Modeling Protocol

AIR QUALITY MODELING STUDY FOR THE FOUR CORNERS REGION

Prepared for

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TABLE OF CONTENTS

Page

1. INTRODUCTION 1-1

1.1 Background 1-1
1.1.1 Purpose of the Modeling Protocol 1-1
1.2 Project Overview 1-2
1.2.1 CAMx Overview 1-3
1.3 Project Management 1-5
1.3.1 Data Gatekeepers 1-5
1.3.2 Communications Plan 1-6
1.3.3 Schedule and Deliverables 1-7

2. MODELING DOMAIN 2-1

3. BASE YEAR MODELING 3-1

3.1 Context for Modeling and Evaluation Approach 3-1
3.2 2005 Base Case Modeling 3-3
3.2.1 Meteorological Inputs 3-3
3.2.2 Emission Inputs 3-5
3.2.3 Initial/Boundary Conditions 3-5
3.2.4 Ancillary Model Inputs 3-5
3.2.5 CAMx Model Options 3-6
3.2.6 Modeling Strategy 3-6
3.3 Model Performance Evaluation 3-7
3.3.1 Available Aerometric Databases for Model Evaluation 3-8
3.3.2 Model Evaluation Process 3-9
3.3.3 Statistical Performance Metrics 3-11
3.3.4 Evaluation of CAMx Model Performance for the 2005 Base Case 3-14
3.3.5 Performance Goals and Benchmarks 3-16

4. FUTURE YEAR MODELING 4-1

4.1 PM Speciated Model Attainment Test 4-1

5. REFERENCES 5-1

TABLES

Table 1-1. Schedule for the Four Corners Air Quality Modeling Study. 1-7
Table 2-1. MM5 vertical layer definitions and mapping to CAMx vertical layers. 2-8
Table 3-1. CAMx meteorological input data requirements 3-4
Table 3-2. Routine statistical measures used in evaluating air quality models against observational data 3-13

FIGURES

Figure 1-1. Project management for the Four Corners Air Quality Study 1-6
Figure 2-1. 2005 36/12/4 km MM5 modeling domain used in the NMED Giant PSD Increment Consumption Study. 2-2
Figure 2-2(a). Maximum potential CAMx 36/12/4 km modeling domain according to the 2005 36/12/4 km MM5 domain from NMED Giant PSD Increment Consumption Study 2-3
Figure 2-2(b). Maximum potential CAMx 12/4 km modeling domain according to the 2005 12/4 km MM5 domain from NMED Giant PSD Increment Consumption Study..... 2-4
Figure 2-3(a). CAMx 36/12/4 km modeling domain to be used for the Four Corners Air Quality Modeling Study 2-6
Figure 2-3(b). CAMx 12/4 km modeling domain to be used for the Four Corners Air Quality Modeling Study 2-7
Figure 3-1. The humidity growth function f(RH) taken from the IMPROVE methodology for reconstructing extinction from ammonium sulfate and ammonium nitrate concentrations 3-12

1. INTRODUCTION

This document constitutes the modeling protocol for the Four Corners Air Quality Modeling Study, which is being carried out by the contractor team of ENVIRON International Corporation and Alpine Geophysics, LLC. This particular component of the study will apply the Comprehensive Air Quality Model with extensions (CAMx), a photochemical/PM dispersion grid model, to project and evaluate criteria pollutants and air quality related values in the Mesa Verde, San Pedro Parks, and Weminuche Class I areas and surrounding Class II areas. The air quality model will be supplied with high-resolution meteorological fields for the entire year of 2005, along with gridded, model-ready emissions for the year 2005 and for several 2018 future year scenarios. The meteorological and emission datasets have been developed under separate projects funded by local industrial stakeholders.

1.1 BACKGROUND

In response to concerns regarding the air quality impacts of growth in many types of sources, especially oil and gas sources and power generation, on Class I and surrounding Class II areas in the Four Corners region, the New Mexico Environmental Department (NMED), together with the Colorado Department of Public Health and Environment, convened the Four Corners Air Quality Task Force (FCAQTF). States, Tribes, Federal Land Managers and other stakeholders have been brought together under the FCAQTF to develop strategies for air quality management in the region. In connection with this effort, the FCAQTF identified a need to model the air quality impacts of potential alternative mitigation strategies being developed by various FCAQTF work groups. Impacts on criteria pollutants (ozone, particulate matter [PM]) and air quality related values (visibility and deposition) are to be evaluated. Impacts in the Mesa Verde, San Pedro Parks, and Weminuche Class I areas and surrounding Class II areas are of primary interest. To facilitate this effort, ENVIRON was contracted by BP America Production Company to develop a gridded, model-ready base case emissions for 2005 and a future year (2018) base case together with five mitigation options to be specified by the FCAQTF. In addition, a high resolution (4 km) MM5 annual simulation for 2005 has been completed, quality assured, and evaluated by Alpine Geophysics, working under subcontract to ENVIRON, at the direction of the NMED in a Prevention of Significant Deterioration (PSD) increment consumption study funded by Giant Petroleum.

In this particular component of the air quality study, the contractor team of ENVIRON and Alpine Geophysics will complete the mitigation option analysis in support of the FCAQTF by applying the CAMx photochemical grid model to the Four Corners region using the emission inventories and meteorological data we have developed as described above.

1.1.1 Purpose of the Modeling Protocol

This Modeling Protocol sets forth the procedures, data sources and modeling approach to be used in performing the air quality modeling and evaluation of air quality related values for the various Class I and Class II areas in the Four Corners area. Its main function is to serve as a means for planning and communicating how the modeling will be performed *before* it occurs. The protocol

guides the technical details of a modeling study and provides a formal framework within which the scientific assumptions, operational details, commitments and expectations of the various participants can be set forth explicitly and means for resolution of potential differences of technical and policy opinion can be worked out openly and within prescribed time and budget constraints. Although the air quality modeling of the Four Corners area is not currently planned to be part of a SIP attainment demonstration, much of EPA's guidance related to the content of Modeling Protocols is directly relevant and provide a road map for our work under this task (EPA, 1991; 2001; 2006; 2007). Note that because some aspects of the Four Corners Air Quality Modeling Study are predetermined (e.g., CAMx has been previously chosen for these analyses, and MM5 meteorological model outputs and emission inputs will be provided from other projects), this Modeling Protocol describes only the air quality modeling and analysis component.

The procedures described herein will be reviewed by the FCAQTF and stakeholders so that a full and complete understanding of the modeling approach will be understood by all. Agencies and Stakeholders are invited to comment on the procedures outlined in the Modeling Protocol; revisions to the protocol will be developed to address issues on an as-needed basis.

1.2 PROJECT OVERVIEW

Details of the technical approach are described in detail in the following sections of this Modeling Protocol. The air quality modeling to be conducted in this project will provide estimates of ozone, PM, sulfur and nitrogen deposition, and visibility impacts in the Four Corners area for 2005 and 2018 base cases, and up to five alternative mitigation scenarios to be defined by NMED/FCAQTF.

The components of the Four Corners Air Quality Study are as follows:

Modeling Protocol: A Modeling Protocol (this document) will be prepared that conforms to the recommendations on Modeling Protocols in EPA's guidance for 8-hour ozone, PM and regional haze modeling (EPA, 2007). The protocol will be provided to the NMED for review, and based on comments received from NMED, a revised Modeling Protocol will be prepared and submitted. Additional Modeling Protocol revisions will be prepared as needed during the course of the study.

Base Case Modeling: A modeling domain comprised of nested grids with 36, 12, and 4 km grid spacing (resolution) will be defined. The 2005 MM5 meteorological data fields will be processed into CAMx inputs for this domain configuration and quality-assured. Emission inputs will be quality assured, and other CAMx 2005 Base Case inputs will be developed. The model will be run for a winter and summer period (e.g., January and July 2005), followed by a preliminary performance evaluation and diagnostic testing (as needed), to identify the optimal model configuration that will be used to perform the full 2005 36/12/4 km CAMx annual base case simulation. CAMx will be run first on the 36 km grid for the full annual period; results from this run will be used to provide boundary conditions (BCs) to the 12 km grid (this is referred to as a "one-way" nesting technique). Then the 12/4 km grids will be run together in a fully two-way interactive manner. A Technical Report and associated presentation will be prepared that documents the Base Case modeling inputs and final configuration.

Model Performance Evaluation: A detailed and comprehensive model performance evaluation will then be conducted on the 2005 Base Case simulation. Available measurements for ozone and other gas-phase species, speciated PM and total PM mass, deposition and visibility will be compared with model output. Existing model evaluation software and techniques will be employed, which have been developed from regional modeling conducted for WRAP and other urban and larger-scale modeling programs. Graphical displays of model performance will be generated including scatter plots, time series plots, quantile-quantile plots, spatial maps of model predictions with superimposed observations, "soccer goal" plots, "bugle" plots and other displays. A Technical Report and associated presentation will be prepared that documents the 2005 CAMx Base Case performance evaluation.

Future-Year Modeling: A 2018 Base Case and 5 future-year mitigation strategies will be simulated using the 2005 36/12/4 CAMx modeling databases and configurations developed above. We will employ EPA guidance techniques to project future-year ozone, visibility and $PM_{2.5}$ concentrations. These techniques use the model in a relative sense to scale the observed values using relative response factors (RRFs). Spatial maps, bar charts and other graphical displays would be used extensively to convey the results. A Technical Report and associated presentation will be prepared that documents the 2018 CAMx Future Year results.

Final Report and Presentation: The results from the 2005 Base Case and 2018 Future Year modeling analyses will be documented in a draft Final Report and submitted to NMED for review by the FCAQTF. After receipt of comments, the report will be updated and resubmitted. A presentation on the study will be developed and presented at the Four Corners Task Force meeting in November 2007.

1.2.1 CAMx Overview

The CAMx modeling system is a publicly available (www.camx.com) three-dimensional multi-scale photochemical/aerosol grid modeling system that is developed and maintained by ENVIRON International Corporation (ENVIRON, 2006). 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 the extension to treat a variety of air quality issues including ozone, particulate matter (PM), visibility, acid deposition, and 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 (referred to as "Probing Tools"), including Process Analysis (IRR, IPR, and CPA), Decoupled Direct Method (DDM), and the Ozone and Particulate Source Apportionment Technology (OSAT/PSAT). CAMx has been widely used in recent years by a variety regulatory agencies for 1-hr and 8-hr ozone and PM_{10} SIP modeling studies as well as by several RPOs for regional haze modeling. Key attributes of the CAMx model include the following:

- Fully interactive two-way grid nesting that supports multiple levels of grids (e.g., 36/12/4 km);
- CB4, CB05 or SAPRC99 gas-phase photochemical mechanisms;
- Two gas-phase chemical solvers, the CAMx Chemical Mechanism Compiler (CMC) Fast Solver or the highly accurate Implicit Explicit Hybrid (IEH) solver;

- Two separate treatments of PM using the same ISOROPIA and RADM chemistry algorithms as CMAQ:
    - A static two-mode (coarse/fine) option comparable to the approach in CMAQ;
    - A multi-section "full-science" approach using the Multi-component Aerosol Dynamics Model (MADM) that treats the effects of condensation/evaporation, coagulation and nucleation upon the particle size distribution.
- Secondary organic aerosol thermodynamics represented using a semi-volatile scheme;
- Multiple numerical algorithms for horizontal transport including the Piecewise Parabolic Method (PPM) and Bott advection solvers;
- Subgrid-scale Plume-in-Grid (PiG) algorithm to treat the near-source plume dynamics and chemistry from point sources;
- Ability to interface with a variety of meteorological models including the MM5, RAMS, and WRF prognostic hydrostatic meteorological models and the CALMET diagnostic meteorological model (others also compatible);

CAMx provides two key options to users interested in simulating PM. For CPU-efficient PM modeling applications, CAMx may be run using a two mode size representation (fine and coarse) similar to the treatment in CMAQ. Alternatively, more rigorous aerosol simulations (perhaps for shorter episodes) may be addressed using the version that treats N-size sections (N is typically 10) and the rigorous, but computationally-extensive MADM multi-section chemistry module.

