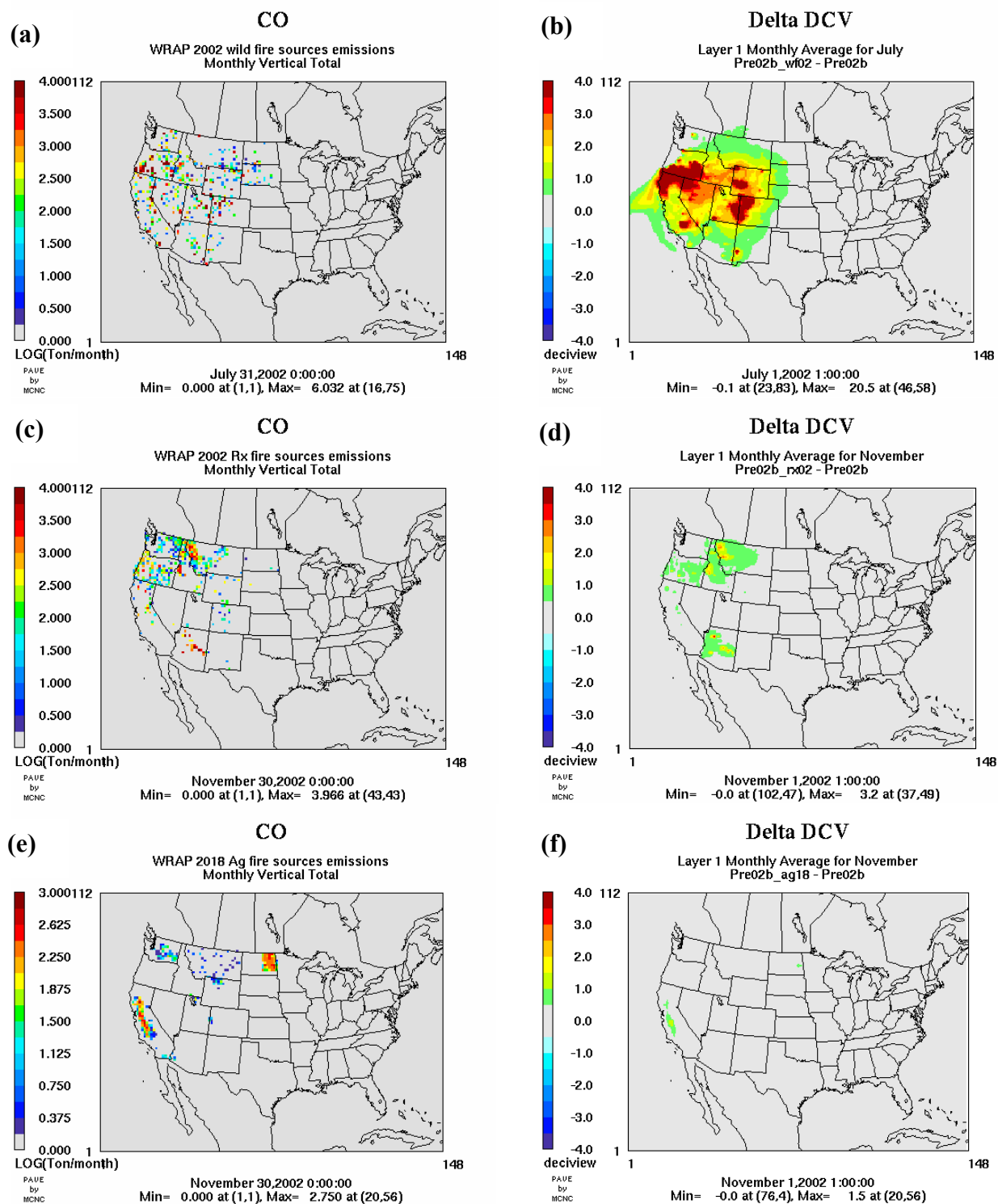


Figure 12-5. Left panels show change in carbon monoxide emissions. Right panels shows the change in visibility from all aerosol species, as monthly average deciviews, for each fire sensitivity case: (b) July wild fires; (d); November prescribed burning; (f) November agricultural burning..

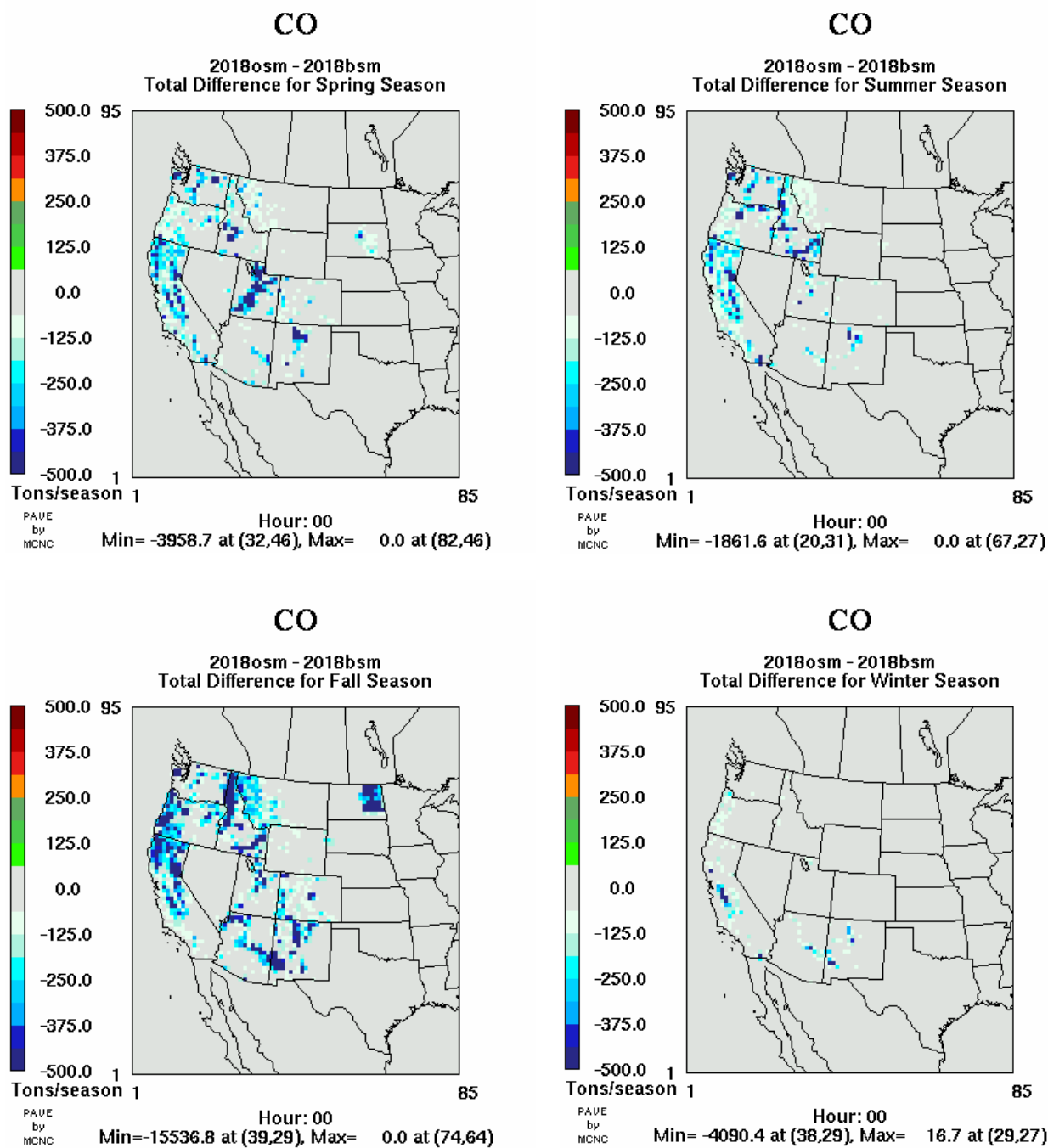


Figure 12-6. Seasonal total change in carbon monoxide emissions for the Optimal Smoke Management emissions compared to the Base Smoke Management emissions.

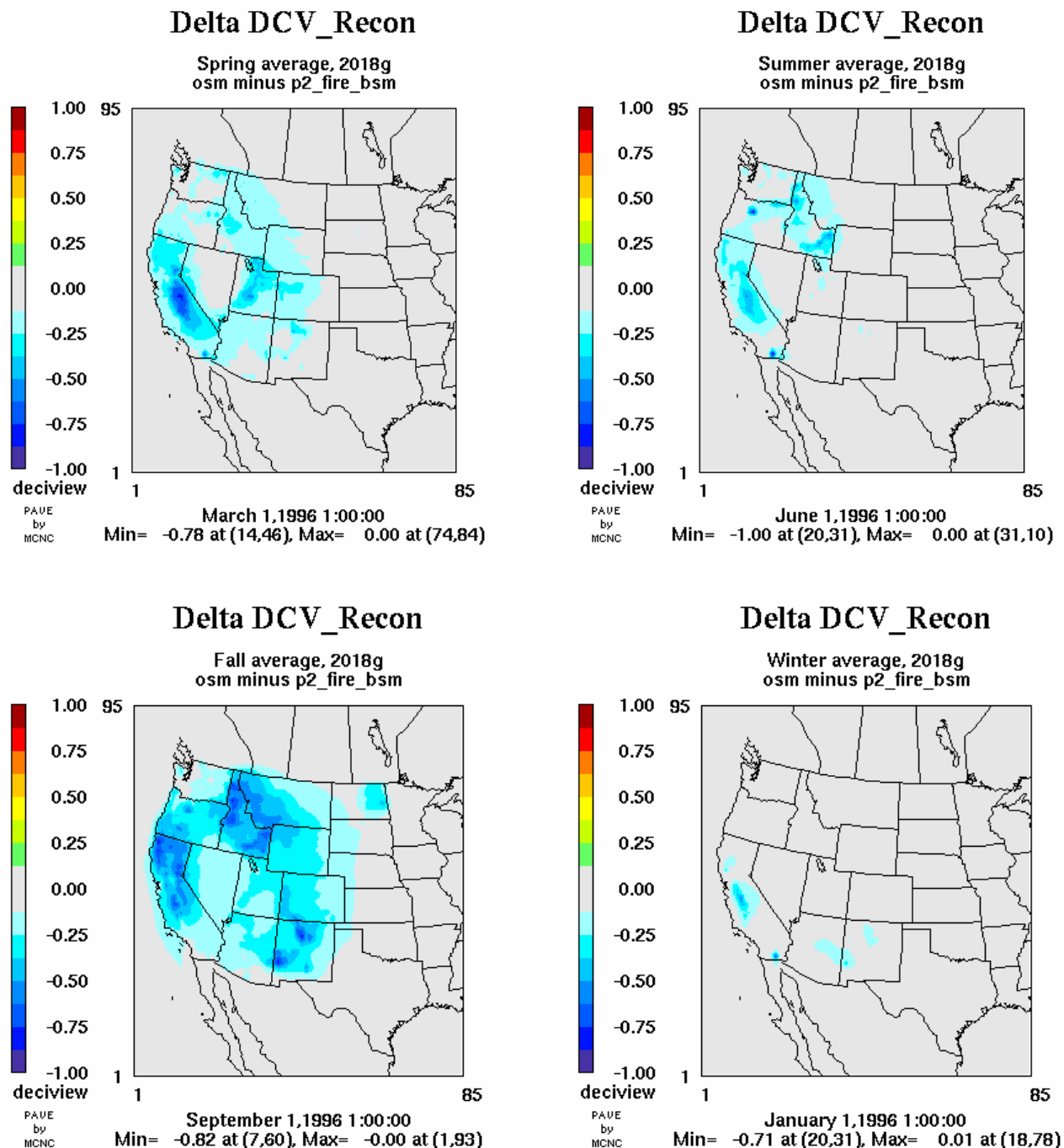


Figure 12-7. Seasonal average change in deciviews showing effect of Optimal Smoke Management emissions compared to Base Smoke Management emissions.

