Draft

Modeling Protocol for the Columbia River Gorge National Scenic Area Air Quality Study

Prepared for:

Paul Mairose

Southwest Clean Air Agency
11815 NE 99th Street
Vancouver, Washington 98682

Prepared by:

Ralph E. Morris

ENVIRON International Corporation
101 Rowland Way
Novato, California 94945

and

Dennis McNally

Alpine Geophysics, LLC
7341 Poppy Way
Arvada, Colorado 80007

February 17, 2006

TABLE OF CONTENTS

Page

TABLES

FIGURES

1.0 INTRODUCTION

This report constitutes the first draft of the Modeling Protocol to perform meteorological, emissions and air quality modeling as part of the Columbia River Gorge National Scenic Area Air Quality Study (Gorge Study) to be performed by the contractor team of ENVIRON International Corp and Alpine Geophysics, LLC. The meteorological, emissions and air quality modeling and analysis is just one component of the Gorge Study.

1.1 Background

In July of 2001, the Columbia River Gorge Technical Team and Interagency Coordination Team, with the assistance of national and global experts in air quality science, developed a phased, technical study plan for the Columbia River Gorge National Scenic Area. In 2003, the Washington Department of Ecology (WDOE), Oregon Department of Environmental Quality (ODEQ) and Southwest Clean Air Agency (SWCAA) asked the Technical Team to develop a "stand alone" study, leveraging other studies and within the available resources, that would:

a) Provide an assessment of the causes of visibility impairment in the Columbia River Gorge National Scenic Area;

b) Identify emission source regions, emission source categories, and individual emission sources significantly contributing to visibility impairment in the Gorge;

c) Provide predictive modeling tools or methods that will allow the evaluation of emission reduction strategies;

d) Provide an initial assessment of air quality benefits to the Gorge from upcoming state and federal air quality programs; and

e) Refine or adapt predictive modeling tools already being developed for visibility or other air quality programs, including but not limited to Regional Haze.

To meet these goals, the Technical Team, drawing on experience in visibility modeling experts across the country, proposed chemical transport modeling as one of the components of the requested study utilizing the state-of-the-science Comprehensive Air Quality Model with extensions (CAMx; ENVIRON, 2005) and EPA's Community Multiscale Air Quality (CMAQ; Byun and Ching, 1999) modeling systems. The Fifth Generation Mesoscale Model (MM5) developed and maintained by the Pennsylvania State University and National Center for Atmospheric Research (PSU/NCAR) will be used to develop hourly meteorological fields. The EPA Sparse Matrix Operating Kernel Emissions (SMOKE) system will be used to develop emissions rate estimates for CMAQ and CAMx.

1.2 Columbia River Gorge Air Quality Study Components

There are several components of the Columbia River Gorge Air Quality Study (SWCAA 2004), including:

> Measurement Program: Collection of additional visibility, particulate matter components, gaseous species and meteorological data during 2003-2005 within and surrounding the Gorge. The enhanced measurement program has been completed and provided to the data warehousing and analysis contractor.
>
> Gradient Haze Study: Analyze visibility measurements within the Gorge to better understand the causes and movement of visibility impairment in the Gorge and identify episodes for more detailed analysis. A Haze Gradient Study report is now available (Green et al., 2006).
>
> Causes of Haze: The Causes of Haze in the Gorge (CaHaGo) analysis is on-going and will be completed in 2006.
>
> Modeling Analysis: The modeling of visibility impairment in the Gorge has just been initiated.

1.3 Overview of Gorge Modeling Approach

The first element of the Gorge Study modeling is the selection and prioritization of episodes to be modeled. Based on the visibility measurements during the enhanced monitoring periods, several episodic periods will be selected and prioritized.

The air quality modeling approach to be used in the Gorge Study is to leverage off of the regional visibility modeling conducted by the Western Regional Air Partnership (WRAP) to address the requirements of the Regional Haze Rule (RHR). The ultimate objective of the RHR is to achieve natural visibility conditions (no man-made impairment) at Class I areas by 2064. Because the Gorge is in close proximity to several Class I areas (e.g., Mount Hood to the south and Mount Adams to the north), efforts to achieve natural visibility conditions at the Class I areas will undoubtedly benefit visibility in the Gorge also.