The databases required to set up and operate CAMx for the Four Corners Air Quality Modeling Study are as follows:

- Three-dimensional hourly meteorological fields generated by MM5 and prepared using the MM5CAMx interface processor;
- Two-dimensional low-level (surface layer) emissions and elevated point source emissions generated by an emissions processor;
- Initial/boundary (IC/BC) inputs for the coarsest (master) grid as prepared by WRAP;
- Photolysis rates look up table;
- Monthly Albedo/Haze/Ozone Column input file prepared from several available global satellite-derived datasets;
- Land use and topography, as prepared for MM5.

All mathematical models possess inherent limitations owing to the necessary simplifications and approximations made in formulating the governing equations, implementing them for numerical solution on fast computers, and in supplying them with input data sets and parameters that are themselves approximations of the full state of the atmosphere and emissions processes. Like all air quality models, a major limitation of CAMx rests with the input fields that characterize emissions, meteorology, and IC/BCs. Key science limitations in the model itself include the nitrate formation chemistry and the secondary organic aerosol (SOA) module. Preliminary modeling by the RPOs (e.g., WRAP, VISTAS and CENRAP) found both CAMx and CMAQ nitrate performance suspect with winter overestimations and summer underestimations (Morris et al., 2004, 2005). While not as poor as CMAQ, the VISTAS and CENRAP modeling also found CAMx performance for Organic Carbon (OC) to be less than ideal; much of the OC performance problems have been due to deficiencies in the SOA module that in the past has failed to account for several known processes important to SOA (e.g., polymerization). Much of these limitations

have been addressed in an improved SOA module now available in CAMx; additional research in this area is on-going.

1.3 PROJECT MANAGEMENT

The Four Corners Air Quality Modeling Study will be conducted by ENVIRON International Corporation and Alpine Geophysics, with input from FCAQTF participants. Organizational commitment is an essential element for developing and implementing a successful research project. The overall project organization is shown in Figure 1-1.

The project management organization established for the ENVIRON/Alpine team is based on the respective expertise of the individual team members. ENVIRON is the prime contractor, and Mr. Till Stoeckenius in ENVIRON's Novato, CA office will serve as the Project Manager; in this role he will be the main point of contact for the NMED, and will be responsible for the timeliness and quality of all project deliverables. Mr. Ralph Morris (also of ENVIRON's Novato office) will serve as Principal-in-Charge for the project. Mr. Morris will ensure that staffing and other resources are made available to the project to meet the needs of NMED. Mr. Dennis McNally will serve as Alpine Geophysics' subcontractor point of contact; he will direct all of Alpine's work on preparation of the MM5 model output for use in CAMx and CAMx model evaluation. ENVIRON has a substantial track record of successfully working together with Alpine Geophysics on complex and high profile air sciences modeling projects and generating high-quality deliverables.

1.3.1 Data Gatekeepers

For quality assurance purposes, we have designated certain key individuals to serve as gatekeepers for data flowing into the modeling analysis. These individuals will be responsible for ensuring that the data provided to the model fulfill the modeling requirement, are consistent with the modeling protocol, have been adequately quality assured, and are ready to be used in the model when needed. Separate air quality, meteorological and emissions gatekeepers have been identified whose roles are defined below.

- **Meteorological Gatekeeper:** As necessary, obtain meteorological data as appropriate for annual 2005 modeling runs and perform data quality checks, together with appropriate documentation of model performance evaluation activities. Chris Emery will serve as the Meteorological Gatekeeper.

- **Emissions Gatekeeper:** Obtain emissions inventory data necessary to support annual 2005 and future year modeling. Assure quality of all emissions data received is consistent with the Modeling Protocol. Ms. Ou Nopmongcol will serve as the Emissions Gatekeeper.

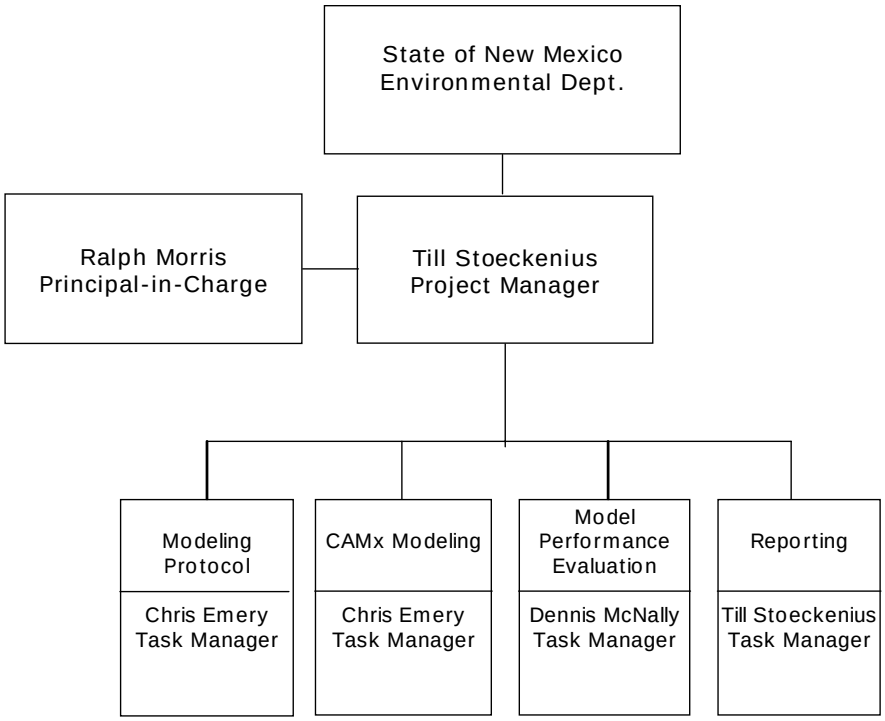


Figure 1-1. Project management for the Four Corners Air Quality Study.

- **Air Quality Data Gatekeeper:** Compile, QA/QC, and maintain the observational database used in the model performance evaluation. Maintain the modeling results and other documents as requested by the FCAQTF to support the modeling tasks. This includes, for example, the storage of model inputs and outputs for annual runs and the transfer (via USB/firewire portable disk or alternative media) of electronic files to NMED and other interested parties. Till Stoeckenius will serve as the Air Quality Data Gatekeeper.

1.3.2 Communications Plan

The ENVIRON team will conduct several activities to ensure smooth project management and communications throughout the project, including:

- Weekly or bi-weekly conference calls among ENVIRON and Alpine Geophysics personnel.
- Monthly calls between the ENVIRON team and NMED personnel; ENVIRON team task managers will participate as appropriate.
- Monthly progress reports prepared by ENVIRON with input as needed from Alpine Geophysics; these reports will summarize project progress, results to date, problems encountered and necessary action items, and plans for the upcoming reporting period..
- Continuous, regular e-mail and telephone contacts as necessary to ensure the communication of progress, issues and their resolution, accuracy of the results, and timely completion of the tasks.

The modeling team members and agency representatives will utilize e-mail as the primary means of routine correspondence and data exchange. Larger data file transfer will require FTP; the largest modeling files are quite volumous and will require shipment via external disk drives. Unscheduled meetings or conference calls will also be held concerning specific issues as the needs arise.

Miscellaneous documents, presentation material, reports, and small data files will be provided on the project FTP site. A web-enabled anonymous FTP site will be set up at: ftp://ftp.environ.org/pub/webaccess/FourCorners.

1.3.3 Schedule and Deliverables

The current schedule for this project is detailed in Table 1-1. All work is to be completed by 30 November 2007. While this is a fairly ambitious schedule, we will be able to complete all of the requested work within this timeframe by combining resources available at ENVIRON and at Alpine Geophysics.

Table 1-1. Schedule for the Four Corners Air Quality Modeling Study.

Task	Description	Due Date
1	Modeling Protocol Progress Reports	30 June 2007 Monthly
2	Draft Technical Report Base Year Modeling	15 September 2007
3	Draft Technical Report Model Performance Evaluation	15 September 2007
4	Draft Technical Report Future Year Modeling	31 October 2007
5	Draft Presentation Final Presentation	31 October 2007 7 November 2007
	Draft Final Report Final Report	16 November 2007 30 November 2007

2. MODELING DOMAIN

The Four Corners air quality modeling will be conducted using CAMx with 2005 meteorological data developed from a 36/12/4 km MM5 simulation conducted as part of the NMED Giant PSD Increment Consumption study. Figure 2-1 displays the MM5 36/12/4 km modeling domain used in the NMED Giant modeling. CAMx will also be similarly applied on a 36/12/4 km grid system that will need to match the MM5 Lambert projection and fit within the respective MM5 grids. CAMx will be run first on the 36 km grid for the full annual period; results from this run will be used to provide boundary conditions (BCs) to the 12 km grid (this is referred to as a "one-way" nesting technique). Then the 12/4 km grids will be run together in a fully two-way interactive manner.

When nesting a CAMx modeling domain within an MM5 modeling domain there are certain rules that must be followed: (1) there must be a buffer of at least 5 grid cells from the MM5 domain boundaries in order to limit artifacts of the MM5 solution near the boundary; and (2) when using two-way grid nesting the modeling domain boundaries of the fine grids must align with the coarsest grid used. Figure 2-2(a) displays the maximum possible CAMx 36/12/4 km modeling domain that can be set within the existing 2005 36/12/4 km MM5 configuration. Also plotted in Figure 2-2(b) are the locations of the IMPROVE and CASTNet monitoring sites in the Four Corners states.

The CAMx 36 km grid will correspond to the Regional Planning Organizations (RPO) continental U.S. domain that is being used by WRAP, CENRAP, MRPO, and VISTAS for their 2002 CAMx/CMAQ regional haze modeling. This will allow the use of WRAP emission databases on the 36 km grid. Note that we considered whether the 36 km grid should be reduced, given our focus on the Four Corners area. However, we took note of recent 8-hour ozone State Implementation Plan (SIP) modeling performed by Clark County (Las Vegas), who reduced the size of the 36 km grid by eliminating the eastern U.S. They found that some of their episodic ozone days were heavily influenced by the eastern boundary conditions. Use of the full 36 km RPO modeling grid is highly advantageous and so will remain unchanged.

However, it is desirable to reduce the size of the 12 km and 4 km domains to increase computational efficiency. Concerning the 12 km CAMx domain, the eastern, western, and northern boundaries will remain at their maximum extent as shown in Figure 2-2. We see no reason to bring in the eastern boundary to reduce its size. It may be important to include transport from California, so the western boundary appears to be appropriate as well. Finally, it will be advantageous to include the Yellowstone and Grand Teton IMPROVE monitors in the model evaluation, so the northern boundary remains unchanged. However, the southern boundary will be moved northward somewhat to make it consistent with 12 km emissions surrogate distributions that ENVIRON has already prepared.