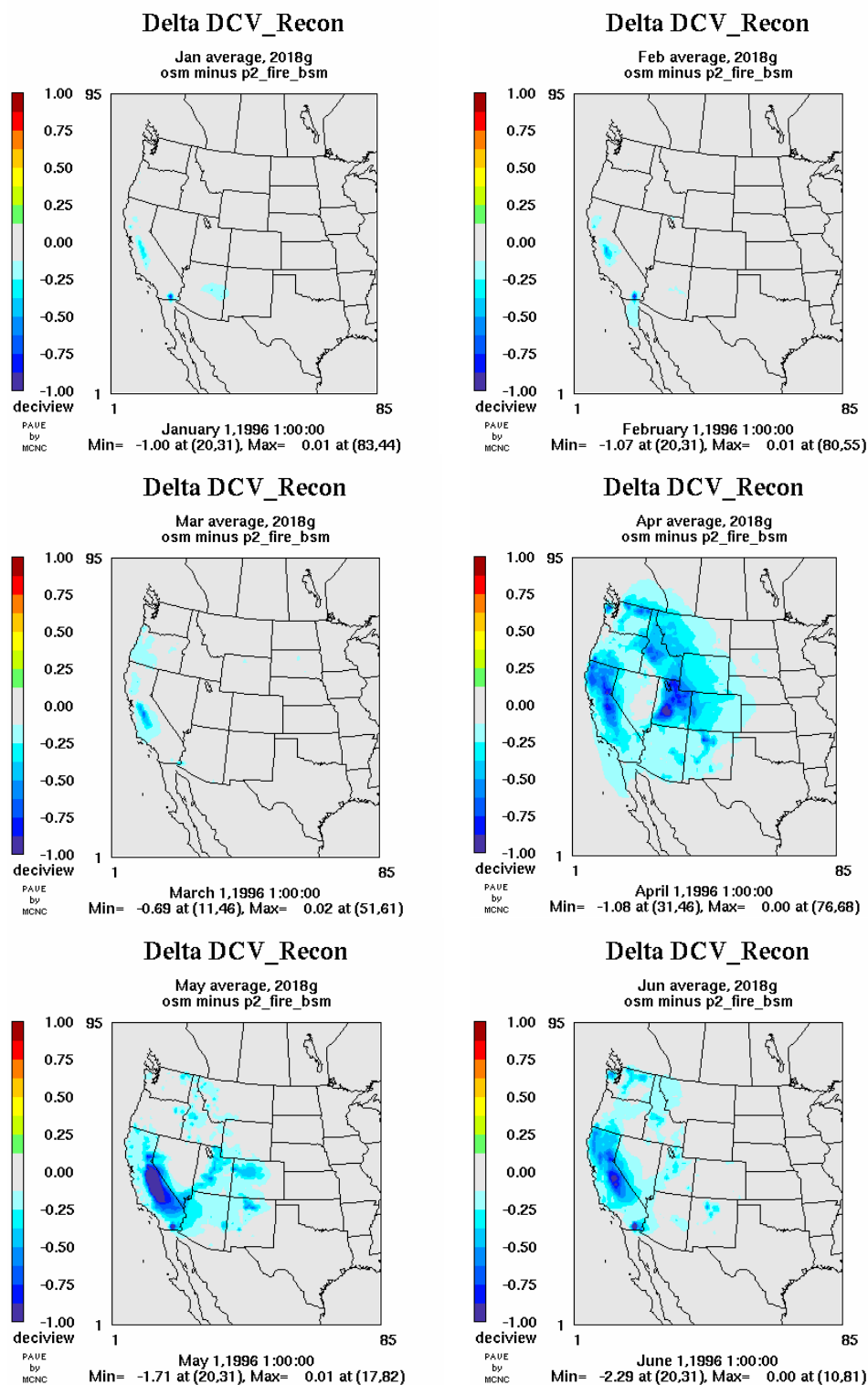


Figure 12-8. Monthly average for January through June (as labeled in each plot) showing effect of Optimal Smoke Management compared to Base Smoke Management emissions.

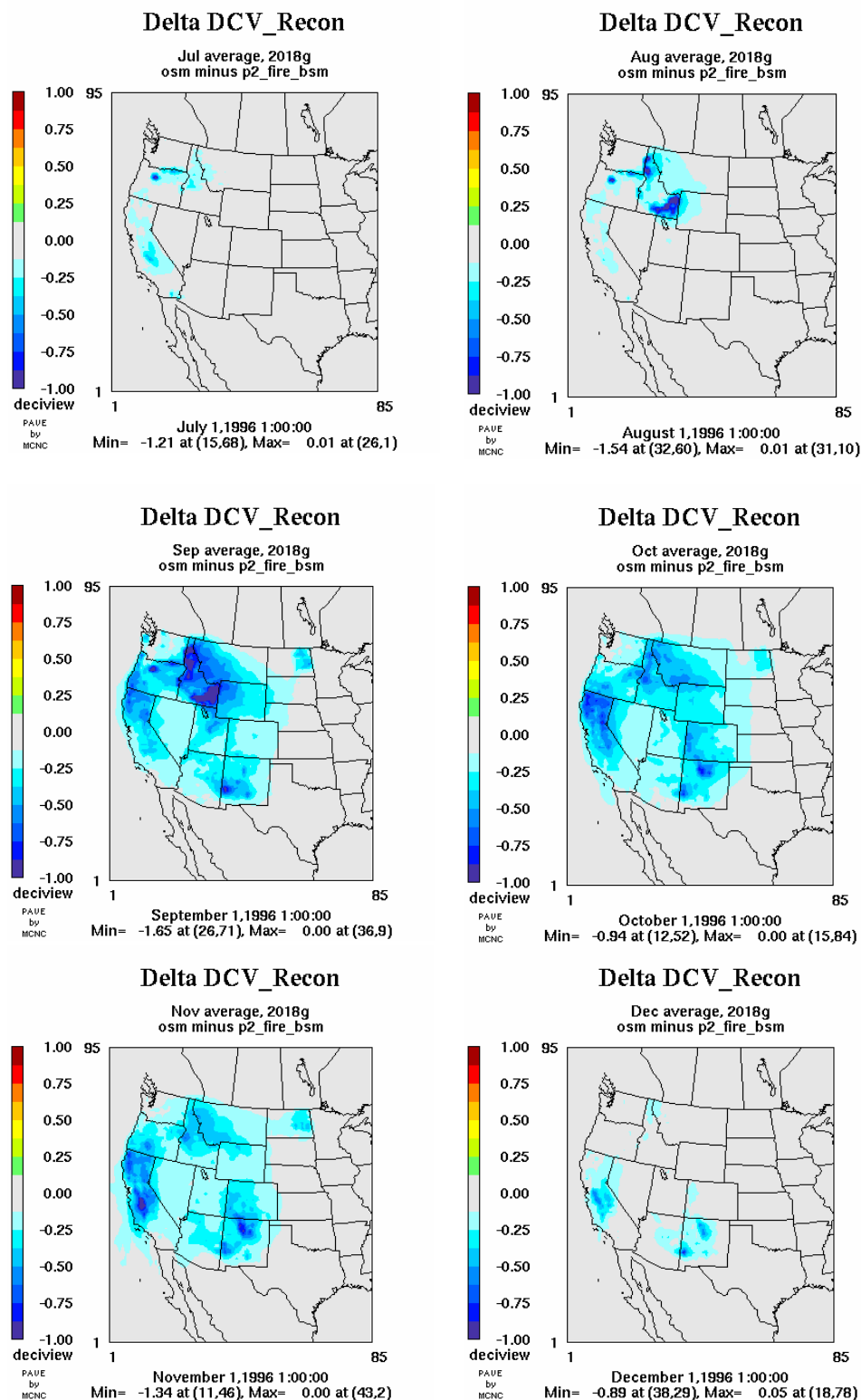


Figure 12-9. Monthly average for July through December (as labeled in each plot) showing effect of Optimal Smoke Management compared to Base Smoke Management emissions.

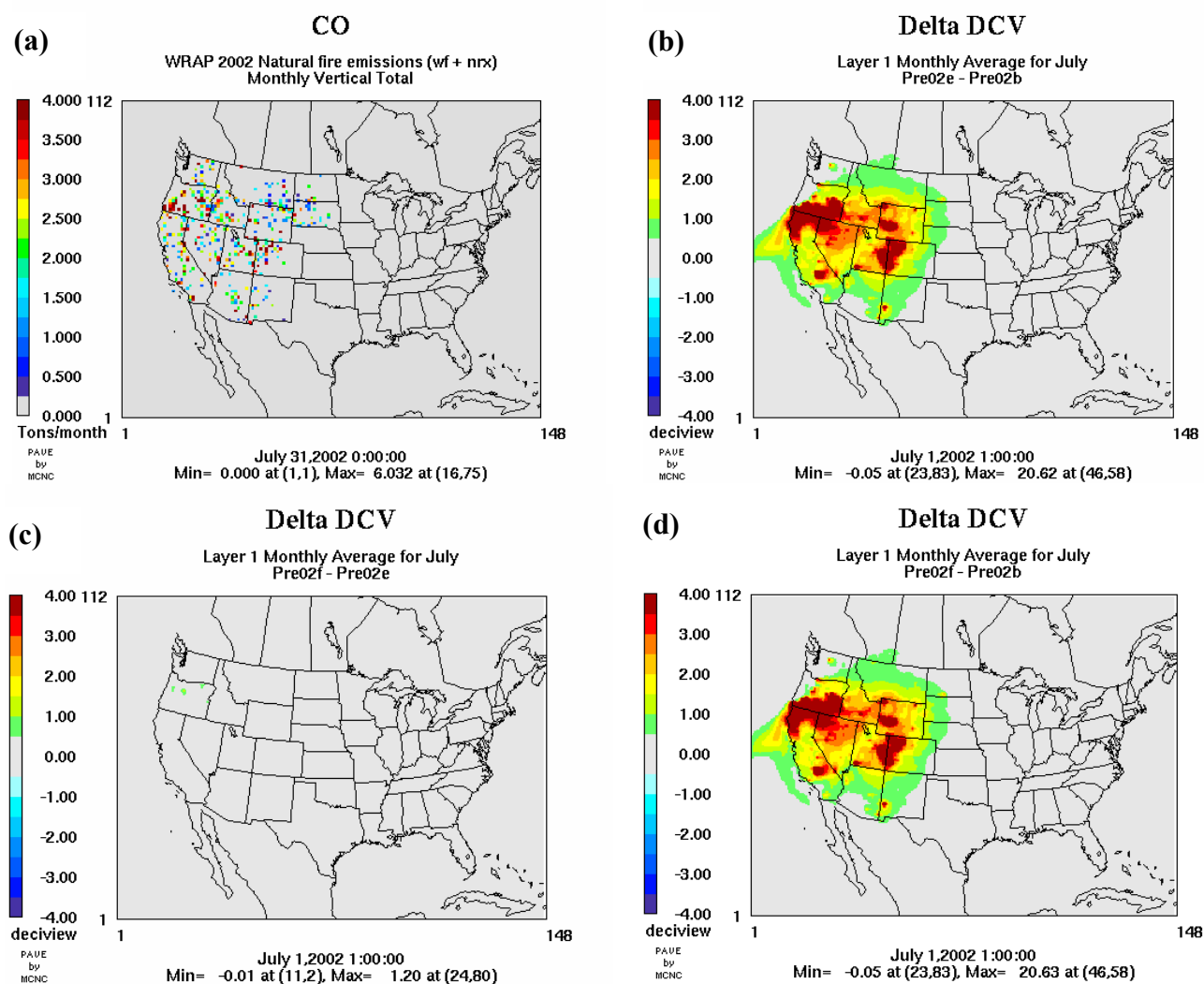


Figure 12-10. (a) The July total natural fire emissions of carbon monoxide. Panels (b) through (d) show the effect of fire sensitivity simulations on visibility, calculated as deciviews and averaged for the month of July, as the difference of each fire sensitivity case minus base case (i.e., Pre02b) for (b) the natural fire sensitivity case; (c) the anthropogenic fire emissions, and (d) the combined natural and anthropogenic fire emissions.

13. Task 12: Preliminary Meteorological, Emissions, and Air Quality Modeling Activities for Alaska

13.1 Introduction

As explained in Section 1.1.1, EPA's Regional Haze Rule calls for state and Federal agencies to work together to improve visibility in 156 Federally mandated Class I areas that include national parks and wilderness areas. The objective of the RHR is to achieve natural visibility conditions in these Federally protected lands by the year 2064. The rule requires that states develop and implement air quality SIPs and TIPS to reduce the pollution that causes visibility impairment. WRAP is charged with implementing regional planning processes to improve visibility in western U.S. Class I areas.

The State of Alaska is developing a plan to protect visibility and comply with the intent of the RHR. Alaska poses some unique challenges for regional haze modeling. Geographically, it is far enough removed from the rest of the WRAP states that using a unified modeling domain would be quite large and inefficient. Also, Alaska has much lower emission densities than the other WRAP states (except during fire events), and there are longer transport distances between the various source regions and Class I areas. In addition, the influence of long-range (international) transport of pollutants from Eurasia may dominate regional haze events on occasion (this phenomenon is known as Arctic haze).

There are four Class I areas in Alaska (Figure 13-1):

- Denali National Park and Preserve
- Tuxedni Wilderness Area
- Simeonof Wilderness Area
- Bering Sea Wilderness Area

Both the Simeonof and Bering Sea Wilderness Areas are quite far away (>500 mi) from Anchorage and Fairbanks, the two largest cities in Alaska. However, the Tuxedni Wilderness Area and Denali National Park are close enough that they may be affected by emissions from, respectively, Anchorage and Fairbanks, as well as other emission sources in the region.

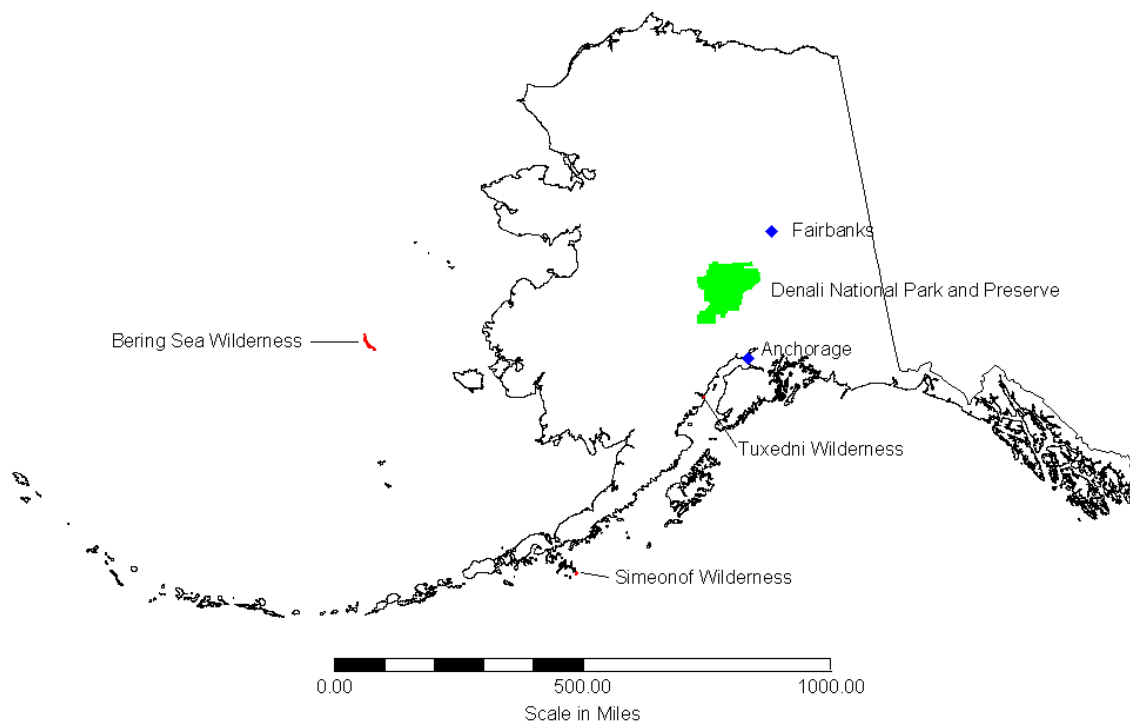


Figure 13-1. Locations of the four Class I areas in Alaska and of the two biggest Alaskan cities, Anchorage and Fairbanks.