The WRAP Regional Modeling Center (RMC) has applied the MM5 meteorological Model on a 36 km continental U.S. and 12 km western U.S. grid for the 2002 calendar year. The SMOKE emissions model is used to generate hourly gridded speciated emissions needed for photochemical grid modeling. WRAP is currently using both the CMAQ and CAMx photochemical grid models to estimate PM components from which visibility impairment is calculated.

The Gorge modeling will also make use of the MM5 meteorological, SMOKE emissions and CMAQ and CAMx air quality models. The WRAP 36 km continental U.S. modeling domain will also be used. However, the Gorge modeling will use a smaller 12 km grid as well as higher resolution 4 km and 1.33 km grids focused on the primary area of study. In addition, the Gorge modeling will focus episodes from the 2003-2005 intensive monitoring periods. The Gorge

Study modeling will spend most of its modeling efforts developing refined modeling inputs for the 12km OR/WA/ID grid, the 4 km Oregon/Washington grid and 1.33 km Columbia River Gorge grid and rely on the WRAP modeling set up for the regional 36 km grid.

1.4 Gorge Study Participants

The Columbia River Gorge National Scenic Area Air Quality Study Technical Study Plan was developed by a Project Technical Team (SWCAA, 2004). The Gorge Study is being administered out of the South West Clean Air Agency (SWCAA). Members of the Project Technical Team are provided in Table 1-1.

Table 1-1. Participants in the Gorge Study Project Technical Team.

Paul Mairose, Chair	Southwest Clean Air Agency (SWCAA)
Robert Bachman	U.S.D.A. Forest Service
Natalia Kreitzer	Southwest Clean Air Agency (SWCAA)
Svetlana Lazarev	Oregon Department of Environmental Quality
Kent Norville	Air Sciences, Inc.
Marc Pitchford	National Oceanic and Atmospheric Administration (NOAA)
Mahbubul Islam	U.S. Environmental Protection Agency, Region X
Ralph Morris	ENVIRON International Corporation
John Vimont	U.S.D.O.I. National Park Service
Mark Green[1]	Desert Research Institute
Frank Van Haren[2]	Washington Department of Ecology
Clint Bowman[2]	Washington Department of Ecology
Sally Otterson[2]	Washington Department of Ecology
Christiana Figueroa-Kaminsky[2]	Washington Department of Ecology

1 Mark Green was a technical advisor to the Team
2 These individuals contributed significantly to the study design, as of July 1, 2003 the Washington Department of Ecology has disinvested in active involvement in visibility work statewide

2.0 MODEL SELECTION

This chapter introduces the regional meteorological, emissions and air quality models to be used in the Columbia River Gorge National Scenic Area Air Quality Study (Gorge Study). The specific science configurations for each modeling system are identified and discussed briefly, where necessary. Although the initial configurations of each modeling system have been selected as the culmination of a review of previous regional haze modeling studies performed in the western (e.g., Tonnesen et al., 2003) and elsewhere in the United States (e.g., Pitchford et al., 2004; Pun, Chen and Seigneur, 2004; Tonnesen and Morris 2004; Morris et al, 2004a; 2003; Baker, 2004), there remains the possibility that certain algorithms and parameter settings may still be updated in the establishment of the final Gorge Study base case simulations and model performance testing. The Gorge Emissions and Air Quality Modeling Team will remain alert to progressive model code improvements, data base refinements, and emergent analysis procedures throughout the entire activity.

2.1 Recommended Models

Based on the previous MM5 forecasting in the Pacific Northwest, AIRPACT, WRAP, VISTAS, CENRAP, MRPO, BRAVO, EPA and other work, The Gorge Study selected the following models for use in modeling particulate matter (PM) and regional haze in the central states:

- **MM5:** The Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Meteorological Model (MM5) is a nonhydrostatic, prognostic meteorological model routinely used for urban- and regional-scale photochemical, fine particulate, and regional haze regulatory modeling studies.

- **SMOKE**: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is an emissions modeling system that generates hourly gridded speciated emission inputs of mobile, nonroad, area, point, fire and biogenic emission sources for photochemical grid models.

- **CMAQ:** EPA’s Models-3/Community Multiscale Air Quality (CMAQ) modeling system is a ‘One-Atmosphere’ photochemical grid model capable of addressing ozone, particulate matter (PM), visibility and acid deposition at regional scale for periods up to one year.

- **CAMx:** ENVIRON’s Comprehensive Air Quality Model with Extensions (CAMx) modeling system is also a state-of-science ‘One-Atmosphere’ photochemical grid model capable of addressing ozone, particulate matter (PM), visibility and acid deposition at regional scale for periods up to one year.