The 4 km domain is reduced from the maximum shown in Figure 2-2 as follows:

- The domain extends sufficiently west and south to include the IMPROVE and nearby CASTNet sites in the Petrified Forest National Park;
- The domain extends as far east to include San Pedro Parks Wilderness Area; and

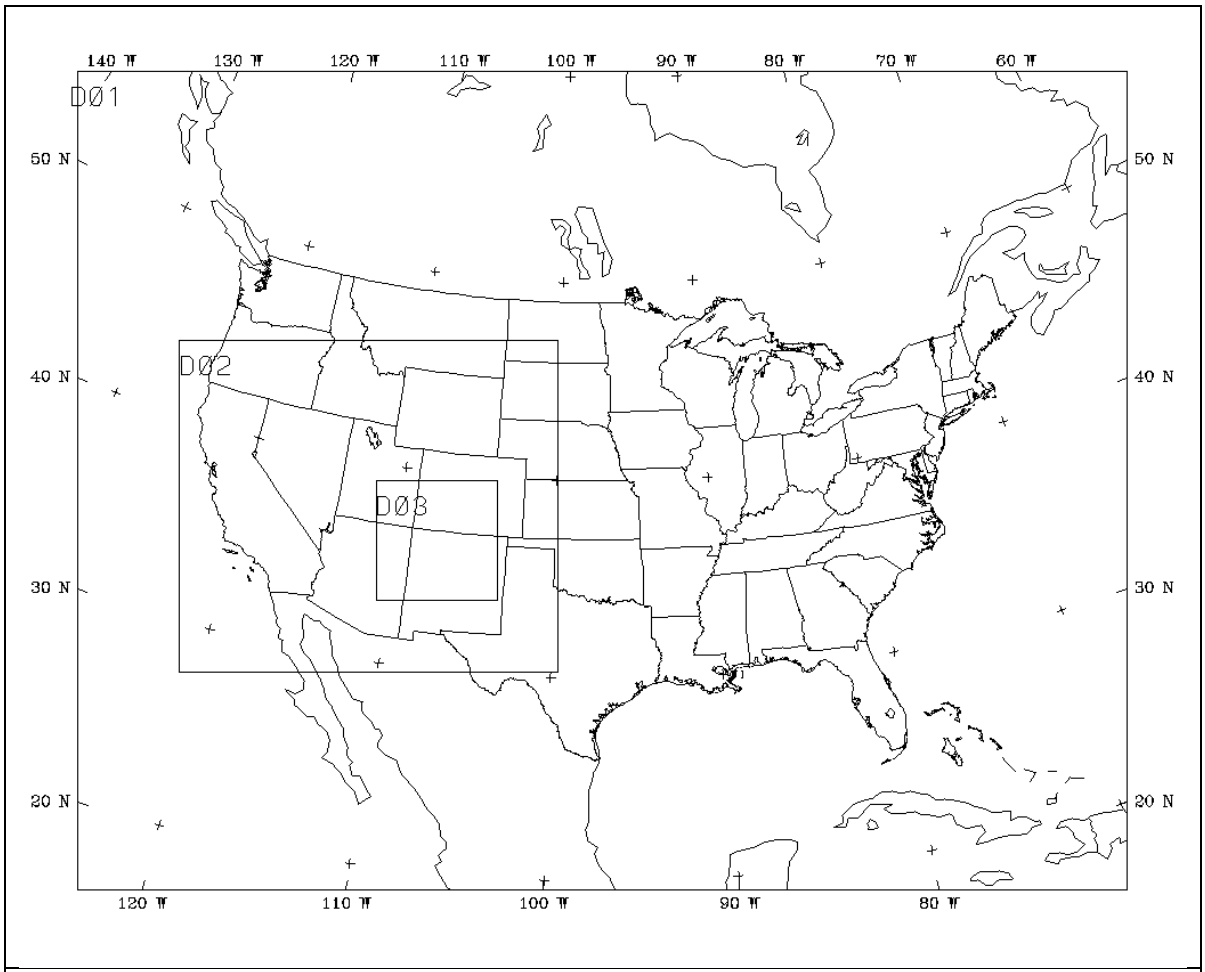


Figure 2-1. 2005 36/12/4 km MM5 modeling domain used in the NMED Giant PSD Increment Consumption Study.

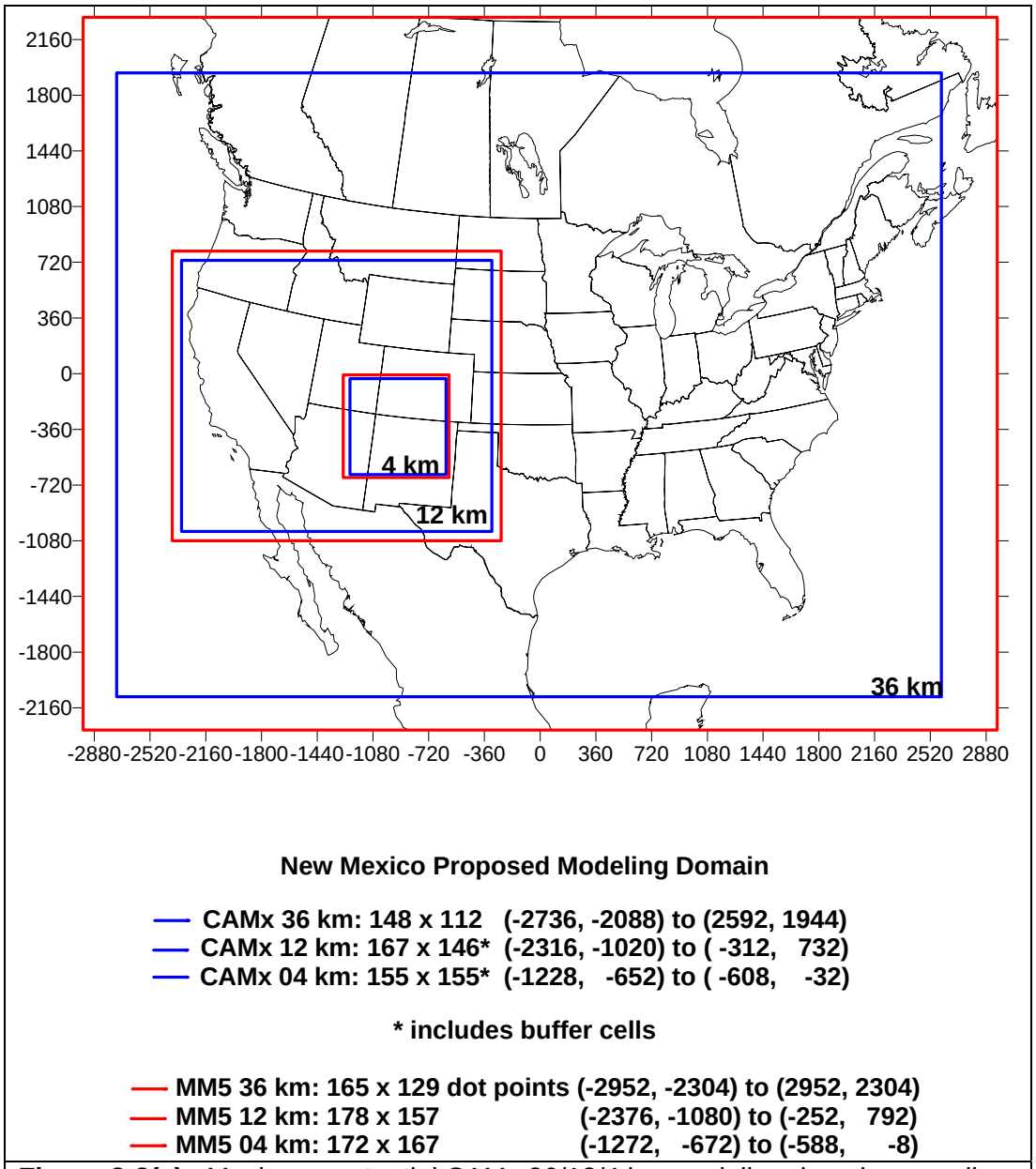


Figure 2-2(a). Maximum potential CAMx 36/12/4 km modeling domain according to the 2005 36/12/4 km MM5 domain from NMED Giant PSD Increment Consumption Study.

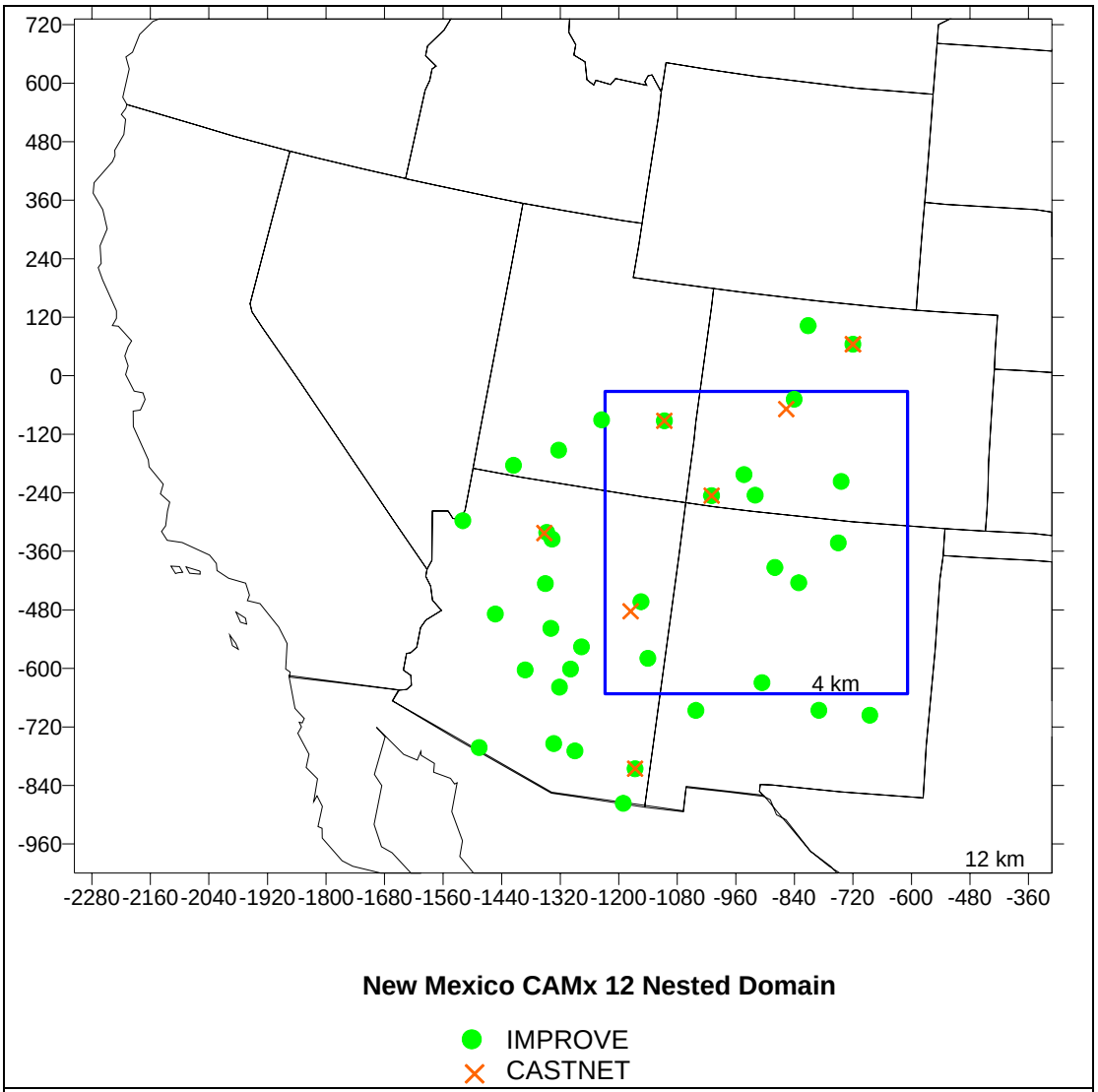


Figure 2-2(b). Maximum potential CAMx 12/4 km modeling domain according to the 2005 12/4 km MM5 domain from NMED Giant PSD Increment Consumption Study.