As part of the WRAP Alaska effort, the RMC is developing techniques for credible modeling of regional haze in Alaska, and providing an initial evaluation of the potential contributions to regional haze in the Alaska Class I areas that are more likely to be affected by in-state emissions: Denali National Park, Tuxedni Wilderness Area, and (less so) Simeonof Wilderness Area. (Due to its remoteness, the Bering Sea Wilderness Area will not be addressed in this initial modeling analysis). There are three main components of regional haze modeling: meteorological modeling, emissions modeling, and air quality modeling.

The State of Alaska is developing a statewide emissions inventory for all sources. It is therefore premature to perform emissions modeling, as not all of the data are currently available in a suitable form. Consequently, it is also premature to perform photochemical grid modeling with a model such as CMAQ, since source-oriented models require complete emissions inventories. Thus, the approach in our WRAP Alaska modeling work is to develop meteorological modeling techniques to simulate the unique and complex meteorological conditions of Alaska, and to perform some preliminary air quality modeling using a simplified Lagrangian (trajectory) model to provide an initial assessment of the potential emissions contributions from Anchorage and Fairbanks, as well as major stationary sources, to visibility at Denali National Park and Tuxedni Wilderness Area. The Lagrangian model chosen for preliminary WRAP Alaska visibility modeling is the California Puff Model (CALPUFF) air quality modeling system.

We are using MM5 to develop hourly meteorological fields for the Alaska region. In the initial modeling phase, MM5 has been applied to simulate two different and diverse episodes (i.e., a

summer and a winter period) to develop appropriate methods for running MM5 over Alaska, including Cook Inlet, the Alaska Range, and the region north of Fairbanks. The meteorological conditions of Alaska, described in Section 13.2.2, required some special consideration.

We have developed a modeling protocol for the meteorological modeling component using MM5, as well as a brief outline of the air quality modeling component, and are proceeding with the meteorological component of the 2002 annual run. Section 13.2 describes the meteorological modeling approach. It overviews MM5 (Section 13.2.1) and the meteorology of Alaska (Section 13.2.2), and discusses the MM5 configuration we chose (based on some preliminary sensitivity studies) and the procedure used to simulate the year 2002 meteorology (Sections 13.2.3 and 13.2.4). Section 13.2.5 presents the plan for evaluating MM5's performance in replicating the evolution of observed winds, temperature, humidity, and boundary layer morphology to the extent that resources and data availability allow; this will be the primary approach to assessing the reliability of the meteorological fields to make sure they adequately characterize the state of the atmosphere for input to CALPUFF. Sections 13.3 and 13.4 briefly discuss the emissions modeling and air quality modeling approaches.

13.2 Meteorological Modeling Approach

The CALPUFF modeling system includes the CALPUFF dispersion model and the diagnostic meteorological preprocessor CALMET (California Meteorological Model). CALPUFF requires inputs of 3-D gridded wind, temperature, humidity, cloud/precipitation, and boundary layer parameters. These fields are generated by CALMET, which can reprocess output fields from MM5 and supply them in a format suitable for CALPUFF. MM5 is a state-of-the-science atmosphere model that has proven very useful for air quality applications and has been used extensively in past local, state, regional, and national modeling efforts. It has undergone extensive peer review, with all of its components continually undergoing development and scrutiny by the modeling community. The MM5 modeling system software is freely provided and supported by the Mesoscale Prediction Group in the Mesoscale and Microscale Meteorology Division of NCAR. For these reasons, MM5 is the most widely used public-domain prognostic model. In-depth descriptions of MM5 can be found in Dudhia (1993) and Grell et al. (1994) and at <http://www.mmm.ucar.edu/mm5>.

13.2.1 Overview of MM5

MM5 is a limited-area, terrain-following (sigma-coordinate), prognostic meteorological model. It solves the full suite of nonhydrostatic prognostic primitive equations for the 3-D wind, temperature, water, and pressure fields. It can be run with multiple one-way or two-way nested grids to resolve a range of atmospheric processes and circulations on spatial scales ranging from one to several thousands of kilometers. The model is highly modular, facilitating the interchange of physics and data assimilation options. Several options exist for boundary layer schemes; resolved and sub-grid-scale cloud and precipitation treatments; soil heat budget models; and radiative transfer. The model equations are solved horizontally on an Arakawa-B grid structure defined on a number of available map projections. The vertical coordinate is a terrain-following normalized pressure coordinate, referred to as "sigma-p." Typically, 30 to 50 vertical levels are used to resolve the troposphere and lower stratosphere to ~15 km.

13.2.2 The meteorology of Alaska

The meteorology of Alaska poses some unique and special challenges for MM5 modeling. In winter, there is little liquid water or insolation, and temperatures and specific humidities are extremely low north of the Alaska Range. In the northern part of the domain, there is extensive sea ice in the winter in the Bering Sea and Arctic Ocean; interactions between sea ice and the air above it have historically been difficult for models to simulate well, and the energy exchange between the sea ice and the overlying air is not well understood (Curry et al., 2001). In the dark of winter, the ice undergoes strong radiative cooling, which sets up a strong temperature inversion near the surface. This also occurs over the snow-covered inland areas from the Alaska Range north. This creates an extremely stable boundary layer, which can then decouple from the flow aloft. It is therefore possible to have air masses with different origins and properties superimposed in the vertical. This can be significant in terms of air quality modeling if the overlying air mass has different chemical properties than the air below it. In addition, it is difficult for an atmosphere model to handle this type of extremely stable boundary layer well, as turbulent flows in stable layers are not well understood (Mahrt, 1998). These stable layers can be broken up by intermittent turbulence, sometimes arising from gravity-wave generation over the Alaska Range. These events are notoriously difficult for an atmosphere model to simulate (Jeff Tilley, University of North Dakota, personal communication, 2004).

MM5-modeled temperature fields are very sensitive to the cloud field. Small errors in cloud cover can produce large errors in the temperatures. Because clouds can be a sub-grid-scale phenomenon, errors in characterization of the cloud field are inevitable, and may lead to significant temperature errors, particularly in winter. For example, in a region with strong radiative cooling over sea ice, if the model places a cloud where there is none in the real world, then the outgoing longwave radiation trapped by the modeled cloud and re-emitted downward will cause a spurious warming below the cloud. This will cause the model to overestimate the surface temperature and underestimate or entirely fail to produce the inversion that should be there. This may have serious implications for subsequent air quality modeling.

Further complicating the characterization of the cloud field is the fact that some Arctic clouds have unusual properties. There are clouds composed of ice crystals that can extend down to the ground, (known as “diamond dust”). Multiple thin cloud decks may appear in the statically stable atmosphere, and convective plumes may appear in gaps in the sea ice (Curry et al., 2001). All of these phenomena may be difficult or impossible to capture in a model running at a maximum resolution of 15 km.

Another issue is that Alaska is so cold in winter that some of the physical assumptions underpinning the parameterizations of moist processes may no longer be valid. MM5 has a POLAR option (Cassano et al., 2001) for use at high latitude that attempts to compensate for this problem.

Given the low population density and often harsh conditions, it is not surprising that the observing network in Alaska is sparse compared to that of the U.S. mainland. This complicates model validation, particularly in a 15-km-resolution domain, where representative observations may be very widely spaced if one or more observing sites are down (Jeff Tilley, personal communication, 2004). The rugged Alaskan terrain can also cause problems in model validation. Many

stations are located in regions where meso-gamma and microscale effects forced by topography can form a significant part of the signal in temperature and winds (Jeff Tilley, personal communication, 2004).

In the spring and fall, the model must account for the breakup and formation of sea ice. Sea ice has a large effect on the surface energy budget, and a mischaracterization of the extent of sea ice will degrade MM5's simulation of the thermal structure of the overlying atmospheric column.

13.2.3 MM5 configuration

The WRAP MM5 modeling system configuration for the Alaska application is based on the work of the Mesoscale Modeling and Applications Group at the University of Alaska Fairbanks (UAF). The UAF group has extensive experience with operational numerical weather prediction in high latitudes using MM5 modeling (<http://knik.iarc.uaf.edu/AtmGroup>). We are building on their experience by incorporating some facets of their MM5 configuration for use in our Alaska application.

13.2.3.1 Modeling domain

We have configured MM5 to run on two grids: a large-scale grid with 45-km grid point spacing, and a smaller, nested grid with 15-km grid point spacing focused on the Class I areas (Figure 13-2). The model is run on both grids simultaneously, but in a “one-way” nesting mode. In this approach, information from the 45-km grid is transferred to the 15-km domain through boundary conditions during the simulation, but there is no feedback of the 15-km fields up to the 45-km domain. Another alternative is “two-way” nesting, wherein MM5 is run for both grids simultaneously and information propagates both down- and up-scale between the two. Our experience suggests that the choice of one-way versus two-way nesting does not significantly affect model performance for regional applications with coarse grid spacing.

Our 45-km Alaska Grid is defined on a polar stereographic projection, with central latitude 59° N and central longitude 151° W. The grid has 109 (east-west) by 90 (north-south) dot points, and 108 (east-west) by 89 (north-south) cross points. The 15-km subregional grid is defined on the same polar stereographic projection, but covers the populated areas and Class I areas (see in Figure 13-2) with 15-km grid point spacing.

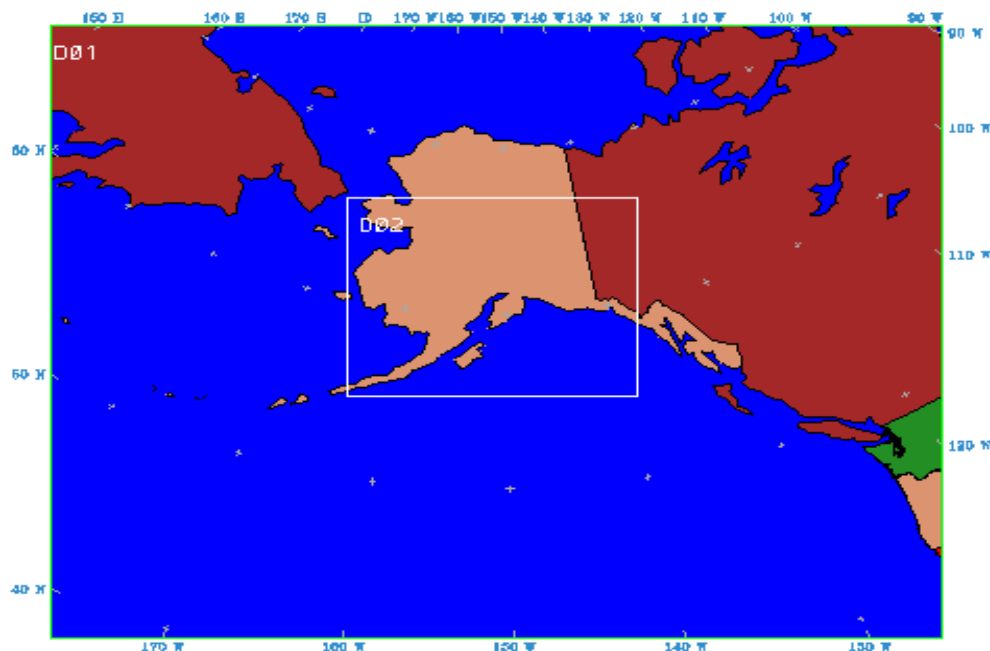


Figure 13-2. Spatial coverage of the Alaska Grid with 45-km grid point spacing (D01) and the nested 15-km grid (D02).

13.2.3.2 Physics options and FDDA

This section details the rationale behind our choices of physics options and FDDA for the Alaska MM5 modeling effort. As mentioned above, the 2002 annual MM5 application has been configured in many aspects according to the optimum arrangement identified by the UAF group. We have also used some information from additional sensitivity tests specific to this application; these tests are discussed below.

When modeling a full year over the Alaska domain, the annual cycle of sea ice must be taken into account. The sea ice, which forms part of the atmosphere's lower boundary condition, grows in spatial extent during fall and winter, and retreats during the spring and early summer. MM5 has an option whereby the sea ice fraction in a grid cell is diagnosed using the sea surface temperature, and this flag must be used during the winter months to ensure adequate treatment of the atmosphere's lower boundary condition. Use of the sea ice option limits the available physics options in MM5, however, as it requires the use of the five-layer land surface model. Thus, for winter modeling, we use the sea ice option, the five-layer LSM, and the Eta PBL scheme. During summer, however, we turn off the sea ice option, which allows us to choose a more detailed land surface model. The NOAH LSM has been shown to be effective in simulating the Alaskan summer when used with the Eta PBL scheme (Jeff Tilley, personal communication, 2004), so we use this configuration as our starting point. Note that although the LSM/PBL/sea ice configuration changes in going from summer to winter, the rest of the physics options are held constant throughout the year.

To treat stratiform clouds, we use the Reisner 2 cloud microphysics scheme (Reisner et al., 1998). Although this scheme is more computationally intensive than the “simple ice” option, EPA recommends that a mixed-phase ice scheme be employed in MM5 to drive aqueous chemistry and wet scavenging in CMAQ. This is because the simple ice approach treats all condensed water forms as a single liquid variable, which when passed to CMAQ overstates the quantity of liquid cloud and precipitation water available for chemistry and removal. Furthermore, the next version of CMAQ will include separate contributions from precipitating ice (graupel). Although the initial Alaska visibility modeling will be done with CALPUFF, subsequent air quality modeling of Alaska may be done with CMAQ, so we selected the Reisner 2 cloud microphysics scheme to allow the use of CMAQ at a later date. For cumulus convection, we selected the Grell scheme, which has been used successfully by the UAF group. Cumulus convection is not expected to play a large role in the Alaska simulation during winter, but significant convection can occur in the summer, particularly in the Denali area. Convection in this region is driven largely by topographic/land surface forcings (Jeff Tilley, personal communication, 2004). Sensitivity tests regarding the cumulus parameterization may be carried out at a later date, depending on model performance.

Next, we needed to select a radiation scheme and an FDDA configuration. We performed several sensitivity tests to determine the appropriate configuration. These tests are summarized in Table 13-1. Below is listing of the various schemes tested in this study and an explanation of the abbreviations used in the table.

- *Land Surface Models:* NOAH LSM; Pleim-Xiu LSM (PX); five-layer LSM
- *Planetary Boundary Layer Schemes:* Eta PBL; Pleim-Xiu PBL (PX)
- *Cumulus Scheme:* Grell
- *Radiation Schemes:* Rapid Radiative Transfer Model (RRTM); Community Climate Model 2 (CCM2); CLOUD
- *IPOlar:* Y = sea-surface temperatures (SSTs) vary with time; N = SSTs do not vary with time
- *IEXSI:* 0 = no sea ice fraction information; 1 = sea ice fraction is diagnosed from SST
- *Cloud Microphysics Scheme:* Reisner 2
- *Four-Dimensional Data Assimilation:* W = wind; T = temperature; RH= relative humidity

Table 13-1. Summary of MM5 configuration for sensitivity tests.

Run ID*	LSM	PBL	Cumulus	Radiation	IPO-LAR	IEXSI	Micro-physics	Analysis FDDA		Obs FDDA
								3-D	Surface	
Run_S1	NOAH	Eta	Grell	RRTM	Y	0	Reisner 2	W/T/RH	W/T/RH	None
Run_S2	NOAH	Eta	Grell	CCM2	Y	0	Reisner 2	W/T/RH	W/T/RH	None
Run_S4	PX	PX	Grell	RRTM	Y	0	Reisner 2	W/T/RH	W/T/RH	None

Run ID*	LSM	PBL	Cumulus	Radiation	IPO-LAR	IEXSI	Micro-physics	Analysis FDDA		Obs FDDA
								3-D	Surface	
Run_W1	5-layer	Eta	Grell	RRTM	Y	1	Reisner 2	W/T/RH	W/T/RH	None
Run_W1b	5-layer	Eta	Grell	RRTM	Y	1	Reisner 2	W/T/RH	W/T/RH	W
Run_W2	5-layer	Eta	Grell	CCM2	Y	1	Reisner 2	W/T/RH	W/T/RH	None
Run_W3	5-layer	Eta	Grell	CLOUD	Y	1	Reisner 2	W/T/RH	W/T/RH	None

*In the run IDs, “S” stands for “summer” (July) and “W” stands for “winter” (January)

The results of the tests are discussed below. As in Section 4, we organize our analysis discussion around soccer plots, which display average performance statistics for a particular modeled time period. Soccer plots are shown for wind speed bias versus wind speed RMSE, temperature bias versus temperature error, and humidity bias versus humidity error. In each plot, a solid blue line indicates the benchmark. The benchmark was generated by considering the performance statistics from approximately 50 MM5 and RAMS simulations performed in support of air quality modeling studies in the continental U.S. (Tesche et al., 2002). A soccer plot, therefore, places the current MM5 model run in the context of prior meteorological databases used for air quality modeling. A data point that falls inside the box represents a model run that meets the performance benchmark. Perfect model performance is indicated by a data point at (0,0). The closer a data point is to the origin, the better the model’s performance. We emphasize that the benchmarks are not used as acceptance/rejection criteria of the MM5 model simulation. Rather, they put the MM5 model performance into perspective and allow the identification of potential problems in the MM5 fields. Furthermore, the benchmarks are mainly for ozone episodes in the continental U.S., which typically occur in meteorological conditions very different from those found in Alaska.

Most prior modeling efforts in Alaska have used the RRTM or CCM2 radiation schemes. They showed that RRTM performed better in some cases while CCM2 did better in others, and there was no guidance to determine a priori which would be the best choice for this application (Jeff Tilley, personal communication, 2004). We tested three MM5 radiation schemes: CCM2, RRTM, and CLOUD. The CLOUD radiative package was widely used before the advent of the RRTM scheme, and has a simpler treatment of the longwave absorption than RRTM, which uses the correlated-*k* method of calculating absorption coefficients. The shortwave treatments in CLOUD and RRTM are similar. We tested the CLOUD scheme in order to have a range of complexity of parameterization when evaluating the sensitivity of the Alaska simulation to the choice of radiation scheme. We ran MM5 for a five-day period in July and a five-day period in January to span the range of climatological conditions the model was likely to encounter in the annual 2002 run. We examined the results on both the 15-km and 45-km domains.

The surface wind performance for the three runs testing the different radiation schemes is shown in Figure 13-3. Runs W1_45km, W2_45km, and W3_45km are otherwise identical 45-km January runs that differ only in the radiation scheme used (the W1b January run, designed to test the effect of observational nudging, is discussed later). The winter runs are shown by blue symbols without borders. The corresponding 15-km model runs are shown by blue symbols with black borders. The summer runs (S1 and S2) are displayed using the same convention for 45- and 15-

km runs, but are shown in red* (the S4 July run, designed to test the effect of LSM scheme, is discussed later).

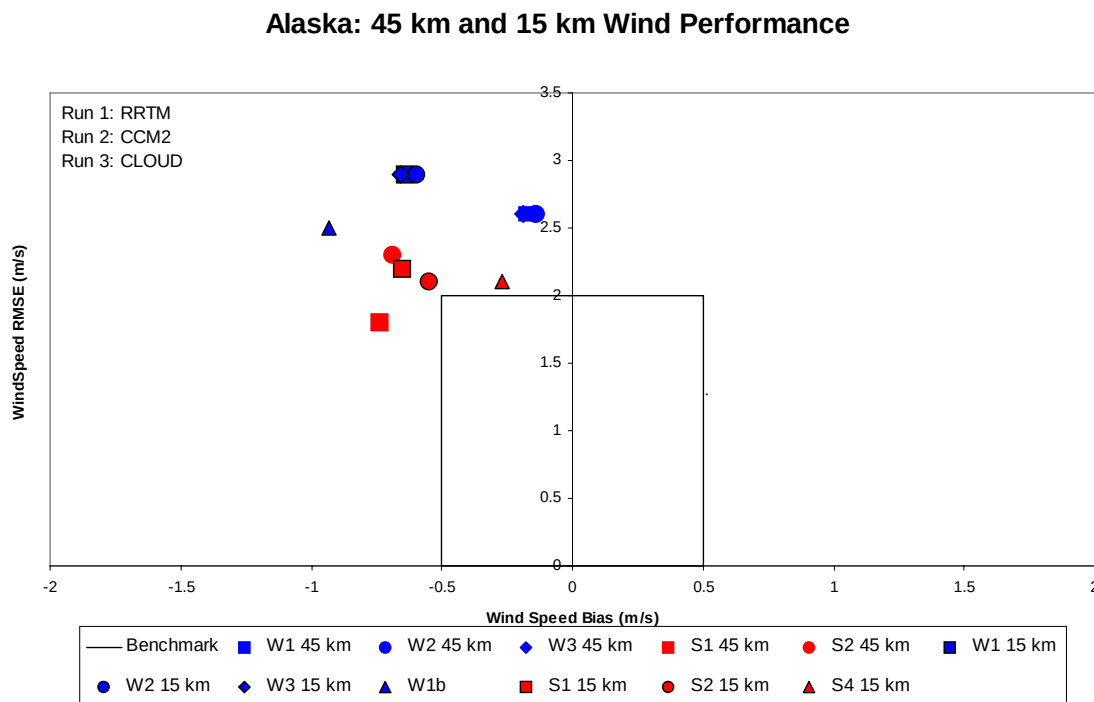


Figure 13-3. Wind soccer plot for winter and summer Alaska sensitivity tests.

A comparison of winter Runs W1_45km through W3_45km shows that there is not much difference among the three radiation schemes in terms of model performance; the three points are tightly clustered and lie outside the benchmark, with a slight low wind speed bias. At 15 km, the three winter runs (Runs W1_15km, W2_15km, W3_15km) were again quite similar in terms of performance, and there was a stronger low wind speed bias on the higher-resolution 15-km grid.

Figure 13-4 displays the temperature performance of the winter runs W1 through W3 and the summer runs S1 and S2. Most of the runs fell within or near the benchmark for bias, but outside the benchmark for error. In the 45-km series of winter runs, the RRTM (Run W1_45km) and CLOUD (Run W3_45km) runs were comparable, but the CCM2 (Run W2_45km) run had a cold bias that was nearly twice as large as those of RRTM and CLOUD. There was little difference in the error among the three runs. In winter at 15 km, the bias changed sign and increased somewhat for RRTM and CLOUD, and the error decreased slightly. For CCM2, however, bias and error both increased.

*Note that the summer runs used different LSM schemes, a different IEXSI setting, and, in the case of run S4, a different PBL scheme than the winter runs (see Table 13-1), so the summer and winter runs are not directly comparable with each other for examining the effects of the radiation schemes.

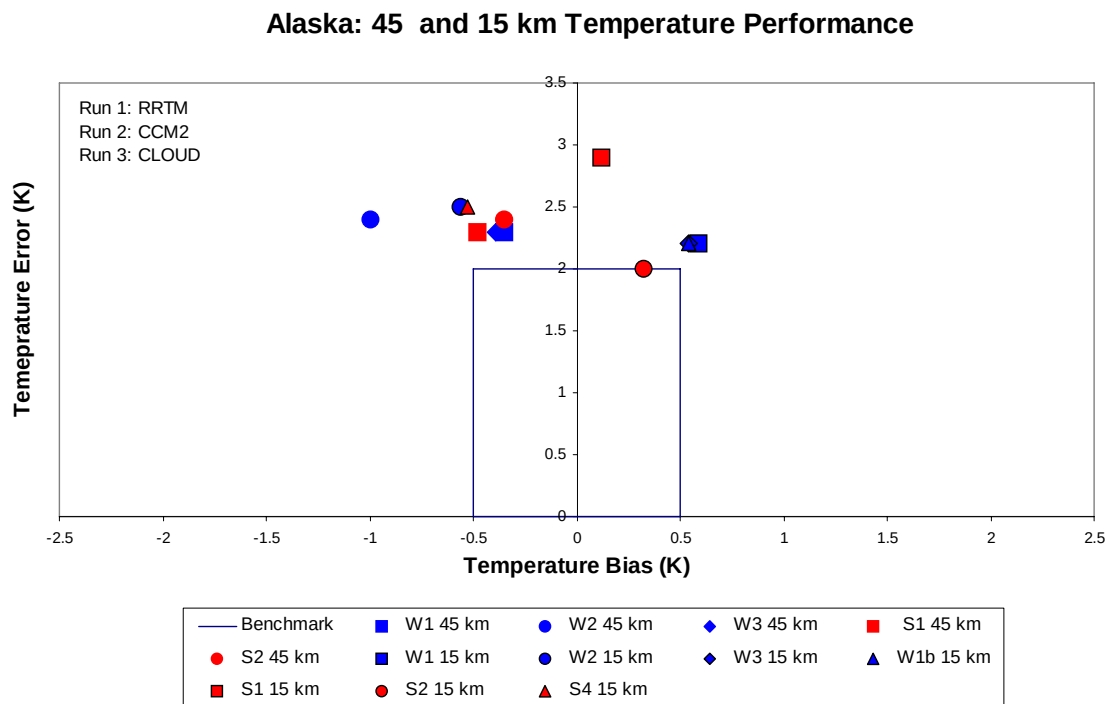


Figure 13-4. Temperature soccer plot for winter and summer Alaska sensitivity tests.

In the summer 45-km runs, there was not much difference in temperature between the RRTM (Run S1_45km) and CCM2 (Run S2_45km). At 15 km, both bias and error in the CCM2 run (Run S2_15km) were reduced to the point where they lay within the benchmark. In the RRTM run (Run S1_15km), on the other hand, the bias decreased but error increased.

The humidity soccer plot (Figure 13-5) shows all runs in summer and winter tightly clustered within the benchmark. Humidity performance is quite good relative to the benchmark, but it is worth noting again that the benchmark is based on MM5 and RAMS simulations of regions in the continental U.S. In these regions, the specific humidities are generally higher than in Alaska, and the fact that the Alaska runs fall within the benchmark may be a reflection of the lower Alaskan humidity rather than an indication of good model performance. Since the humidity performance was consistent across the sensitivity tests, humidity was not a useful metric for selecting a radiation scheme.