- The domain extends as far north to include Mesa Verde National Park and Weminuche Wilderness Area.

The resultant CAMx 36/12/4 km modeling domain for the 2005 Four Corners Air Quality Modeling Study is displayed in Figure 2-3(a). Figure 2-3(b) displays the 12/4 grid domain and the locations of the IMPROVE, CASTNet and NADP monitoring sites. The 4 km domain includes 5 IMPROVE, 5 CASTNet and 2 NADP monitoring sites.

Table 2-1 displays how the CAMx vertical grid will be meshed with the MM5 vertical grid structure. This mapping is taken from the methodology used by WRAP. Note that 19 CAMx layers will comprise an aggregation of 34 MM5 layers. This is done to increase computational efficiency, while maintaining higher resolution in the planetary boundary layer (lowest ~3 km of the atmosphere) where the bulk of pollutant chemistry and transport take place. Such layer collapsing is performed in nearly every regulatory modeling exercise, and is especially necessary to maximize model speed for annual simulations. Early testing by WRAP found nearly identical air quality modeling results were obtained using no layer collapsing (i.e., 34 vertical layers that exactly match MM5) and 19 vertical layers. However, more aggressive layer collapsing (e.g., 12 layers) affected the surface predicted concentrations. Thus, in Table 2-1 we have proposed a 19 vertical layer structure that is consistent with WRAP, CENRAP and VISTAS.

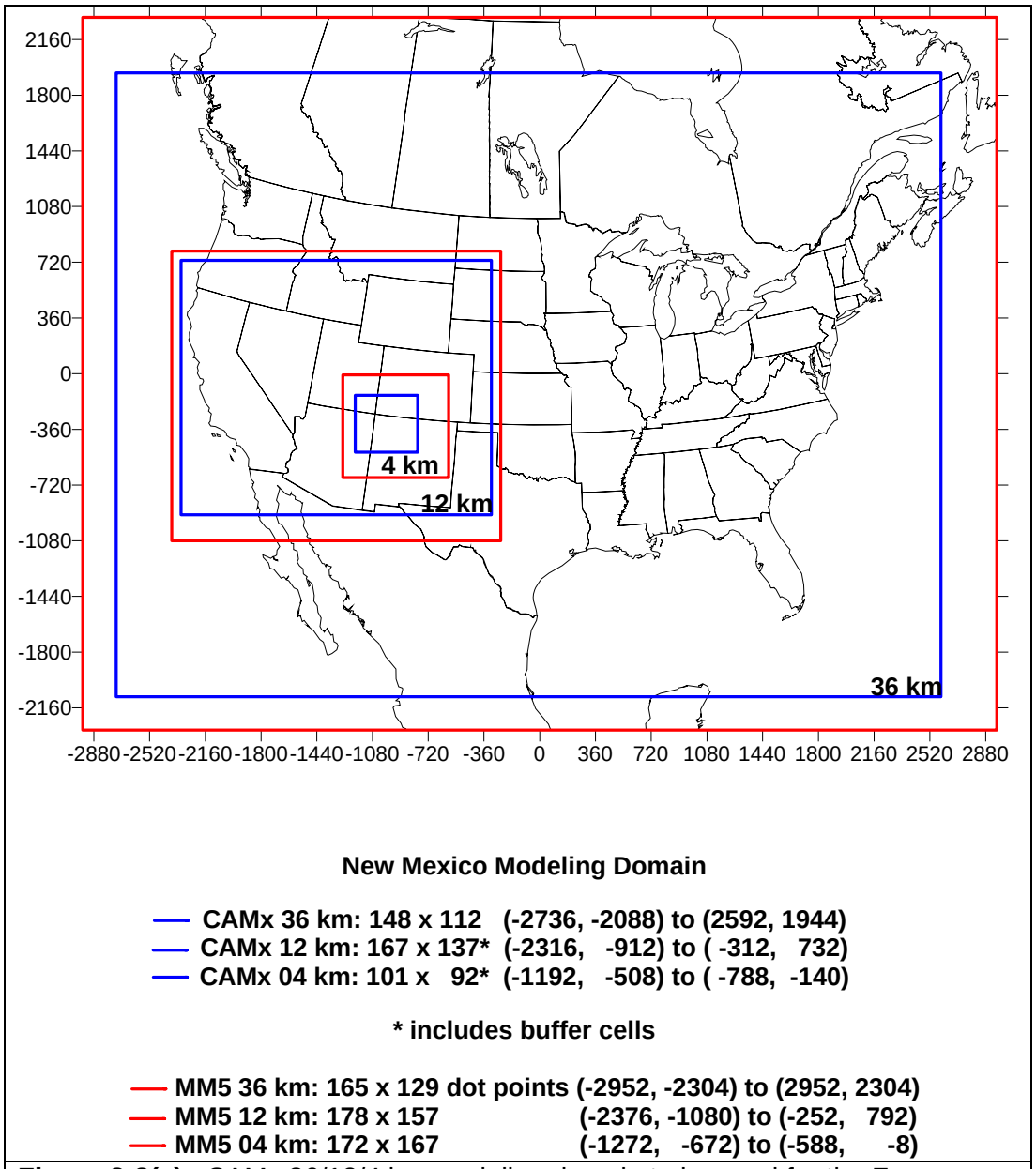
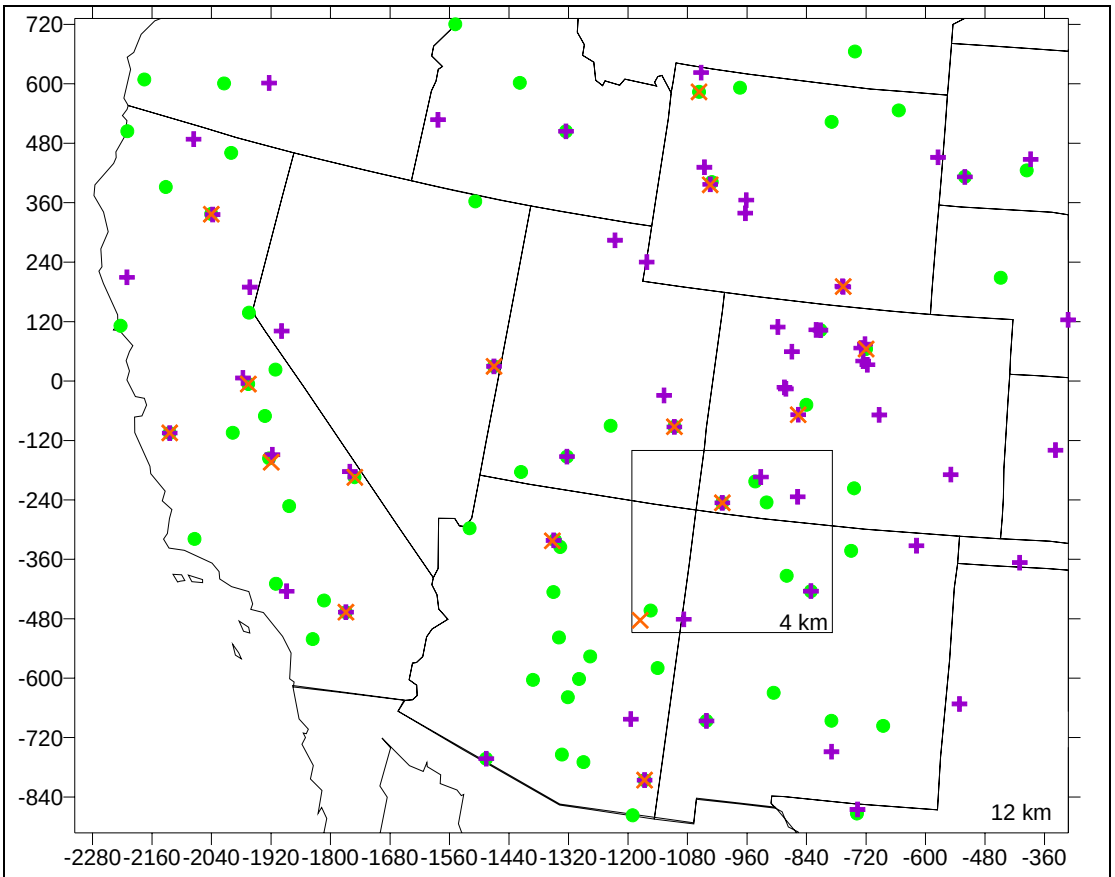


Figure 2-3(a). CAMx 36/12/4 km modeling domain to be used for the Four Corners Air Quality Modeling Study.



New Mexico CAMx 12 km Nested Domain

● IMPROVE
× CASTNET
✚ NADP

CAMx 12 km: 167 x 137* (-2316, -912) to (-312, 732)
CAMx 04 km: 101 x 92* (-1192, -508) to (-788, -140)

* includes buffer cells

Figure 2-3(b). CAMx 12/4 km modeling domain to be used for the Four Corners Air Quality Modeling Study.

Table 2-1. MM5 vertical layer definitions and mapping to CAMx vertical layers.

MM5 Vertical Layers					CAMx Vertical Layers		
K (MM5)	sigma	Press (mb x 100)	Height (m)	Depth (m)	K (CAMx)	Height (m)	Depth (m)
34	0.000	10000	15674	2004	19	15674	7053
33	0.050	14500	13670	1585			
32	0.100	19000	12085	1321			
31	0.150	23500	10764	1139			
30	0.200	28000	9625	1004			
29	0.250	32500	8621	900	18	8621	2467
28	0.300	37000	7720	817			
27	0.350	41500	6903	750			
26	0.400	46000	6153	693	17	6153	1942
25	0.450	50500	5461	645			
24	0.500	55000	4816	604			
23	0.550	59500	4212	568	16	4212	1104
22	0.600	64000	3644	536			
21	0.650	68500	3108	508	15	3108	896
20	0.700	73000	2600	388			
19	0.740	76600	2212	282	14	2212	556
18	0.770	79300	1930	274			
17	0.800	82000	1657	178	13	1657	353
16	0.820	83800	1478	175			
15	0.840	85600	1303	172	12	1303	341
14	0.860	87400	1130	169			
13	0.880	89200	961	167	11	961	249
12	0.900	91000	794	82			
11	0.910	91900	712	82	10	712	163
10	0.920	92800	631	81			
9	0.930	93700	550	80	9	550	80
8	0.940	94600	469	80	8	469	80
7	0.950	95500	389	79	7	389	79
6	0.960	96400	310	78	6	310	78
5	0.970	97300	232	78	5	232	78
4	0.980	98200	154	39	4	154	39
3	0.985	98650	115	39	3	115	39
2	0.990	99100	77	38	2	77	38
1	0.995	99550	38	38	1	38	38
0	1.000	100000	0	0	0	0	0

3. BASE YEAR MODELING

3.1 CONTEXT FOR MODELING AND EVALUATION APPROACH

Although the emergence of affordable and fast Linux PCs allows for annual/continental air quality modeling using photochemical grid models on nested grids, it remains a challenge to achieve the best model performance possible given: the many factors associated with evaluating performance for ozone, multiple $PM_{2.5}$ species, and wet/dry deposition; uncertainties associated with the meteorology and emissions; and variations in the important physio-chemical processes associated with different locations and times of the year. With the limitations imposed by the schedule and resource availability, as well as the extensive computer requirements associated with annual ozone/PM modeling, the number of model iterations required to develop a well performing base case, as done for episodic SIP modeling, will not be possible[1]. Thus, much of the technical approach to be applied in this project builds from our past experience with ozone/PM/visibility modeling, tailored to the specific and unique conditions of the Four Corners region. Some elements in our recent past experience that we would put to use in the Four Corners air quality study include the following:

- We have amassed a history of model performance expectations for ozone, $PM_{2.5}$ and regional haze from which general model performance attributes can be gleaned:

  Ozone: Current photochemical grid models generally perform well for ozone in most urban and rural applications, with perhaps a tendency for under prediction. In most cases ozone model performance achieves EPA's performance goals and adequate ozone model performance is attainable. Reasons for ozone underestimation tendencies likely include misrepresented emission rates and VOC speciation, limitations in the photochemical mechanisms themselves, improperly characterized vertical mixing, and/or inadequate treatment of other processes, often specific to each area, that are important to ozone formation.