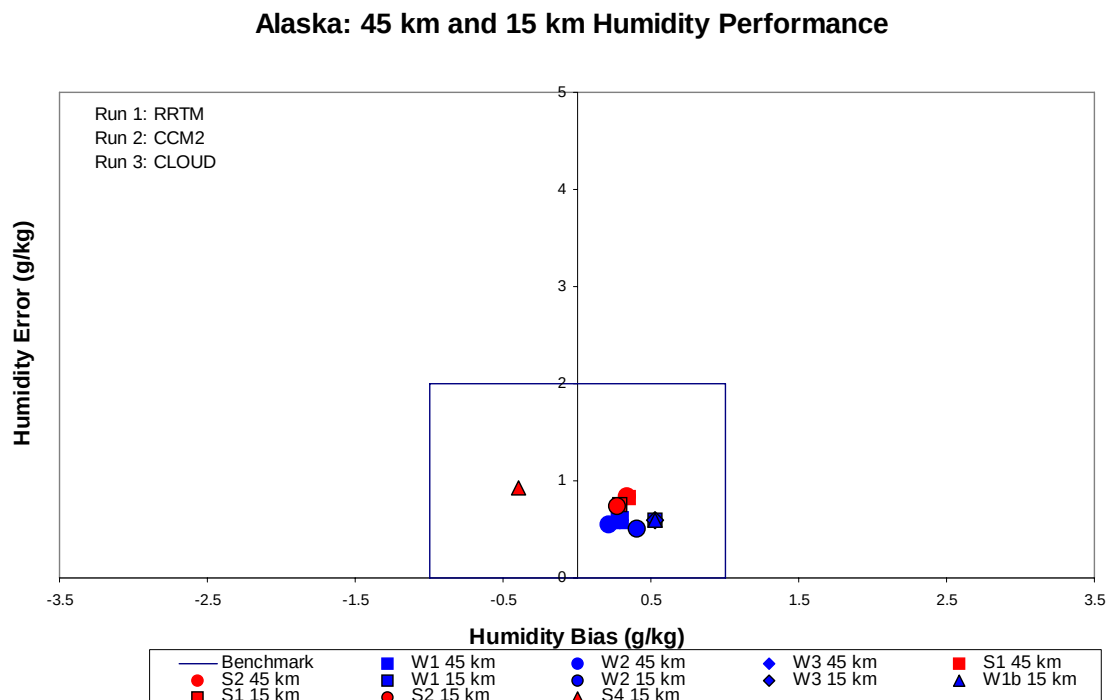


Figure 13-5. Humidity soccer plot for winter and summer Alaska sensitivity tests.

Based on the surface wind and temperature performance, the CCM2 scheme did not sufficiently improve MM5 performance to justify its added computational burden (~20%), so we selected the RRTM parameterization to be the radiation scheme for summer and winter.

In the next sensitivity test we looked at the choice of LSM for the summer months. Recall that in winter, we must use the five-layer LSM in order to turn on the sea ice parameterization. In summer, however, we are free to select the best-performing LSM scheme for this application. The Pleim-Xiu scheme has been shown to perform well over the continental U.S. (Olerud and Sims, 2003; Kemball-Cook et al., 2004) and also allows use of the Pleim deposition scheme in subsequent CMAQ modeling; we therefore made a run (S4) using the Pleim-Xiu scheme and the RRTM radiation scheme for the July time period. The 15-km results for wind (Figure 13-3) show a reduction in the low wind speed bias relative to the other 15-km summer runs, and little change in the RMSE. For temperature (Figure 13-4), the bias increased and the error decreased relative to the other 15-km run that used the RRTM radiation scheme (Run S1_15km). The humidity soccer plot (Figure 13-5) shows a change of sign in the bias, and a small increase in error. Overall, the Pleim-Xiu scheme did not cause significant improvement, so we elected to use the NOAA/Eta LSM/PBL combination for summer.

In summary, Tables 13-2 and 13-3 give the MM5 physics options we used for the winter and summer months, respectively.

Table 13-2. Physics options selected for the 2002 WRAP winter Alaska MM5 simulation.

Physics Option	Parameterization
Cloud microphysics	Reisner 2
Cumulus parameterization	Grell
Planetary boundary layer	Eta
Land surface model	Five-layer Model
Radiation	RRTM
Shallow convection	None
Varying SST with time? (IPOLAR)	Yes
Sea ice (IEXSI)	Yes
Snow cover	Simple Snow Model

Table 13-3. Physics options selected for the 2002 WRAP summer Alaska MM5 simulation.

Physics Option	Parameterization
Cloud microphysics	Reisner 2
Cumulus parameterization	Grell
Planetary boundary layer	Eta
Land surface model	NOAH
Radiation	RRTM
Shallow convection	None
Varying SST with time? (IPOLAR)	Yes
Sea ice (IEXSI)	No
Snow cover	No

Regarding FDDA capabilities to use in the Alaska simulations, we configured MM5 to use FDDA to nudge the model toward observed wind, temperature, and moisture fields on both the 45-km and 15-km grids throughout the 2002 annual simulation. Specifically, analysis (or grid) nudging was performed at three-hourly intervals for both the 2-D surface fields and the 3-D fields aloft, excluding the boundary layer depth. Excluding the boundary layer in the FDDA process removes the potential for damping out resolved mesoscale forcings in the model that are important to boundary layer development and thus the vertical fluxes of momentum, heat, and moisture into the free atmosphere and to the surface. Two-dimensional surface nudging was based on NCAR/National Centers for Environmental Prediction (NCEP) Reanalysis Project (NNRP) surface analyses, but were enhanced via the “little_R” program using hourly NWS

surface observations from NCAR dataset ds472.* The analysis nudging coefficients we chose to use are shown in Table 13-4.

Table 13-4. FDDA analysis nudging coefficients (s^{-1}).

Data Type	45 km	15 km
Wind	2.5×10^{-4}	1.0×10^{-4}
Temperature	2.5×10^{-4}	1.0×10^{-4}
Water vapor	1.0×10^{-5}	1.0×10^{-5}

In addition to analysis nudging, FDDA may be used to nudge the model solution toward observational data at individual measurement sites (i.e., “station” or “observational” nudging). Usually this option is best suited for smaller, high-resolution grids in which data from a very dense network of measurement sites are available (such as an intensive field study). The next sensitivity test was designed to test the effect of observational (obs) nudging using the ds472 surface meteorological observation network (Figure 13-6). Obs nudging of the winds was performed for the winter W1 configuration (Run W1b in Table 13-1), and the effect on the surface wind speed performance is shown in Figure 13-3. With obs nudging turned on, the low wind speed bias increased and the RMSE decreased relative to the comparable un-nudged run W1. For temperature (Figure 13-4) and humidity (Figure 13-5), the difference in performance between runs W1 and W1b is nearly indistinguishable. Although this test of nudging was not conclusive, we elected to proceed with observational nudging of winds.

* Note that the NNRP analysis fields are used instead of the usual EDAS fields because Alaska falls out of the EDAS domain.

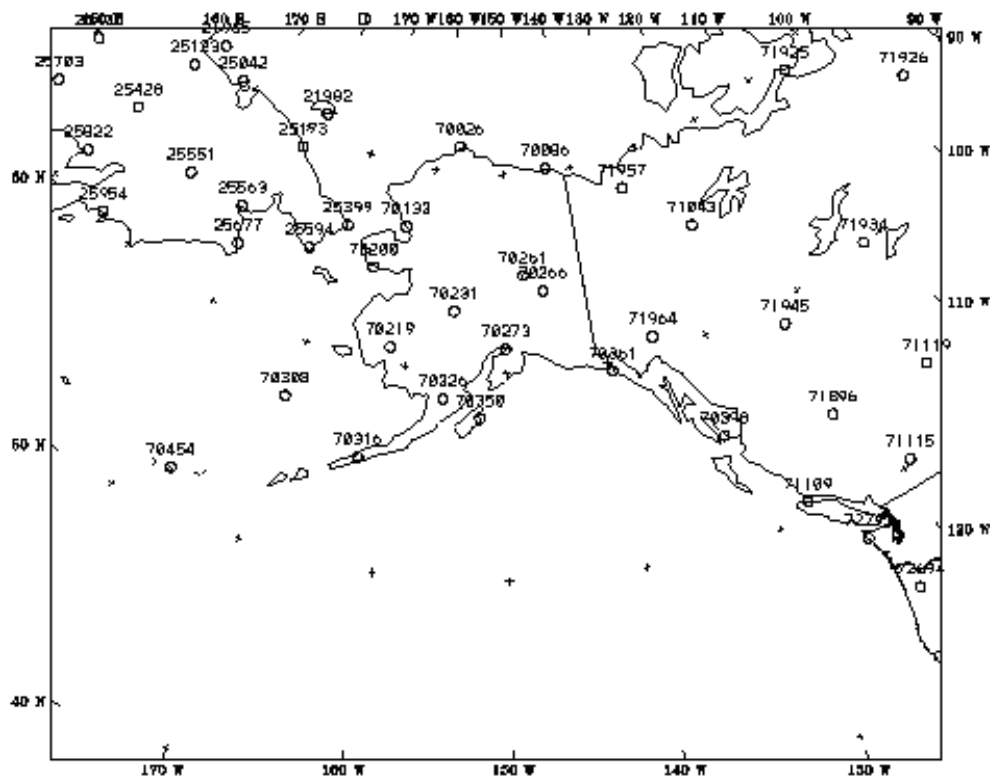


Figure 13-6. Stations contributing data used for observational nudging.

13.2.4 Procedure to simulate the year 2002

Once we had selected model configurations for summer and winter that would ensure reasonable model performance in both seasons, the annual simulation for the year 2002 was begun. The January-June 2002 time period of the simulation was done at UCR and July-December 2002 was done at ENVIRON. The 2002 annual simulation was made in sequential five-day run segments, each with an initial spin-up period of 12 h that overlaps the last 12 h of the preceding run. This is done so that the air quality model can be started at either 00Z or 12Z without including the MM5 re-initialization period. MM5 was re-initialized at the beginning of each five-day period to reduce error propagation through the simulation. The 2002 annual simulation included the final two weeks of December 2001 to allow sufficient spin-up time for photochemical/visibility applications with start dates at the beginning of January 2002. The model was run with 90-s and 30-s time steps on the 45-km and 15-km grids, respectively. The MM5 annual run for 2002 is now complete, and analysis of the results is underway.

13.2.5 Evaluation procedures for the 2002 annual run

13.2.5.1 Overview

The goal of the evaluation is to determine whether the meteorological fields are sufficiently accurate to properly characterize the transport, chemistry, and removal processes in CALPUFF.

If errors in the meteorological fields are too large, the ability of the air quality model to replicate regional pollutant levels over the entire base year will be compromised. To provide a reasonable meteorological characterization to the photochemical/visibility model, MM5 must represent the following with some fidelity:

- Large-scale weather patterns (i.e., synoptic patterns depicted in the 850-300-mb height fields), as these are key forcings for mesoscale circulations
- Mesoscale and regional wind, temperature, PBL height, humidity, and cloud/precipitation patterns
- Mesoscale circulations such as sea breezes and mountain/drainage circulations
- Diurnal cycles in PBL depth, temperature, and humidity

For visibility applications, the moisture and condensate fields are particularly important, as they significantly impact PM chemical formation, removal, and light scattering efficiency. In addition, cloud and precipitation fields are a good measure of the integrated performance of the model because these are model-derived quantities and not nudged to observations. Because of the coarse resolutions of 45 and 15 km, the model cannot be expected to faithfully simulate the pattern or variability of the convective precipitation, but should reproduce the synoptic precipitation and cloud patterns.

In this study, the basis for the performance assessment is a comparison of the predicted meteorological fields with available surface and aloft data that are collected, analyzed, and disseminated by NWS. This is being carried out both graphically and statistically to evaluate model performance for winds, temperature, humidity, and the placement, intensity, and evolution of key weather phenomena. For example, Figure 13-7 shows a comparison of modeled and observed upper-air soundings for a weather station in the Alaska domain. A specific set of statistics has been identified for use in establishing benchmarks for acceptable model performance (Emery et al., 2001); these benchmarks, similar to current EPA guidance criteria for air quality model performance, are intended to allow for a consistent comparison of various meteorological simulations for important variables at the surface and in the boundary layer. ENVIRON has developed a statistical analysis software package, METSTAT, to calculate and graphically present the statistics described above.

13.2.5.2 Surface statistical analyses

The statistical evaluation of the Alaska MM5 surface fields using NCAR dataset ds472, which contains hourly observations of the commonly measured variables from airports in the U.S. and Canada. The network of ds472 stations used in the Alaska MM5 evaluation is shown in Figure 13-8. Variables in the ds472 data set include temperature, dew point, wind speed/direction and gusts, cloud cover fraction and cloud base for multiple cloud layers, visual range, precipitation rates and snow cover, and a descriptive weather code. The key data of interest were extracted for the modeled domain, and processed into the appropriate formats for METSTAT that is used to generate time-series plots of observed and modeled surface wind, temperature, and humidity and relevant performance statistics. Example time series of observed and estimated temperature performance for a preliminary Alaska MM5 simulation for January 2002 are shown in Figure 13-9.