  Sulfate (SO4): Model performance for SO4 has been fairly good, which is probably due to well characterized emissions (e.g., known point source emissions rates) and relatively simple chemistry.

  Nitrate (NO3): Performance for NO3 has been challenging for the current models. This is due to the complex chemical cycle that transforms NOx to total nitrate, the partitioning of total nitrate between gaseous nitric acid and particle NO3 (which depends strongly on ambient SO4, ammonia and meteorology), very large uncertainties in ammonia emissions, and the strong roll of wet and dry deposition pathways. It is also very difficult to measure, given its volatility. This is an area that will be evaluated very closely in the Four Corners Modeling Study.

  Ammonium (NH4): Performance for NH4 has been mixed and generally follows the performance for SO4 and NO3 in a particular application, depending upon which acid is

[1] For example, ENVIRON's work with the State of Texas for a recent ozone SIP required over 40 base case simulations in order to achieve an adequate level of model performance.

dominant. Performance evaluations have been limited by the fact that many PM monitoring networks do not measure NH4 (such as IMPROVE), and complicated by the fact that ammonia emissions are very uncertain and that NH4 salts can take on many forms depending upon the relative quantities of the various acids and environmental conditions.

Elemental Carbon (EC): With the exception of fire events, performance for EC has been fairly good. Again, well characterized emissions from combustion sources and no chemistry are likely causes for this good performance.

Organic Carbon (OC): Performance for OC has been mixed, and depends upon the model formulation, the region of interest, and the mix of contributing sources. OC is typically one of the largest components of $PM_{2.5}$ and regional haze; it is often dominated by wildfire emissions in the western U.S. OC is complicated because there are both primary (e.g., combustion) and secondary contributors, and its volatile components are difficult to measure. There is currently an intense area of research investigating the sources and chemistry of secondary organic aerosol (SOA), and the SOA chemistry modules in both CMAQ and CAMx have been updated to include new biogenic sources of SOA. The modeling team will use the latest version of CAMx, which incorporates a new SOA module that includes SOA pathways from biogenic sesquiterpene, isoprene, and terpenes. However, this would require that biogenic emissions be generated with the new MEGAN biogenic emissions model.

Inorganic Primary Fine PM (IP): Performance for IP has been poor. This is due to: (1) PM speciation profiles that allocate unidentified PM to this species; (2) miss-matches between what the modeled and measured values represent; and (3) emission sources that are poorly characterized, episodic and uncertain (e.g., wind blown and fugitive dust).

Coarse Mass (CM): CM performance has also been poor as a large part of the measured contribution is due to local fugitive dust sources whose emissions are poorly characterized and not appropriately modeled with regional models (e.g., the fact that the vast majority of CM from specific sources settles upon nearby vegetation and structures soon after being emitted cannot be handled in grid models, since emissions are instantaneously diluted to grid scale).

- An important issue to consider is that different PM monitoring networks may use different measurement approaches that “measure” different amounts of the same species, which further differ from the form of the modeled species. It is often difficult to gauge model performance against specific measurements, since we must emulate “how” the PM is measured (i.e., the form of sulfate reported, loss of carbon and nitrate via volatilization, etc.). Such measurement issues can introduce an apparent model bias that may not be truly there. In other words, measurements do not necessarily always represent “truth”; as modelers, we must build in a large margin for what is “acceptable” performance when comparing model results to measurement data.

- It is difficult to perform comprehensive diagnostic testing on annual simulations due to the computational requirements and the vast amount of data generated. Consequently, we will perform initial diagnostic model testing over two representative months to identify

an optimal model configuration for the annual run. We have used this same approach for the VISTAS (Morris et al., 2004), and other studies (e.g., CENRAP, WRAP and the ongoing St. Louis 8-hour ozone and $PM_{2.5}$ modeling study).

The CAMx model evaluation protocol concentrates on an operational evaluation of 1-hour and 8-hour ozone concentrations and PM species concentrations that are consistent between the model and measurements (i.e., SO_4, NO_3, NH_4, OC, EC, IP, and CM). Where feasible and supported by sufficient measurement data, we will also evaluate the modeling system for its ability to accurately estimate gas-phase oxidant and precursor/product species since correct, unbiased simulation of gas-phase photochemistry is a necessary element of reliable secondary PM formation. This evaluation will focus on available measurements within the 4 km Four Corners domain; however an evaluation across the full 12/4 km western U.S. on a month-by-month basis will be relied upon heavily to build confidence that the modeling system is operating correctly in the Four Corners region. With this context in mind, we next turn to the actual steps in the CAMx Base Case model application and evaluation process.

3.2 2005 BASE CASE MODELING

The modeling team will develop CAMx modeling inputs on the 36/12/4-km nested modeling domain for a 2005 Base Case simulation. Preliminary model testing and evaluation will be performed over two months of the year to establish the model configuration and any input modifications needed, after which a full 2005 annual simulation will be performed.

3.2.1 Meteorological Inputs

Meteorological data for this project will be derived from MM5 modeling of the calendar year 2005 on a similar 36/12/4 km nested grid structure (as described in Section 2). The MM5 simulation has been completed by the ENVIRON/Alpine Team for the Giant/NMED project. Details of the MM5 application are described in the Giant/NMED work plan and final report (ENVIRON and Alpine Geophysics, 2006; McNally and Schewe, 2006).

It is necessary to convert raw output from the MM5 meteorological model to formats and variables used by CAMx specifically. The MM5CAMx translation processor will be used to complete this task. The software includes the ability to interpolate data from the native map projections used by the meteorological model to any projection to be specified for the air quality model (CAMx may be applied on Lambert Conformal, Polar Stereographic, or UTM Cartesian projections, or in geodetic latitude/longitude).

CAMx requires meteorological input data for the parameters described in Table 3-1. All of these input data are derived from the MM5 results. MM5CAMx performs several functions:

Table 3-1. CAMx meteorological input data requirements.

CAMx Input Parameter	Description
Layer interface height (m)	3-D gridded hourly time-varying layer heights
Winds (m/s)	3-D gridded hourly wind vectors (u,v)
Temperature (K)	3-D gridded hourly temperature and 2-D gridded surface temperature
Pressure (mb)	3-D gridded hourly pressure
Vertical Diffusivity (m^2/s)	3-D gridded hourly vertical exchange coefficients
Water Vapor (ppm)	3-D gridded hourly water vapor mixing ratio
Cloud Cover	3-D gridded hourly cloud and precip water contents
Landuse Distribution	2-D gridded static landuse/landcover distribution

1. Extracts data from the MM5 grids to the corresponding CAMx grids; in this study, the extraction includes a simple one-to-one mapping from the MM5 Lambert Conformal grid to the CAMx Lambert Conformal grid, with appropriate windowing to remove the extra row/columns in the MM5 grids.
2. Performs mass-weighted vertical aggregation of data for CAMx layers that span multiple MM5 layers.
3. Diagnoses key variables that are not directly output by MM5 (e.g., vertical diffusion coefficients and some cloud information).

The MM5CAMx program has been written to carefully preserve the consistency of the predicted wind, temperature and pressure fields output by MM5. This is the key to preparing mass-consistent inputs for CAMx, and therefore for obtaining high quality performance from CAMx.

The MM5CAMx processor will be used to process the 2005 MM5 output data fields from each modeling grid to the CAMx grids, variables and formats. We will employ layer collapsing to reduce the number of vertical layers from the 34 used in the MM5 modeling (as described in Section 2). Vertical diffusivities (Kv) are an important input to the CAMx simulation since they determine the rate and depth of mixing in the planetary boundary layer (PBL) and above. In general, our experience has been that diffusivities from meteorological models require careful examination before they are used in air quality modeling. This may be because the air quality model results are much more sensitive to diffusivities than the meteorological model results. We will evaluate the CAMx diffusion inputs by comparing the Kv values from several diagnostic calculation approaches. Two sets of vertical turbulent diffusivity files will be generated by MM5CAMx:

- Use of the O'Brien scheme (OB70);
- Use of the CMAQ scheme.

Sensitivity simulations will be undertaken with the two variations. Additionally, MM5CAMx will be set up to apply both 0.1 m^2/s and 1.0 m^2/s minimum Kv values, which will be evaluated in these same sensitivity tests. The choice of minimum Kv value is an area of ongoing investigation by both the CMAQ and CAMx developers. The problem relates to simulating the proper degree of the pollutant buildup during stable (e.g., nighttime) conditions. A value that is too small often results in over predictions of PM and ozone precursors such as NOx that can

artificially remove ozone, while a value that is too large may lead to significant under predictions. These problems have been seen to impact daytime photochemistry and the calculation of 24-hour PM levels.

As described in Section 1, we have established a Meteorological Gatekeeper to provide independent review and QA/QC of the meteorological inputs. Mr. Chris Emery will serve as the Meteorological Gatekeeper for this study. He will provide a final level of QA/QC on the model-ready meteorological inputs processed by the MM5CAMx program, and ensure that data are transferred to the model correctly.

3.2.2 Emissions Inputs

CAMx emissions inputs for the study are being developed by ENVIRON under separate funding. Documentation on the development of model-ready emissions will be prepared at the conclusion of that project. Thus, for this work effort, we are expecting that speciated, hourly, model-ready emissions for 2005 on the 36/12/4 km CAMx grids will be fully available.

As described in Section 1, we have established an Emissions Gatekeeper to provide independent review and QA/QC of the emission inputs. Dr. Ou Nopmongcol will serve as the Emissions Gatekeeper for this study. She will provide a final level of QA/QC on the model-ready emissions, and ensure that data are transferred to the model correctly.

3.2.3 Initial/Boundary Conditions

For the WRAP/CENRAP/VISTAS modeling of the 2002 year, boundary conditions for the continental U.S. 36 km RPO domain were based on a 2002 simulation of the GEOS-CHEM global transport and chemistry model. The GEOS-CHEM 2002 output was processed as 3-hourly spatially varying boundary conditions along the edges of the 36 km RPO grid. For modeling years other than 2002, we have processed the GEOS-CHEM 2002 data into monthly average, diurnally varying boundary conditions (BCs). This approach has been successfully used for several recent SIP modeling efforts in the Southwest U.S. (e.g., Phoenix, Las Vegas). We will similarly use the 2002 monthly average, diurnally varying BCs for this study.