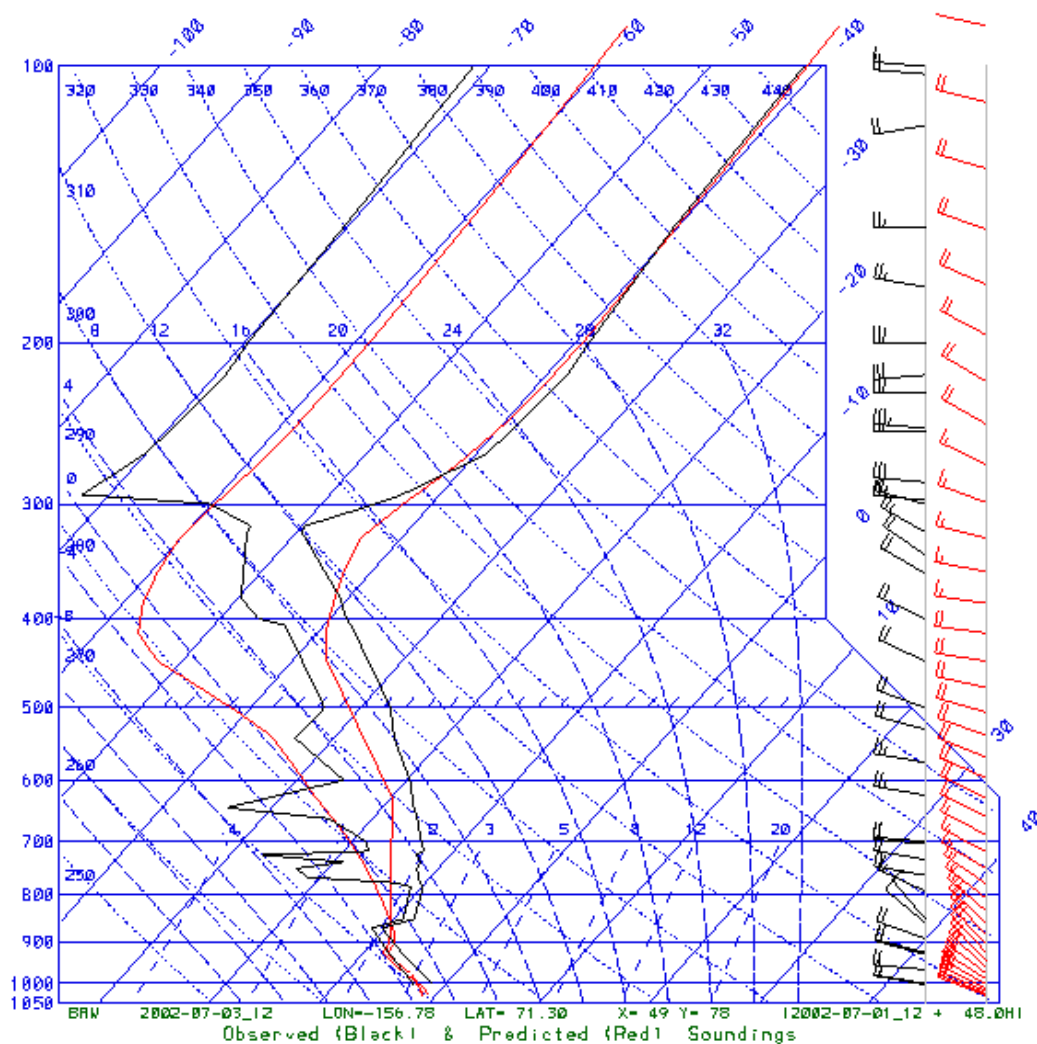


Figure 13-7. Observed (black) and modeled (red) temperature and dew point soundings for a sample weather station (BRW) in the Alaska domain for July 3, 2002.

ds472 Stations in the Alaska Modeling Domain

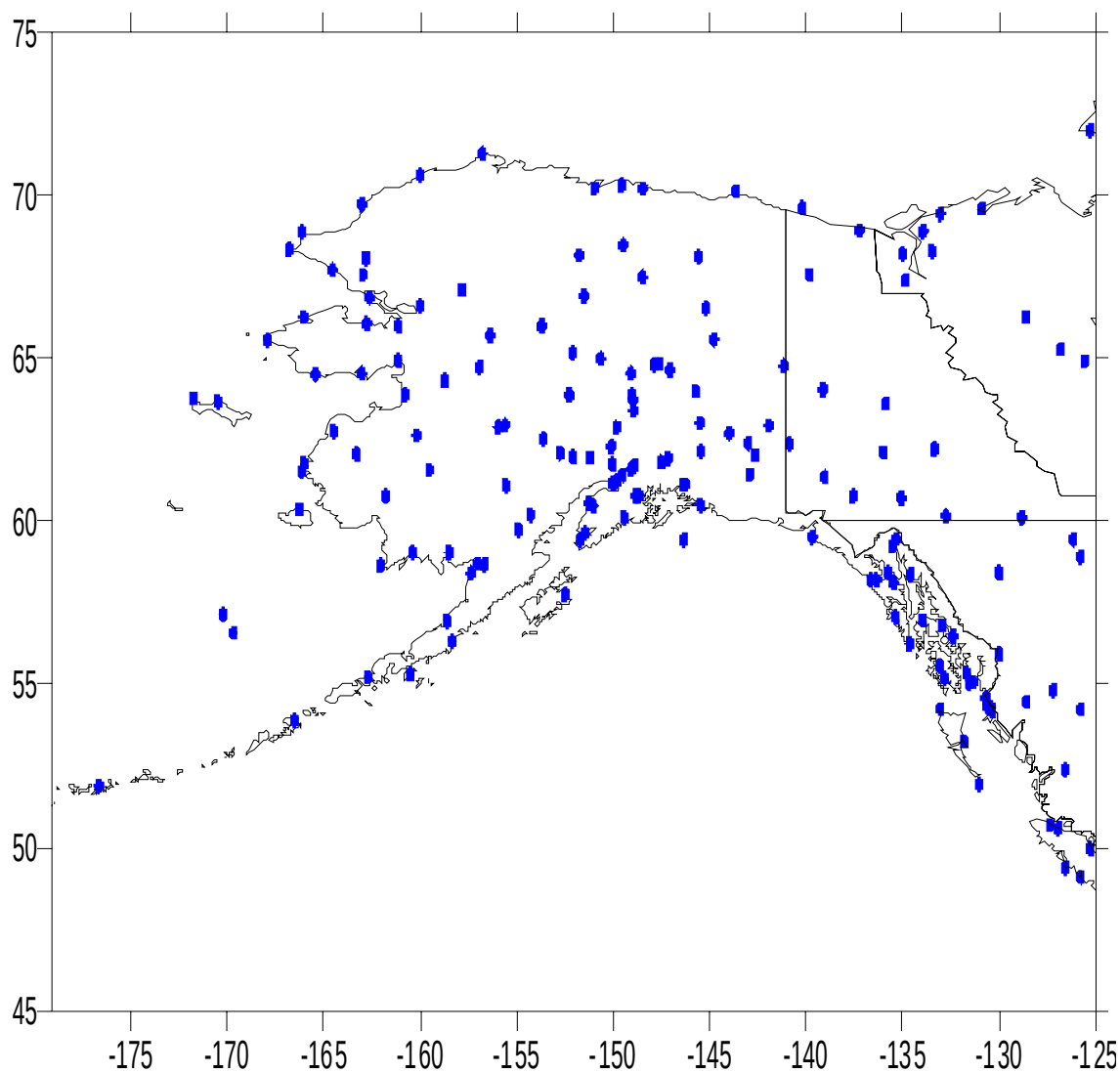


Figure 13-8. NCAR ds472 surface observing network stations in the 45-km Alaska domain.

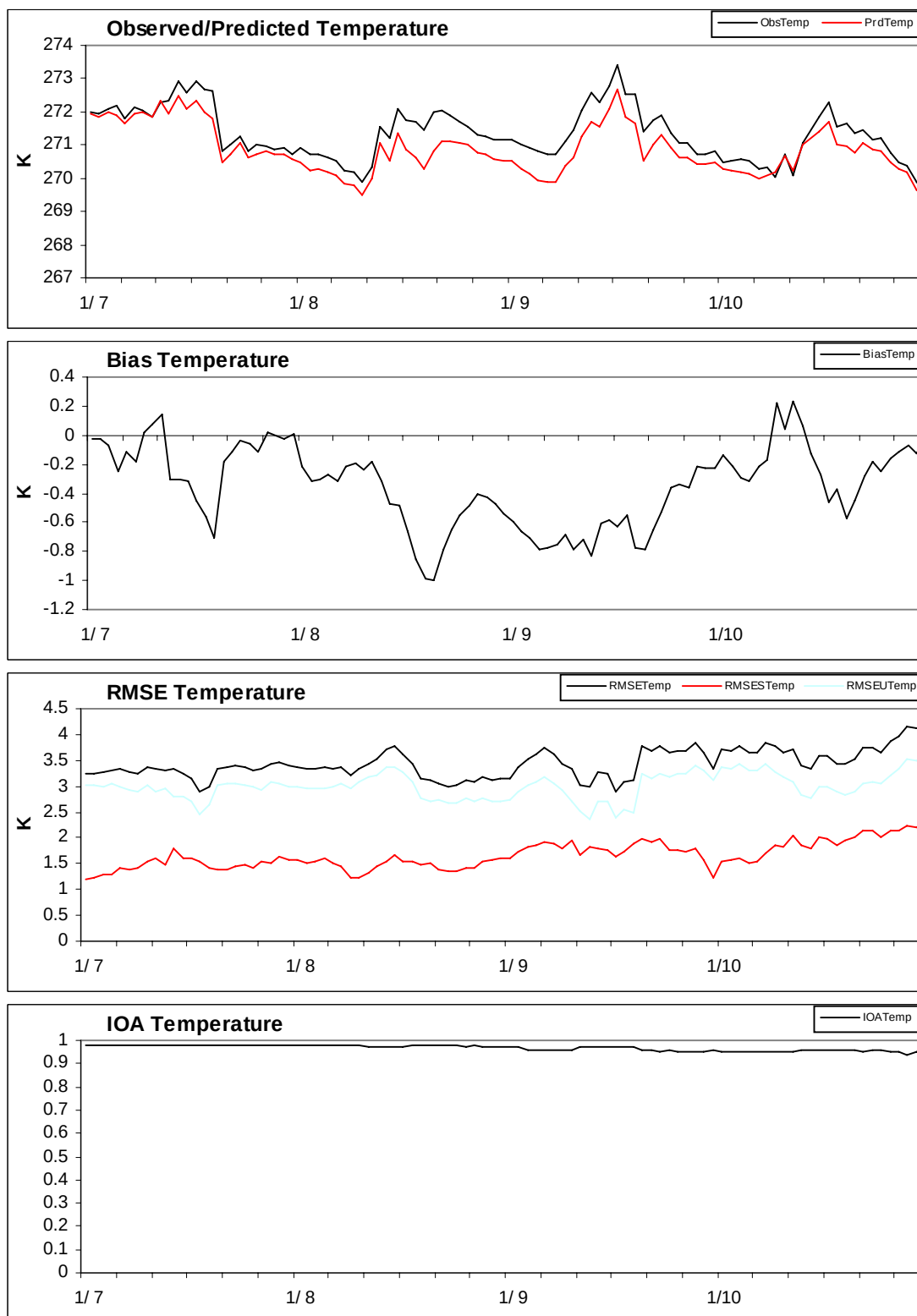


Figure 13-9. Example of METSTAT graphics from a WRAP Alaska January 2002 sensitivity test.

As described above, care must be taken in selecting an area for averaging when calculating model performance statistics. One problem with average evaluation statistics is that the more data pairings a given metric includes, the better the statistic generally looks, so calculating a single set of statistics for a very large area would not yield significant insight into performance. Therefore, a balance must be struck between taking an area large enough to create a representative sample but not choosing such a large area as to smear out the signal of interest. For Alaska, the observing network is sufficiently sparse that we must average over the entire domain or else we may not have enough data points to form a meaningful average. However, special attention needs to be given to the meteorological model performance near the Class I areas of interest.

The METSTAT statistical package is used to calculate hourly and daily statistical measures, and compare them against the Emery et al. (2001) benchmarks (see Section 13.2.5.1) for acceptable model performance. Potential reasons for any poor statistical performance for particular variables, times, and/or subregions are being investigated and documented in an evaluation report.

13.2.6 CALMET modeling

To generate the 3-D gridded wind, temperature, humidity, cloud/precipitation, and boundary layer parameters required by CALPUFF for air quality modeling, the CALMET meteorological preprocessor was used. As we noted earlier, CALMET can reprocess output fields from MM5 and supply them in a format suitable for CALPUFF. The 2002 MM5 output discussed in Section 4 was processed using the CALMM program to create files of the format and with the variables needed by CALMET. CALMET was run initially using the MM5 data as input in the NOOBS mode; this mode uses the MM5 data only, without any surface or upper-air observations. The feasibility of running with meteorological observations in addition to the MM5 data is being investigated along with the evaluation of the use of 15-km versus 5-km grid resolution for CALMET/CALPUFF modeling.

13.3 Emissions Modeling Approach

In June 2004, the Alaska Department of Environmental Conservation (ADEC) submitted 2002 annual emissions for major point sources and railroad emissions to EPA for inclusion in EPA's initial 2002 NEI. These data are undergoing corrections and will be resubmitted in the future. Previously, ADEC submitted 1999 criteria pollutant inventories for Anchorage, Fairbanks, and Juneau for all source categories (point, area, and mobile) that are included in the EPA 1999 NEI Version 2 (NEI99 v2). Day-specific 2002 emissions for major point sources, such as EGUs, are available from EPA's Acid Rain Database (ARDB). ADEC intends to have additional 2002 emissions data ready by the March-April 2005 time frame. Also, WRAP has contracted to obtain aviation and rural area emissions for Alaska that should be ready in spring 2005.

The Alaska air quality sensitivity modeling was initiated in late 2004 and will be completed during 2005. The following approach is being used to develop an Alaskan emissions inventory for sensitivity modeling:

- Acquire (1) the latest 2002 point-source and railroad emissions inventories and (2) the 1999 Anchorage, Fairbanks, and Juneau criteria pollutant emissions inventories for the three main Alaska urban areas.
- Download the Alaska 2002 major-point-source emissions from the ARDB.
- Combine the 2002 ARDB, 2002 point-source and railroad, and 1999 criteria pollutant emissions databases, eliminating duplicate sources by keeping the source characteristics according to the following priorities: 2002 ARDB, 2002 point/railroad, and 1999 criteria.
- Process emissions into CALPUFF format in separate files by major source categories, such as major point sources, minor point sources, railroads, on-road mobile sources, and other sources.

13.4 Air Quality Modeling Approach

As discussed at the beginning of Section 13.2, preliminary air quality modeling using the 2002 MM5 meteorological fields for Alaska, processed first through CALMET (see Section 13.2.6), will be conducted using CALPUFF, a Lagrangian (trajectory) puff model. This model is typically used to simulate the concentration and deposition impacts due to a source or group of sources. Species that CALPUFF treats include primary PM (e.g., PM_{2.5}, PM₁₀, EC, and OC), SO₂, NO_x, and secondary sulfate and nitrate PM. We will use the model to simulate the effect of primary emissions of PM, NO_x, and SO₂ on atmospheric PM (e.g., primary PM and SO₄ and NO₃) in Alaska, including the three Class I areas in the Alaska CALMET/CALPUFF modeling domain. Separate CALPUFF simulations will be made by major source category, and the results will be summed by CALPOST to estimate visibility impairment at the Class I areas.

At this time we are not proposing to use a more comprehensive photochemical grid model, such as CMAQ, to simulate air quality in Alaska because such models require emissions data from all sources, which as noted in Section 13.3 are not yet available for Alaska. The CALPUFF air quality modeling of Alaska is ongoing and will be completed in 2005.

13.5 Status of Task 12 Deliverables

Table 13-5 gives the status of each Task 12 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 13-5. Status of the Task 12 deliverables.

Deliverable	Status
Conduct 2002 MM5 sensitivity runs for January and July 2002	Completed December 2004
Conduct 2002 annual MM5 simulations	Completed February 2005
Initiate CALMET/CALPUFF runs	To be completed in 2005

14. Task 13: Training Courses for the WRAP States and Tribes

14.1 Work Performed from March 2004 through February 2005

Training needs were uncertain at the beginning of 2004, so a contingency fund was included in the 2004 funding to allow training to be conducted as needed. Basic training in CMAQ and SMOKE is routinely being provided through the Community Modeling and Analysis System (CMAS) Center, which is hosted at UNC-CEP. Since this is the most efficient method to provide basic SMOKE/CMAQ training, it was determined that the RMC would provide “advanced training.” Based on discussions with WRAP members, we developed a one-day training class for managers (i.e., non-modeling staff) that provides an introduction to the technical aspects of the modeling program, including definition of terminology, an introduction to the modeling system, and explanations of the products from the modeling activity and how to access them. A major goal of this class is to enhance the ability of managers to present and explain modeling results to their constituents.

The content of the training was selected after extensive discussions with WRAP members. An initial one-day training class was conducted in conjunction with the Attribution of Haze meeting held in September 2004. Additional training classes will be offered as needed.

During 2004, another training opportunity emerged: training to assist staff at state and tribal air pollution agencies in setting up and operating the visibility modeling system, including the aspects of hardware, operating systems, and installation and operation of models and datasets and the associated computers. We are engaged in several activities related to this need. For example, we are producing a frequently asked questions (FAQ) sheet that explains how to install an operating system and the modeling system on a Linux PC, and includes recommendations for computer hardware appropriate for the modeling system users’ needs. This FAQ sheet will be posted on the project web page.

After providing some assistance to one state in setting up a specialized operating system for managing parallel computers, we determined that the best use of RMC resources would be to limit the assistance we provide to supporting a single, standard installation of Linux and the modeling system.

The original funding budgeted for training and technology transfer in the 2004 RMC work plan was \$85,000, with activities to be defined depending on training needs during 2004. Per agreement with the WRAP Modeling Forum, some of these funds were rebudgeted for other activities. On July 30, 2004, we rebudgeted \$20,000 to perform additional MM5 testing and sensitivity simulations to improve the meteorology data used in the air quality modeling. The additional MM5 testing was a high priority because the MM5 performance in the WRAP region was inferior to that in other regions of the United States. The additional MM5 sensitivity testing resulted in new parameters for the MM5 configuration that substantially improved MM5’s

performance in the WRAP states. In a September 2004 conference call, we rebudgeted an additional \$20,000 to purchase new computer equipment, including additional RAID5 disk storage and parts to build eight additional dual-CPU compute nodes. UCR charged \$25,000 for training activities in 2004. At the end of December 2004, UCR carried over a balance of \$100,420, which included funding of \$20,000 budgeted for training and technology transfer.

14.2 Status of Task 13 Deliverables

Table 14-1 gives the status of each Task 13 deliverable listed in the 2004 WRAP RMC work plan, plus any additional deliverables agreed upon after the work plan was prepared.

Table 14-1. Status of the Task 13 deliverables.

Deliverable	Status
Develop material for a one-day introductory training class	Completed. Training agenda and PowerPoint files are available at http://pah.cert.ucr.edu/aqm/308/reports/training/Model_Training.htm
Offer first class in Salt Lake City in September 2004	Completed.
Provide support in computer systems configuration to Arizona DEQ	Initial support task complete. Additional support available as needed.
Develop a hardware and software FAQ sheet to be accessed on the RMC web site	In progress; to be updated periodically.

15. Summary of Work for March 1, 2004, through February 28, 2005

15.1 Task 0.5: 2002 Ammonia Emissions Inventory for WRAP Region

The RMC has developed an ammonia emissions inventory that includes livestock operations, fertilizer application, native soils, domestic sources, and wild animals, to be used for gridded modeling in the WRAP region. The inventory was created using the improvements and estimation methodologies described in Section 2 and documented in detail in Chitjian and Mansell (2003a,b). These inventory enhancements were associated with the effects of environmental parameters on the emission factors, and with the temporal and spatial allocation of NH_3 emissions for several source categories. The improvements were based on the results of a literature survey of recent research in NH_3 emissions inventory development. We developed a GIS-based NH_3 emissions modeling system and applied it for calendar year 2002 to generate a gridded, hourly emissions inventory for the WRAP modeling domain at a spatial resolution of 36 km. The data sources and environmental factors used in the inventory improvements were presented previously and in more detail in the draft task report (Mansell, 2004a).

On a regional scale, the 2002 NH_3 emissions inventory is dominated by fertilizer application and livestock operation emissions. This result is entirely consistent with the current understanding of NH_3 emission within the air quality and emissions modeling community. Ammonia emission from native soils, while a major component of the overall inventory, remains highly uncertain. This uncertainty arises mainly from the current differences of opinion in the research community with respect to whether soils act as a source or a sink of NH_3 . Ammonia emission from domestic sources, while only a small contributor to the total regional NH_3 inventory, can be a major source of emissions on smaller, urban scales. The wild animal NH_3 emissions are only a small portion of the inventory.

Section 2.3.6 compares the WRAP NH_3 inventory with similar results obtained from the CMU Ammonia Model; this is discussed in greater detail in Mansell (2004a). Based on state-level comparison, the results of this task are seen to be consistent with existing NH_3 emissions inventories. Evaluation of the differences and similarities, and a further investigation of the two inventories for detailed source categories at the county level, may provide useful insight into potential improvements and enhancements to the inventory and to the emissions modeling system.

Based on the results of this task, we make a number of recommendations (see Section 2.4.2) regarding improvements in data quality and refinements to the NH_3 inventory and emissions modeling system.

15.2 Task 1: Project Administration

The major activities in this task included:

- Communication with WRAP to define the scope of work, approach and specific tasks, and deliverables, and to communicate project results
- Coordination among the three contractors (one prime contractor, two subcontractors)
- Computer systems administration, including computer hardware, software, project web site, and mailing lists
- Contract administration

Because of the evolving and sometimes uncertain nature of the regulatory framework and guidance for visibility SIPs and TIPs, extensive discussion is required to carefully define the scope of work and deliverables. Moreover, because the RMC includes three different contractors who receive data from several WRAP contractors and WRAP forums, the project requires frequent communication. Project communication and coordination is handled through monthly conference calls with the WRAP modeling forum cochair on the second Monday of each month, and through a conference call with the WRAP Modeling Forum on the following Monday of each month. Additional conference calls are scheduled as needed, typically at least one call per week, for detailed follow-up on specific tasks. Progress and refinement of task definitions are also frequently discussed by e-mail and phone communications.

Computer systems for the RMC are maintained at UCR. ENVIRON and UNC staff have accounts on these computer systems so that all project staff can perform simulations on the RMC computers. Because there are “down times” between model simulations, computer resources funded by WRAP and other agencies can be shared. This provides an important efficiency in the use of computer resources and allows WRAP to benefit by having access to a larger number of computers when WRAP simulations are being performed.

The RMC web site and e-mail listserv are the primary method of communicating project results. These are updated regularly.

Finally, contract administration is also a complex and time-consuming activity that involves contract administration staff at WGA, UCR, UNC, and ENVIRON. Difficulty in communicating with or between administrative staff members at these institutions can sometimes be a significant source of frustration and delay in managing the project.

15.3 Task 2: Test, Improve, Quality Control, Obtain External Peer Review, and Finalize 36-km and 12-km MM5 Simulations for Eventual Use in CMAQ

The RMC has carried out MM5 simulations for the entirety of 2002 to support CMAQ visibility modeling for the §308 SIPs/TIPs. During the fall of 2003, we made an initial MM5 run for 2002 on the RPO Unified Continental 36-km Modeling Grid domain. This simulation used an MM5 model configuration similar to what has been used by the other RPOs (i.e., VISTAS, CENRAP,

MRPO). For this run, the modeling system performed better in the central and eastern United States than in the West, and in general performed better in winter than in summer (Morris et al., 2004a; Kemball-Cook et al., 2004). In the western U.S., the amplitude of the diurnal temperature cycle was persistently underestimated during the summer, especially in the Southwest. In the desert Southwest, the humidity was greatly overestimated during the summer as well, and there was a pronounced cold bias.

WRAP then requested that we perform further MM5 sensitivity tests to identify a better-performing model configuration for the western states. We ran sensitivity tests in which four physics options were changed: (1) the cumulus parameterization, (2) the LSM, (3) the PBL model, and (4) the FDDA. As a result of these tests, we obtained an improved MM5 configuration that provided better results.

The 36-km MM5 runs we made with this improved configuration showed a dramatic reduction in the summertime cold, wet bias in the desert Southwest. The surface temperature and humidity performance are now within benchmarks for all WRAP subdomains, except the desert Southwest for temperature. The new configuration gives a more accurate representation of the diurnal temperature cycle in the desert Southwest as well as a more realistic precipitation pattern over the western United States. Model performance over the eastern U.S. also improved.

After settling on a configuration for the 36-km annual run, we turned our attention to MM5's performance on the nested WRAP 12-km grid. Further sensitivity tests at this resolution were undertaken, allowing for the possibility that the 36-km physics options might differ from those selected for the 12-km run. Improved MM5 performance using the new configuration was also seen on the 12-km grid. Therefore, a new annual 36/12-km 2002 MM5 simulation was conducted and the results subjected to a model performance evaluation. The revised WRAP 2002 MM5 36-km results were compared against those for the initial WRAP 2002 36-km simulation, as well as the CENRAP and VISTAS 2002 36-km MM5 simulations. The results from the new WRAP 36-km and 12-km results were also compared. Details of these activities can be found at http://pah.cert.ucr.edu/aqm/308/mm5_reports04.shtml.

15.4 Task 3: 2002 Base Year Emissions Modeling, Processing, and Analysis

The four preliminary 2002 emissions simulations conducted by the RMC during this project year have served to prepare us for the final 2002 simulation and emissions sensitivities that will begin in 2005. The WRAP emissions modeling QA protocol—which includes the generation of comprehensive documentation, implementation of the Bugzilla project management system, and using CVS for version control—has proved to be a success. Using a team of emissions modelers, each with well-defined roles, worked well for managing the complex emissions modeling project at the RMC.

A summary of the major emission modeling tasks completed in 2004 by the WRAP RMC includes the following:

- *2002 WRAP emissions inventory database development:* This task included collection, QA, and enhancement of 2002 emissions inventories for the U.S., Canada, and

Mexico. We collected inventory data from WRAP inventory contractors, other RPOs, and EPA to build the WRAP inventory database for preliminary 2002 emissions modeling. The database is hosted at the RMC and will provided the basis for the final 2002 modeling that will be completed in 2005.

- *Simulation Pre02a_36*: We used this first preliminary 2002 simulation to test the emissions modeling QA protocol, collect a first set of 2002 inventories, and diagnose any problems with the emissions modeling system.
- *Simulation Pre02b_36*: The annual extension of simulation Pre02a_36, this simulation contained some data updates and produced the first results used in CMAQ modeling by the RMC.
- *Simulation Pre02c_36*: This annual simulation was created by the addition of actual 2002 wildfires and prescribed fires and typical-year agricultural fires to Pre02b_36.
- *Simulation Pre02c_36s01*: A one-month sensitivity to test the effects of the diesel retrofit emissions control program in the WRAP region.
- *Simulation Pre02d_36*: Several data updates, including new 2002 fires, actual 2002 VISTAS inventories, windblown dust, and anthropogenic ammonia emissions, created the last annual simulation of the year.
- *Simulation Pre02d_12*: An annual fine-grid nest of simulation Pre02d_36 on the WRAP 12-km modeling grid.
- *Simulation Pre02e_36*: An annual fire sensitivity to test the effects of natural fires.
- *Simulation Pre02f_36*: An annual fire sensitivity to test the effects of the updated 2002 fire inventories.

With the emissions modeling and QA infrastructure now fully developed, we are well prepared to begin the final 2002 emissions modeling, as well as the host of derivative sensitivities for evaluating the impacts of natural emissions on regional haze (Task 6 in the 2004 work plan, to be continued in 2005).