Default initial concentrations developed for RPO CMAQ simulations will be used to specify CAMx initial conditions (ICs). A 15-day spin-up period will be run before each quarter to eliminate any significant influence of the arbitrary initial conditions.

3.2.4 Ancillary Model Inputs

Additional CAMx model inputs will be prepared using standard data sources and processors. For example, total integrated ozone column data for 2005 will be obtained from the TOMS satellite database (http://jwocky.gsfc.nasa.gov/) and processed as input into CAMx using the AHOMAP preprocessor. Ozone column data will be processed for each month of 2005, according to the monthly average files obtained from that web site. Surface characteristics will be defined based on land cover data taken from the MM5 simulation (as processed by

MM5CAMx). This will include monthly snow cover. Photolysis rates will be prepared using the NCAR TUV radiation transfer pre-processor, which will ingest the monthly ozone column and surface characteristics data described above. TUV will prepare a monthly photolysis look up table that is directly input to CAMx; the table defines photolysis rates for six photolytic reactions over a range of solar zenith angles, altitudes, ozone column, surface ultraviolet albedo, and haze turbidity.

3.2.5 CAMx Model Options

The latest version of CAMx (ver 4.50 or newer) will be employed. The CAMx configuration options for the preliminary model performance will include the following:

- CAMx will be run separately on the 36-km grid (resulting in "one-way" grid nesting between the 36 and 12 km grids);
- CAMx will be run on the 12/4-km nested grid system (resulting in interactive "two-way" grid nesting between the 12 and 4 km grids);
- Plume-in-Grid (PiG) subgrid-scale plume chemistry and dynamics module will be used for major stationary sources (e.g., San Juan and Four Corners EGUs);
- PPM advection solver will be employed;
- CB05 gas-phase chemistry will be employed (requiring the VOC emissions inventory to be prepared according to the speciation needed by CB05);
- CMC chemical solver will be employed;
- CF static two-mode aerosol chemistry mechanism will be employed, which invokes RADM aqueous-phase chemistry, ISORROPIA inorganic aerosol thermodynamics (sulfate/nitrate/ammonium equilibrium), and the latest updates to the SOAP secondary organic aerosol chemistry module;
- Dry and wet deposition will be active;
- Probing Tools will not be employed (these include source apportionment, decoupled direct method of sensitivity analysis, process analysis, and reactive tracers).

3.2.6 Modeling Strategy

An initial CAMx simulation will be performed for the entirety of 2005 on the 36 km continental RPO domain. Output will be processed to generate BCs for the interactive two-way 12/4 km model simulations. The strategy for performing the annual simulation will be to run CAMx separately for each of four quarters of the year (January-March, April-June, July-September, and October-December). A 15 day "spinup" period will be added prior to the start of each quarter as a way to remove the influence of initial conditions, which as described above, will be specified in very simple terms. Our tests on the RPO grid suggest that at least two weeks are needed to remove a significant fraction of the initial conditions from such large domains. The CAMx simulation for each quarter will comprise a series of single-day simulations, in which the model is restarted at midnight local time. This will facilitate the use of various day-of-week specific emissions that need to be provided to the model on a daily basis.

As was done in several recent annual modeling studies (e.g., VISTAS, CENRAP, WRAP, St. Louis $PM_{2.5}$ SIP, etc.), we will initially select two representative monthly periods to perform diagnostic and sensitivity testing with CAMx on the 12/4-km nested grid system. We will select a summer month characterized by high ozone and anthropogenic PM (e.g., SO4) and a winter month characterized by high NO3 (note that EC and OC occur year round and are heavily associated with natural emissions). The actual modeling periods will be chosen according to an analysis of the 2005 air quality data in the Four Corners region. Using the 12/4-km emissions and meteorology, and the BCs generated from the 36 km 2005 annual run, we will perform an initial 2005 Base Case simulation for the chosen summer and winter months of 2005, and conduct a preliminary model performance evaluation. We will then perform a series of diagnostic and sensitivity tests designed to identify the optimal model configuration for simulating ozone and PM air quality in the Four Corners region. The specific types of tests to be performed will depend upon the initial model performance and our assessment of the quality and uncertainties of the model inputs.

The summer and winter diagnostic tests could include, but not be limited to, the following:

- Vertical Mixing
  - O'Brien Kz profile from MM5CAMx
  - CMAQ Kz profile from MM5CAMx
  - Various versions of minimum surface Kz
- Other Meteorological Variables
  - Account for bias in MM5 temperature
  - Precipitation Adjustments
  - Other
- Emissions (increases/decreases)
  - Ammonia
  - VOC
  - NOx
  - Other
- Boundary Conditions
- Photolysis Rates

Once we have identified an optimum configuration for the summer and winter 2005 periods, we will perform a full annual CAMx simulation on the 12/4 km grids to establish the 2005 Base Case scenario. The 12/4-km annual simulation will follow the technique used for the 36-km run, with four quarterly simulations and 15 days of model spinup prior to each.

3.3 MODEL PERFORMANCE EVALUATION

In general, a model performance evaluation (MPE) is the process of testing a model's ability to accurately estimate observed atmospheric properties over a range of synoptic and geophysical conditions. To the extent possible given available data, the MPE should provide evidence that the modeling system is properly simulating the observed conditions for the correct reasons, and not through a serendipitous combination of compensatory errors (i.e., arriving at the right answer for the wrong reason). Likewise, the MPE process should also provide evidence that the model

properly responds to changes in emissions, allowing us to judge the suitability of the CAMx air quality modeling system as an effective tool to evaluate alternative mitigation strategies. When conducted thoughtfully and thoroughly, the process focuses and directs the continuing cycle of model development, data collection, model testing, diagnostic analysis, refinement, and re-testing.

The objective of the model performance evaluation (MPE) to be conducted for this project will be to evaluate the ability of CAMx, through the use of common statistical measures and graphical procedures, to appropriately replicate the spatial/temporal distribution of ozone and PM species concentrations, and deposited mass, as measured at various monitoring sites in the western U.S. over the 2005 period. Below we summarize the philosophy and objectives that will govern the evaluation of the CAMx regional air quality modeling system (and supporting preprocessor models) for the Four Corners Air Quality Modeling Study. To the extent possible given data availability in the Four Corners region, this evaluation plan conforms to the final procedures published by the EPA (2007) for 8-hour ozone, $PM_{2.5}$, and regional haze attainment demonstration modeling.

3.3.1 Available Aerometric Databases for Model Evaluation

Ideally, concentration measurements from a number of monitoring networks will be used to the fullest extent possible in the CAMx model performance evaluation. Drawn from a wide variety of state and federal monitoring networks in New Mexico, Colorado, Arizona, and Utah as well as in surrounding states, these surface measurements include ozone, NOx, CO, SO_2, some VOCs, PM_{10}, $PM_{2.5}$, PM species components, light scattering/extinction, and deposited mass. The first is the routine gas-phase concentration measurements for ozone, NOx and CO archived in EPA's Aerometric Information Retrieval System (AIRS/AQS) database. Other sources of information come from the various PM monitoring networks in the U.S. These include the: (a) Interagency Monitoring of Protected Visual Environments (IMPROVE), (b) Clean Air Status and Trends Network (CASTNET), (c) EPA $PM_{2.5}$ and PM_{10} Mass Networks (EPA-FRM), (d) EPA Speciation Trends Network (STN); and (e) National Acid Deposition Network (NADP). Typically, these networks provide ozone, other gas phase precursors and product species, PM, and visibility measurements.

Unfortunately, in our previous modeling work for the NMED in the San Juan/Four Corners 8-hour ozone EAC SIP study (Tesche et al., 2003), the available photochemical data sets for CAMx evaluation were extremely limited. In particular, hourly surface observations provided by EPA's AQS database were available from only 17 ozone monitoring sites in the 4 km grid used in the EAC modeling, and from only 2 to 5 NOx and CO sites. Within the San Juan Basin (a smaller region of the 4 km domain focusing on just the Four Corners area), no CO data were available and there were only two NO monitors (Bondad and Ignacio). NO_2 monitoring data were available at four monitors (Bondad, Ignacio, Substation, and Bloomfield). No ambient monitoring of volatile organic compounds (VOCs), either speciated or total mass, was available within the 4 km modeling domain.

Care must be taken in the PM model performance evaluation to assure the PM measurements and modeled concentrations are consistent with the measured quantities, as discuss previously. Although the focus of the CAMx PM evaluation will be on PM component performance in the

Four Corners region, since data are lacking in this area, it will be important to evaluate the model for PM and gas species throughout the entire 12/4-km modeling domains to assure that the "right answer is obtained for the right reason". Fortunately, gas, PM, and visibility data are available within the 12 km grid domain and these will likely serve as the principal basis upon which the model's performance for secondary aerosol and visibility impacts will be based.

As described in Section 1, we have established an Air Quality Data Gatekeeper to provide independent review and QA/QC of the various types of ambient measurement data. Mr. Till Stoeckenius will serve as the Air Quality Data Gatekeeper for this study. He will provide a final level of QA/QC on the data, and ensure that data are used in the model performance evaluation correctly.

3.3.2 Model Evaluation Process

The CAMx regional photochemical modeling system will be evaluated through a logical, proven process of model performance evaluation and diagnostic analysis. The operational evaluation of the model's reliability in simulating 8-hour ozone, 24-hour and annual PM concentrations, regional haze (visibility), and deposition for the 2005 base year will be quantified through the following model testing process:

- Exercise the modeling system for the base case, attempting to replicate the time and space behavior of 1-hour and 8-hour ozone concentration fields as well as concentrations of gas-phase and particulate precursor and product species; primary (e.g., EC, OC, IP) and secondary aerosol species (e.g., nitrate, sulfate, SOA); total PM, and visibility;

- Evaluate the model's fidelity in simulating gas-phase (e.g., ozone) and particulate precursor/product species using a two-step process consisting of: (a) an initial "screening model performance evaluation" (SMPE) process; and if the modeling results pass the screening analysis, (b) a "refined model performance evaluation" (RMPE) consisting of progressively more stressful testing procedure involving multi-species, multi-scale (e.g., 36/12/4 km grids) surface model evaluations;

- Identify sources of error and/or compensating biases, through examination of preprocessor models (e.g., MM5), air quality model inputs, mass budgets and conservation checks, process analysis, etc. (as time and budget permit);

- Through a documented process of diagnostic and sensitivity investigation, pinpoint and correct specific performance problems through model refinement, additional data collection and/or analysis, or theoretical considerations (as time and budget permit);

- Re-run the model for the base case and re-evaluate performance until adequate performance is achieved consistent with project time and resource allocations.

It is stressed that the process outlined above should avoid a model "tuning" exercise, wherein specific non-physical, unrealistic, or uncorroborated adjustments are made simply to obtain a better answer.

In addition to 1-hour and 8-hour ozone performance, the performance evaluation will focus on the evaluation of CAMx to estimate PM concentrations and PM components (SO4, NO3, NH4, EC, OC, IP and CM) at different averaging times (e.g., 24-hour, weekly, monthly, quarterly and annually). Model performance for wet deposition of sulfur and nitrogen species at the NADP monitoring sites will also be made. The ability of the model to simulate visibility impairment will also be evaluated using the IMPROVE reconstructed mass extinction equation and direct visibility measurements as available (e.g., via comparison against nephelometer and transmissometer measurements).