15.5 Task 4: Air Quality Model Evaluation for 2002 Annual Simulation

The RMC performed a CMAQ 2002 annual model simulation on the RPO Unified Continental 36-km Modeling Grid domain and the WRAP western U.S. 12-km domain using the final WRAP 2002 MM5 meteorological fields and the Base Case D (pre02d) emissions inputs. We then conducted an operational model performance evaluation that compared the CMAQ model estimates against observations from the IMPROVE, CASTNet, STN, and NADP networks in the WRAP region.

- Model performance for sulfate was reasonably good, albeit with a winter overestimation bias of 20% to 80% and a summer underestimation bias that reached as low as -20%.
- Nitrate performance was generally poor, with a winter overestimation (~ +100%) and summer underestimation (~ -100%) bias and large (100%-140%) errors. With the

exception of California, summer NO_3 levels are low, so the summer underestimation bias is not as big a concern as the overestimation bias in winter, when NO_3 makes up a larger fraction of the visibility extinction.

- Organic carbon performance exhibited less seasonal variation and is overstated in the winter. The CMAQ 36-km and 12-km OC performances are quite different from each other: summer OC bias was generally within $\pm 10\%$ using the 36-km grid, but OC is underestimated by -30% when the 12-km grid is used.
- Performance for elemental carbon was generally fairly good, with low ($< \pm 20\%$) monthly bias across the year, although with a fair amount of scatter (i.e., errors of 60% - 80%).
- “Other fine PM” (soil) was overstated in the winter, with fairly low bias in the summer. Coarse mass, on the other hand, was understated throughout the year, with winter bias of -40% to -80% and summer bias exceeding -100% . The reasons for the poor soil and CM performance are related to (1) model-versus-measurement incommensurability, whereby modeled soil and CM may include different components from those included in the measured values; (2) uncertainties and missing emissions (e.g., windblown dust); and (3) local (sub-grid-scale) impacts that are not captured by the model.

In summary, although there are noticeable areas of improvement needed in the 2002 CMAQ pre02d model performance, the performance is substantially better than the CMAQ 1996 simulation used in the §309 analysis. Performance for SO_4 and EC is generally fairly good, whereas performance of NO_3 and CM is poor.

15.6 Task 5: Preparation and Reporting of Geographic Source Apportionment Results

During 2003, UCR developed the Tagged Species Source Apportionment (TSSA) algorithm in CMAQ version 4.2.2 to assess source attribution. In 2004 we ported this code to a beta release of CMAQ version 4.4. However, it was discovered that there were problems with mass conservation in the model that made it difficult to fully attribute PM mass at receptor sites to emissions sources. We expended significant effort in the source attribution modeling task, which included debugging and refining the algorithm, completing the annual source attribution model simulation, and presenting and providing results to WRAP and its other contractors. Some uncertainty remains in the source attribution because of problems with mass conservation in CMAQ. This creates uncertainty in some of the source attribution results, especially with respect to the contribution of boundary conditions. However, we have more confidence in the ranking of the relative source attribution for the tagged sources other than boundary conditions. As part of Task 7, we also performed source attribution simulations for February and July using the CAMx Particulate Source Apportionment Technology (PSAT). In general the PSAT results were consistent with the CMAQ TSSA results, although there were significant differences in the relative ranking of sources at some receptor sites. Any additional source attribution modeling should be performed using the CAMx PSAT model while we complete further testing of the TSSA algorithm in a new release of CMAQ that corrects some mass conservation errors.

15.7 Task 6: Further Analysis of Model Performance in Regard to the Contribution of Natural Emissions to Visibility Impairment

The RMC used 2004 to focus on identifying the sources of haze impacting the WRAP region. By reviewing cursory model simulations we performed in 2003, EPA regional haze guidance documentation, and research completed by other RPOs, we established a direction for defining the distinction between natural and anthropogenic emissions sources contributing to regional visibility impairment. We circulated a memorandum in 2004 defining the various natural emissions sources that would be the focus of continuing research. Based on this memo, we completed a literature review to identify the availability of emission factors for modeling natural emissions sources. We used this information to develop emissions estimates for previously unaccounted-for natural sources of haze, and to implement new inventories created by the WRAP Emissions Forums that define natural versus anthropogenic emissions. We now have the information needed to begin modeling to assess the impacts of natural emissions sources on visibility impairment in the WRAP region.

15.8 Task 7: Evaluation and Comparison of Alternative Models

The CMAQ modeling system is the primary modeling tool being used in the WRAP 2002 modeling. However, there are many advantages to operating alternative models, such as being able to diagnose model performance, corroborate the primary model's results, quantify model uncertainty, and provide a backup modeling tool. A review of available alternative models identified the Comprehensive Air-quality Model with extensions (CAMx) as the optimal alternative model because it's similar state-of-science formulations as CMAQ, its use by several other RPOs (e.g., MRO and CENRAP) and availability of a PM Source Apportionment Technology (PSAT) capability. The CAMx modeling system was applied for February and July 2002 on the RPO Unified Continental 36-km Modeling Grid domain, and the model performance compared with CMAQ. In general CMAQ and CAMx exhibited similar model performance attributes with neither model exhibiting superior model performance across all species and subregions. The CAMx PSAT sulfate source apportionment was also compared with the PM source apportionment modeling results from the CMAQ TSSA runs. The CAMx PSAT and CMAQ TSSA sulfate source apportionment produced similar rankings of source region contributions to sulfate at western Class I areas, with the exception that the TSSA "Other" category that includes non-tagged sources, mass adjustments and mass conservation errors is not present in the PSAT results that accounts for the contributions of all sources.

15.9 Task 9: Testing and Further Improvements to the Windblown Dust Emissions Modeling Methodology

In 2004 we implemented the Phase II estimation methodology for PM dust emissions from wind erosion for calendar year 2002 on the RPO Unified Continental 36-km Modeling Grid domain. A number of sensitivity simulations were performed to investigate the effects of the various assumptions regarding dust reservoir characteristics and disturbance levels of the soils across the domain.

Based on a review of recent studies concerning dust emission from wind erosion, we developed a general estimation methodology. Emission rates were developed by soil type and wind speed. Land use/land cover data came from the NLCD database were used to determine the surface roughness lengths necessary for estimating threshold surface friction velocities. Wind speed, precipitation rates, and soil temperatures were based on MM5 model simulation results at a spatial resolution of 36 km. Although we improved the overall estimation methodology compared with our Phase I methodology, a number of assumptions were still required to implement the methodology (see Section 10.3).

The results, presented and discussed in Section 10.4, qualitatively appear to be consistent with the various assumptions made. Variations in estimated dust emissions by land use type and season are described in that section. A more detailed analysis of the model results and a comparison with ambient data are currently underway and will be documented in the final task report.

Although the results of the project are still being reviewed, we can already make a number of recommendations with regard to improvements in data quality and in the estimation methodology. These include incorporating more detailed land use type and soil characteristics data, implementing the model using higher-resolution meteorological data, applying transport fractions to the estimated dust emissions, and validating the methodology using a smaller-scale local domain.

15.10 Task 10: Continued Improvement to Model Evaluation Software

We continued to revise and improve the model performance evaluation (MPE) software during 2004. Because model performance guidance does not yet exist for visibility modeling, we continue to explore new evaluation methods and sometimes discover improved methods for presenting model results that necessitate changes in the MPE software. In particular, during 2004 we experimented with various types of plots for summarizing and effectively presenting the results of the model-to-ambient-data comparisons, including soccer plots and bugle plots. Beginning in January 2005 we also adapted a Microsoft Access Database program originally developed by Air Resources Inc. to produce stacked-bar time-series plots.

Although we continue to compute a wide variety of model performance metrics, we typically use mean fractional bias (MFB) and mean fractional error (MFE) when presenting evaluation results because these metrics provide the most balanced and symmetrical approach for characterizing model underpredictions and overpredictions.

We currently recommend presenting model evaluation results using a combination of bugle plots, stacked-bar time-series plots, and soccer plots. We are continuing to modify the MPE software to make it easier to generate these plots. We still need guidance from EPA on official criteria for defining acceptable performance for visibility modeling.

The MPE software is available for use to all WRAP contractors and WRAP members. We plan to release a public version of the MPE after completing revisions to the MPE documentation. A draft of the MPE user's guide is included as Appendix F.

15.11 Task 11: Sensitivity Studies Designed to Evaluate Uncertainties in Fire Emissions

With the Fire Emissions Joint Forum and Air Sciences Inc., the RMC developed several emission scenario combinations to study the effect of fires on air quality in general, and on visibility in particular. We completed CMAQ simulations for each of these scenarios and compared the results to the CMAQ results with no fire emissions. Fire emissions were classified as wildfires, prescribed burning, or agricultural burning. They were further classified as either natural or anthropogenic, with wildfires defined exclusively as natural, prescribed burning divided between natural and anthropogenic, and agricultural burning defined as exclusively anthropogenic. The fire scenario evaluations completed include the following:

- Comparison of the 2018 Base Smoke Management (BSM) and Optimal Smoke Management (OSM) strategies.
- Comparison of natural versus anthropogenic emissions.
- Evaluation of individual contributions of wildfires, prescribed burning, and agricultural burning.
- Evaluation of the sensitivity of the CMAQ results to changes in the vertical distribution of agricultural burning emissions.

Wildfires and natural fire emissions were the major component of the fire emissions inventory and by far the largest contributors among the three categories to ambient PM. Anthropogenic emissions had a relatively small effect on visibility because of the small magnitude of agricultural burning compared to total fire emissions. However, anthropogenic fire emissions might show larger effects in model simulations that use finer grid resolution. This would be a special concern for emissions located in or near Class I area. Thus, the significance of anthropogenic emissions should not be discounted based on these results, and additional studies should be performed at finer grid resolutions.

The CMAQ results were not sensitive to changes in the vertical distribution of agricultural burning emissions because these were small compared to the wildfire emissions. However, we would expect a different result for large wildfires for which the plume rise height may extend into the free troposphere, and which also have much larger emissions than agricultural burning, and therefore a larger effect on visibility in general. Additional sensitivity simulations should still be performed to evaluate the effects of plume rise height for large fires.

15.12 Task 12: Preliminary Meteorological, Emissions, and Air Quality Modeling Activities for Alaska

The State of Alaska is developing a plan to protect visibility and comply with the intent of the RHR. As part of the WRAP Alaska effort, we are developing techniques for credible modeling of regional haze in Alaska, and providing a preliminary evaluation of the potential contributions to regional haze in the Alaska Class I areas that are more likely to be affected by in-state emis-

sions. There are three main components of regional haze modeling: meteorological modeling, emissions modeling, and air quality modeling.

The State of Alaska is developing a statewide emissions inventory. It is thus premature to perform emissions and photochemical grid modeling, as not all of the data are currently available in a suitable form. Therefore, our current modeling approach for Alaska is to begin by developing meteorological modeling techniques to simulate the unique and complex meteorological conditions of the region. The MM5 model was applied for year 2002 on a 45/15-km grid and evaluated against available surface, upper-air, and synoptic data. The 2002 MM5 data are being used to perform preliminary air quality modeling using a simplified Lagrangian (trajectory) model in 2005 to provide an initial assessment of the potential effects of emissions from Anchorage and Fairbanks, as well as major stationary sources, on visibility at Denali National Park and Tuxedni Wilderness Area. The Lagrangian model we will use for preliminary WRAP Alaska visibility modeling is CALPUFF. CALPUFF is being applied for 2002 and the results compared against available observations for reasonableness.

15.13 Task 13: Training Courses for the WRAP States and Tribes

Basic CMAQ and SMOKE training classes are available through the CMAS Center. Therefore, the RMC focuses its efforts on advanced training and technology transfer. A one-day training class on the use of visibility modeling results was developed and offered in conjunction with the Attribution of Haze meeting held in September 2004.

The primary training need concerns the transfer of the models and datasets to the states and tribes, and instruction or assistance in setting up the modeling system. This includes aspects of hardware, operating systems, and installation and operation of models and datasets and the associated computers. We are engaged in several activities related to this need. For example, we are producing a frequently asked questions (FAQ) sheet that explains how to install an operating system and the modeling system on a Linux PC, and includes recommendations for computer hardware appropriate for the modeling system users' needs. This FAQ sheet will be posted on the project web site.

After providing some assistance to one state in setting up a specialized operating system for managing parallel computers, we determined that the best use of RMC resources would be to limit the assistance we provide to supporting a single, standard installation of Linux and the modeling system.

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Appendices A through E: Five Appendices to Section 5, “Task 3: 2002 Base Year Emissions Modeling, Processing, and Analysis”

Five appendices are referred to in Section 5, which covers Task 3. They are contained in a separate file located at

http://pah.cert.ucr.edu/aqm/308/reports/final/2004_RMC_final_report_Appendices_A-E.pdf

The titles of the appendices are as follows:

- **Appendix A:** Complete Listing of Simulation Pre02d_36 Input/Output Files and SMOKE Configuration Settings
- **Appendix B:** Area-Source Agricultural SCCs Replaced by Process-Based NH₃ Emissions Model
- **Appendix C:** Preliminary 2002 Emissions Density Maps
- **Appendix D:** Preliminary 2002 Bar Charts
- **Appendix E:** SMOKE QA Checklist for Simulation Pre02d_36

Appendix F: Appendix to Section 11, “Task 10: Continued Improvement to Model Evaluation Software”

One appendix is referred to in Section 11, which covers Task 10. This appendix is a draft of the model performance evaluation (MPE) documentation prepared by RMC staff at CE-CERT, University of California, Riverside and titled “User’s Guide: Air Quality Model Evaluation Software, Version 2.0.1.” The appendix is contained in a separate file located at

http://pah.cert.ucr.edu/aqm/308/reports/final/2004_RMC_final_report_Appendix_F.pdf