When designing a model performance evaluation, it is important to understand how the modeling results will ultimately be used. EPA has published draft guidance for fine particulate and regional haze modeling (EPA, 2001), utilizing a Fine Particulate Guidance Workgroup to provide technical input in its development[2]. More recently, EPA provided an informal update on the PM/regional haze modeling guidance (Timin, 2002) and conducted a PM model evaluation workshop (see, for example, Timin, 2004; Boylan, 2004) shedding additional light on what the final guidance document would contain (final guidance was released by EPA in April 2007). A key concept in the guidance for addressing annual PM issues is that the modeling results should be used in a relative sense to scale or roll back the observed ozone and PM concentrations from the current observed levels to the projected future-year levels.

Here, the total PM mass is assumed to be the sum of the component concentrations:

$$PM = [SO4] + [NO3] + [NH4] + [OC] + [EC] + [IP] + [PBW] + [CM] + [Blank]$$

where,

[SO4] is the sulfate concentration;
[NO3] is the particulate nitrate concentration;
[NH4] is the ammonium concentration;
[OC] is the organic mass carbon concentration (=POA+SOA);
[EC] is the elemental carbon concentration;
[IP] is the inorganic primary fine particulate (< 2.5:) concentration excluding primary sulfates and nitrates;
[PBW] is fine mass associated with particle bound water;
[CM] is the total coarse mass; and
[Blank] is the passive blank corrections for the measurement.

CAMx does not directly estimate visibility, instead it estimates PM and gaseous species concentrations from which visibility can be estimated, usually in a post-processing step. The most frequent equation to convert PM species concentrations to light extinction is the original IMPROVE reconstructed mass equation:

[2] Members of the Four Corners modeling team participated on the EPA fine particulate modeling work group over the two-year span of its activities.

$$b_{ext} = 3\times f(RH)\left[(NH_4)_2SO_4\right] + 3\times f(RH)\left[NH_4NO_3\right] + 4\times f'(RH)\left[OC\right] + 10\times\left[EC\right] + 1\times\left[IP\right] + 0.6\times\left[CM\right] + b_{rayleigh}$$

where:

b_{ext} is the estimated total light extinction coefficient (Mm^{-1});
$[(NH_4)_2SO_4]$ is the sulfate concentration assumed to be ammonium sulfate;
$[NH_4NO_3]$ is the particulate nitrate concentration assumed to be ammonium nitrate;
$[OC]$ is the total organic mass concentration (=POA+SOA);
$[EC]$ is the elemental carbon concentration;
$[IP]$ is the inorganic primary fine particulate (< 2.5 μm) concentration excluding primary sulfates and nitrates;
$[CM]$ is the primary coarse particulate (> 2.5 μm and <10 μm) concentration;
$b_{rayleigh}$ is the natural atmospheric Rayleigh scattering (assumed to be 10 Mm^{-1});
$f(RH)$ is a relative humidity adjustment factor for the sulfate and nitrates; and
$f'(RH)$ is a relative humidity adjustment factor for OC (set to a constant 1.0).

The numerical factors in front of each term of the extinction equation are referred to as "extinction efficiencies." A unique efficiency is used for each PM species, and converts concentration to an extinction coefficient in units of inverse megameters (1/Mm). Total extinction is determined from the sum of scattering components (SO4, NO3, OC, IP, CM, and natural atmospheric Rayleigh scattering) and absorbing components (EC). The relative humidity adjustment factor $f(RH)$ accounts for the growth of sulfate and nitrate aerosols as they hydrate with increasing humidity. As these salts absorb water, they grow into sizes that are more efficient at scattering light, and as they continue to take on water near 100% relative humidity, they transform form large haze particles to small cloud droplets. The humidity adjustment function defined by IMPROVE is shown in Figure 3-1.

3.3.3 Statistical Performance Metrics

The current $PM_{2.5}$ guidance document (EPA, 2007) focuses more on a holistic model evaluation approach compared to the original 1-hour ozone and draft PM guidance (EPA, 1991; 2001). Not only should we assess how well the model matches the observation, but we also need to determine whether the model is correctly simulating the processes that produce the elevated concentrations, which includes comparing against a conceptual model. Table 3-2 lists a standard set of statistical performance measures that can be used to evaluate fine particulate models. These performance measures will be calculated using several model performance evaluation software tools, including:

UCR Analysis Tool: Operates on a Linux platform, performs species and temporal matching of the predictions and observations and generates statistical performance measures, scatter plots and time series plots for user specified subdomains and across all sites and all days, for each site and all days and for each day across all sites.

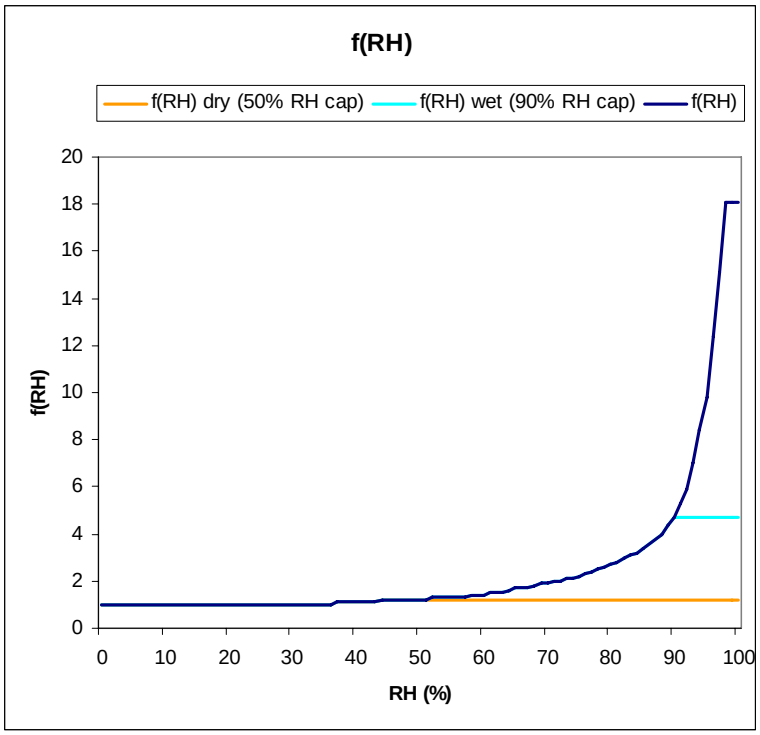


Figure 3-1. The humidity growth function *f*(*RH*) taken from the IMPROVE methodology for reconstructing extinction from ammonium sulfate and ammonium nitrate concentrations. Two alternative curves are shown; (1) the cap at 50% is intended to mirror the behavior of "dry" nephelometer scattering, and (2) the cap at 90% is used to compare to "wet" nephelometers and for reconstructing IMPROVE extinction.

Alpine Geophysics MAPS Software: Also operates on a Linux platform generating statistical measures, scatter plots, time series plots and spatial comparisons of predictions and observations. MAPS also produces spatially averaged performance summaries (e.g., time series of bias and error) that are useful for synthesizing model performance.

PAVE by MCNC: Used on a Linux platform to generate spatial maps (tile plots) of model predictions with super imposed observations as colored symbols.

ENVIRON Performance Software: Calculates performance statistics and exports them along with the predictions and observations to be used with macros operating standard Windows software such as Excel and SURFER to generate graphical displays of model performance that can be customized by the user where the data are also available for further analysis if desired.

The Four Corners CAMx evaluation will strive to use each of these evaluation packages to some extent to elucidate model performance.

Table 3-2. Routine statistical measures used in evaluating air quality models against observational data.

Statistical Measure	Shorthand Notation	Mathematical Expression	Notes
Accuracy of paired peak (***A_p***)	**Paired_Peak**	$\frac{P - O_{peak}}{O_{peak}}$	P_{peak} = paired (in both time and space) peak prediction
Coefficient of determination (***r^2***)	**Coef_Determ**	$\frac{\left[\sum_{i=1}^{N}(P_i - \overline{P})(O_i - \overline{O})\right]^2}{\sum_{i=1}^{N}(P_i - \overline{P})^2 \sum_{i=1}^{N}(O_i - \overline{O})^2}$	P_i = prediction at time and location i; O_i = observation at time and location i; $\overline{P}$ = arithmetic average of P_i, i=1,2,…, N; $\overline{O}$ = arithmetic average of O_i, i=1,2,…,N
Normalized Mean Error (***NME***)	**Norm_Mean_Err**	$\frac{\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\sum_{i=1}^{N} O_i}$	Reported as %
Root Mean Square Error (***RMSE***)	**Rt_Mean_Sqr_Err**	$\left[\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2\right]^{1/2}$	Reported as %
Fractional Gross Error (***F_E***)	**Frac_Gross_Err**	$\frac{2}{N}\sum_{i=1}^{N}\left\lvert\frac{P_i - O_i}{P_i + O_i}\right\rvert$	Reported as %
Mean Absolute Gross Error (***MAGE***)	**Mean_Abs_G_Err**	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert$	
Mean Normalized Gross Error (***MNGE***)	**Mean_Norm_G_Err**	$\frac{1}{N}\sum_{i=1}^{N}\frac{\lvert P_i - O_i\rvert}{O_i}$	Reported as %
Mean Bias (***MB***)	**Mean_Bias**	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$	Reported as concentration (e.g., $\mu g/m^3$)

Statistical Measure	Shorthand Notation	Mathematical Expression	Notes
Mean Normalized Bias (***MNB***)	**Mean_Norm_Bias**	$\frac{1}{N}\sum_{i=1}^{N}\frac{(P_i - O_i)}{O_i}$	Reported as %
Mean Fractionalized Bias (Fractional Bias, ***MFB***)	**Mean_Fract_Bias**	$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$	Reported as %
Normalized Mean Bias (***NMB***)	**Norm_Mean_Bias**	$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N}O_i}$	Reported as %
Bias Factor (***BF***)	**Bias Factor**	$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{P_i}{O_i}\right)$	Reported as BF:1 or 1: BF or in fractional notation (BF/1 or 1/BF).

3.3.4 Evaluation of CAMx Model Performance for the 2005 Base Case

The CAMx performance evaluation will be carried out in two sequential phases, beginning with the SMPE of modeled and observed ground-level ozone and aerosol species concentrations (SMPE), progressing to the RMPE with potentially more illuminating analyses if necessary (e.g., examination of precursor and product species, comparisons of pollutant ratios and groupings).

The formal procedures outlined in EPA's final ozone, $PM_{2.5}$, and regional haze modeling guidance (EPA, 2007) will be used. In particular, we will consider all six means for assessing photochemical model performance as specified in the guidance, to the extent feasible given available measurement data bases and project time/schedule constraints. These methods include:

- Use of computer generated graphics;
- Use of ozone and PM metrics in statistical comparisons;
- Comparison of predicted and observed precursor emissions or species concentrations;
- Comparison of observed and predicted ratios of indicator species;
- Comparison of predicted source category contribution factors with estimates obtained using observational models; and
- Use of retrospective analyses in which air quality differences predicted by the model are compared with observed trends.

Obviously, a comprehensive measurement database for gas phase species including ozone and particulate aerosol precursors requires an extensive monitoring network to support all six of

these analyses. This is clearly not possible with the current 2005 Four Corners data base, particularly in regards to precursor measurements, since no intensive field measurements were conducted in this area during the 2005 year. Therefore, the evaluation approach will consist of a blend of those points above and the steps outlined below. To the extent possible, each of the performance procedures described by EPA's final guidance will be addressed, and at a minimum, an explanation of why certain components cannot be fulfilled will be provided.

Initial screening of the CAMx base case ozone and PM predictions (i.e., the SMPE) will be performed for the 2005 base case in an attempt to identify obviously flawed model simulations and to implement improvements to the model input files in a logical, defensible manner. If the initial screening phase reveals no obvious flaws or compensating errors exist in the simulation(s), we will progress to the refined model performance evaluation (RMPE) operational evaluation.

The screening SMPE will employ some of the more appropriate ozone performance statistics and plots; examples of the types of graphical displays that may be helpful in the SMPE include the following:

- Spatial mean ozone and PM2.5 time series plots;
- Ozone and aerosol time series plots;
- Ground-level ozone and particulate aerosol isopleths;
- Ozone and PM2.5 concentration scatterplots;
- Bias and error stratified by concentration; and
- Bias and error stratified by time.

This screening is intended to identify obviously flawed simulations. Experience in photochemical modeling is the best basis upon which to identify obviously flawed simulation results. Efforts to improve photochemical model performance, where necessary and warranted (i.e., to reduce the discrepancies between model estimates and observations), should be based on sound scientific principles. A "curve-fitting" or "tuning" activity is to be avoided.

The following principals will govern the model performance improvement process (to the fullest extent possible given the project schedule):

- Any significant changes to the model or its inputs must be documented;
- Any significant changes to the model or its inputs must be supported by scientific evidence, analysis of new data, or by re-analysis of the existing data where errors or misjudgments may have occurred;
- All significant changes to the model or its inputs should be reviewed by the project sponsors and/or other advisory group(s); and
- Changes to the modeling approach need to be documented in the Modeling Protocol.

If the initial screening of the CAMx ozone and particulate aerosol results does not reveal obvious flaws, the refined model performance evaluation will be carried out. If the SMPE is not passed, the period will be subjected to further model diagnosis, quality assurance of the input files and related model performance improvement analyses. That is, the full refined model performance evaluation will not be carried out on an obviously flawed model simulation as it would be wasteful of project resources and schedule.

Assuming the SMPE is passed, the formal operational evaluation in the RMPE will consist of three steps. First, the graphical displays utilized previously for ozone may be generated for NOx, VOC, and key product species (e.g., HNOx, PAN). Note that model performance for VOC and many product species may not be tested since there is a limited quantity of relevant ambient measurements collected in the Four Corners region. The graphical displays for ozone precursor and product species will be examined for obvious flaws. Should these be detected, the model diagnosis and performance improvement efforts may be needed to fully identify and correct (if possible) the noted problems. Second, the ozone and NOx predictions will be examined both at the ground and aloft. Where aloft data are lacking or in short supply, the modeled fields should nevertheless be examined to assess their reasonableness. Finally, a limited number of model sensitivity and/or uncertainty simulations may be performed to help elucidate model performance and response to changes in key inputs. Sensitivity analysis, often an important component of the evaluation process, may be performed to aid in understanding the air quality model's response to key input parameter uncertainties.

The extent to which sensitivity simulations with CAMx will be needed can only be assessed after the initial model evaluations are performed. Sensitivity experiments may be conducted as part of the CAMx model performance evaluation analysis as appropriate. However, much of these diagnostic tests will have been performed using the Jan/Jul 2005 diagnostic testing.

3.3.5 Performance Goals and Benchmarks

Establishment of performance goals and criteria for modeling is a necessary but difficult activity, and has been an area of ongoing research and debate (Morris et al., 2005). Here, performance *goals* refer to targets that we believe a good performing model should achieve, whereas less stringent performance *criteria* represent a minimal level of model performance that a model should achieve for use in regulatory modeling. Performance goals are necessary in order to provide consistency in model applications and expectations across the country, while criteria provide standardization in how much weight may be accorded modeling study results in the decision-making process. It is a problematic activity, though, because many areas present unique challenges and no one set of performance goals is likely to fit all needs. Equally concerning is the very real danger that modeling studies will be truncated when the "statistics look right" before full assessment of the model's reliability is made. This has the potential for breeding built-in compensating errors as modelers strive to achieve good statistics as opposed to searching for the explanations for poor performance and then rectifying them.

Decades ago EPA established performance goals for 1-hour ozone centered on the use of normalized bias (<15%) and error (<35%). However, when these evaluation metrics were later adapted to PM and its components, difficulties arose because performance statistics that divide by low concentration observations (such as nitrate, which is often zero) become practically meaningless. In time, this has led to the introduction of the fractional bias and error metrics. EPA draft fine PM modeling guidance (EPA, 2001) notes that PM models may not be able to achieve goals similar to those of ozone, and that better performance should be achieved for those PM components that make up the major fraction of total PM mass than those that are minor contributors. In fact, differences in measurement techniques for some PM species likely exceed the more stringent ozone performance goals. For example, recent comparisons of PM

measurements using the IMPROVE and STN technologies found differences of ~20% for sulfate and ~50% for elemental carbon (Morris et al., 2005).

As with ozone in the 1980s, actual experience with PM models has led to the development of the current performance expectations for these models. For example, PM_{10} SIP model performance goals of 30% and 50% (normalized gross error) have been used for southern California and Phoenix, respectively. Boyland and Russell (2006) have proposed fractional bias and error goals of 30% and 50%, and fractional bias and error criteria of 60% and 75%, respectively. Furthermore, they proposed that these goals and criteria values vary as a function of concentration, such that below 2 $\mu g/m^3$, they expand exponentially to 200% (the maximum of fractional bias and error) at zero observed concentrations.

The following levels of model performance criteria have been adopted for VISTAS regional visibility modeling using CMAQ, and we carry these forth into the Four Corners modeling assessment:

Fractional Bias	Fractional Error	Qualitative Performance
≤ ±15%	≤ 35%	Excellent
≤ ±30%	≤ 50%	Good
≤ ±60%	≤ 75%	Average, each PM component should meet for regulatory modeling
> ±60%	> 75%	Poor, indicating fundamental problems with the modeling system

4. FUTURE YEAR MODELING

Future year CAMx model-ready emission inputs will be available on the 36/12/4 km grid configuration for a 2018 Base Case and up to five (5) mitigation scenarios. Thus, the modeling team will be running a total of six (6) annual CAMx simulations. To maximize efficiency, our approach will be to run the 2018 Base Case similarly to the 2005 Base Case, with a separate simulation on the 36 km, which will provide BCs to a nested 12/4 km grid simulation. The mitigation runs will only be run on the 12/4 grids using the same 2018 Base Case BCs, since we expect that the mitigation scenarios will likely focus more on "local" controls in the Four Corners states (the exact definitions will be determined by the NMED).

The meteorological inputs will be held constant, based on the 2005 36/12/4 km MM5 simulations described in Sections 2 and 3. The BCs around the edges of the 36 km domain will also be held constant, based on the 2002 GEOS-CHEM simulation.

The 2018 modeling results will be interpreted using both relative and absolute methodologies. EPA guidance suggests using the relative changes in the modeling results to project future-year ozone, PM2.5 and regional haze measurements (EPA, 2007). EPA has developed a new Modeled Attainment Test Software (MATS) that incorporates 8-hour ozone Design Value projection techniques and the Speciated Modeled Attainment Test (SMAT) for $PM_{2.5}$ and regional haze (visibility). MATS will be used with the 2018 modeling results. These approaches use the relative changes in the modeling results between the 2005 Base Case and 2018 emission scenarios to project or scale the observed concentrations (e.g., Design Values). MATS also includes procedures for interpolating the observed concentrations to make projections for unmonitored areas (which are important for Class II assessments).

We will also analyze the absolute modeling results for the 2018 Base Case and mitigation scenarios. When looking at changes in emissions from specific sources, the absolute modeled incremental impact may be enlightening in addition to analyzing the model results in a relative sense. The types of displays will include the following:

- Spatial maps of modeled ozone, PM speciated and total mass, regional haze (visibility), wet deposition, and differences between the modeled values for the different scenarios;
- Time series of species concentrations and changes in visibility at specific monitoring sites and locations;
- Comparison of changes in concentrations, visibility and deposition against thresholds that are used to judge significance;
- Development of visibility trend lines in terms of total light extinction and deciview;
- Other displays to be determined.

4.1 PM SPECIATED MODEL ATTAINMENT TEST

EPA guidance for projecting $PM_{2.5}$ and regional haze to future year conditions relies on the SMAT technique, which applies model results in a relative sense to scale observed $PM_{2.5}$ concentrations from the current to future year. The scaling factors are called Relative Response

Factors (RRFs) and are specific to each monitor and PM species; they are based on the ratio of the future-year to current-year modeling results. The SMAT procedures consists of two components: (1) the combination of total $PM_{2.5}$ mass measurements from the FRM network with speciated $PM_{2.5}$ measurements such as those from the STN or IMPROVE networks; and (2) the use of modeling results to scale the speciated FRM $PM_{2.5}$ observations to obtain future-year projected $PM_{2.5}$ levels.

Speciated $PM_{2.5}$ measurements are routinely collected on the same 1-in-3 day sampling schedule as used by the FRM network. The FRM, STN, and IMPROVE networks use different measurement technologies and each exhibits its own measurement artifacts. For example, FRM uses a single Teflon filter to measure total $PM_{2.5}$ mass, and includes water in the measurement (after equilibration at ~35% relative humidity). Particulate nitrate may volatilize off of the FRM Teflon filter. The STN measurement technology uses Teflon, Nylon and Quartz filters for measuring the speciated PM and does not measure the water component. The STN Quartz filters are also not blank-corrected which results in inaccurate OC measurements. IMPROVE also uses multiple filters and does not include ammonium in its measurements.

As the FRM is the de-facto regulatory definition of $PM_{2.5}$, EPA has developed procedures for adjusting the STN and IMPROVE speciated $PM_{2.5}$ measurements to account for the measurement artifacts of the different networks and to make the speciated PM measurements consistent with the FRM $PM_{2.5}$ mass measurements. These adjustments include the following:

- Adjust nitrates downward to account for volatilization off of the FRM nylon filter;
- Add particle-bound water (PBW) that is assumed to be associated with nitrate and sulfate in the FRM measurements (hydroscopic species); and
- Estimate total carbonaceous mass accounting for the lack of blank-correction in the STN measurements.

The resultant fine particle chemical speciation approach has been named the Sulfates, Adjusted Nitrates, Derived Water, Inferred Carbonaceous mass and estimated aerosol acidity (H+), or SANDWICH. Details on the SANDWICH procedures are given in EPA (2007).

The SMAT scaling/projection procedure involves the following steps:

1. Use the ratio of base to future year model-estimated PM components at each monitor and for each of the four annual quarters to develop monitor-, quarter- and PM species-specific Relative Response Factors (RRFs).

2. Apply the monitor-, quarter- and species-specific RRF to each observed quarterly PM species concentrations to obtain quarterly PM species concentrations representative of the future year.

3. Recalculate the Particle Bound Water (PRB) component from the future year projected quarterly sulfate and nitrate concentrations.

4. Average the four quarterly future year species concentrations to derive annual average PM species concentrations at each monitor.

5. Compare the projected annual average $PM_{2.5}$ concentrations against the NAAQS $PM_{2.5}$ in the attainment test, and use the scaled PM species concentrations to calculate total extinction and deciview levels to assess visibility changes.

The SANDWICH and SMAT RRF projection techniques are both included in EPA's MATS analysis software package.

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