2.2 MM5 Mesoscale Prognostic Model

Over the past decade, researchers at the Pennsylvania State University (PSU) and the National Center for Atmospheric Research (PSU/NCAR) have collaborated in the refinement and extension of the PSU Mesoscale Meteorological Model leading to the current version of the system, MM5 (ver 3.6, MPP). Originally developed in the 1970s at PSU and first documented by Anthes and Warner (1978), the MM5 modeling system maintains its status as a state-of-the-science model through enhancements provided by a broad user community (e.g., Chen and Dudhia, 2001; Stauffer and Seaman, 1990, 1991; Xiu and Pleim, 2000). The MM5 modeling system is routinely employed in forecasting projects as well as refined investigations of severe weather. Utilization of MM5 within air quality applications is also a common practice. In recent years, the MM5 modeling system has been successfully applied in continental scale annual simulations for the years 1996 (Olerud et al., 2000), 2001 (McNally and Tesche, 2003), and 2002 (Johnson, 2004; Kemball-Cook et al., 2005). Due to its ongoing scientific development worldwide, extensive historical applications, broad user community support, public availability, and established performance record compared with other applications-oriented prognostic models, the Gorge Study selected the MM5 as the preferred meteorological model. This section provides an overview of the MM5 and its data input requirements.

2.2.1 MM5 Overview

The non-hydrostatic MM5 model (Dudhia, 1993; Grell et al., 1994) is a three-dimensional, limited-area, primitive equation, prognostic model that has been used widely in regional air quality model applications (Seaman, 2000). The basic model has been under continuous development, improvement, testing and open peer-review for more than 20 years (Anthes and Warner, 1978; Anthes et al., 1987) and has been used world-wide by hundreds of scientists for a variety of mesoscale studies, including cyclogenesis, polar lows, cold-air damming, coastal fronts, severe thunderstorms, tropical storms, subtropical easterly jets, mesoscale convective complexes, desert mixed layers, urban-scale modeling, air quality studies, frontal weather, lake-effect snows, sea-breezes, orographically induced flows, and operational mesoscale forecasting.

MM5 is based on the prognostic equations for three-dimensional wind components (u, v, and w), temperature (T), water vapor mixing ratio (q_v), and the perturbation pressure (p'). Use of a constant reference-state pressure increases the accuracy of the calculations in the vicinity of steep terrain. The model uses an efficient semi-implicit temporal integration scheme and has a nested-grid capability that can use up to ten different domains of arbitrary horizontal and vertical resolution. The interfaces of the nested grids can be either one-way or two-way interactive. The model is also capable of using a hydrostatic option, if desired, for coarse-grid applications.

MM5 uses a terrain-following non-dimensionalized pressure, or "sigma", vertical coordinate similar to that used in many operational and research models. In the non-hydrostatic MM5 (Dudhia, 1993), the sigma levels are defined according to the initial hydrostatically-balanced reference state so that the sigma levels are also time-invariant. The gridded meteorological fields produced by MM5 are directly compatible with the input requirements of ‘one atmosphere’ air-quality models (e.g., CMAQ and CAMx).

Distinct planetary boundary layer (PBL) parameterizations are available for air-quality applications, both of which represent sub-grid-scale turbulent fluxes of heat, moisture and momentum. These parameterizations employ various surface energy budget equations to estimate ground temperature (T_g), based on the insolation, atmospheric path length, water vapor, cloud cover and longwave radiation. The surface physical properties of albedo, roughness length, moisture availability, emissivity and thermal inertia are defined as functions of land-use for numerous categories via a look-up table. One scheme uses a first-order eddy diffusivity formulation for stable and neutral environments and a modified first-order scheme for unstable regimes. The other uses a prognostic equation for the second-order turbulent kinetic energy, while diagnosing the other key boundary layer terms.

Initial and lateral boundary conditions are specified from mesoscale three-dimensional analyses performed at 12-hour intervals on the outermost grid mesh selected by the user. Additional surface fields are analyzed at three-hour intervals. A Cressman-based technique is used to analyze standard surface and radiosonde observations, using the National Meteorological Center's (NMC) spectral analysis as a first guess. The lateral boundary data are introduced into MM5 using a relaxation technique applied in the outermost five rows and columns of the most coarse grid domain.

A major feature of the MM5 is its use of state-of-science methods for Four Dimensional Data Assimilation (FDDA). The theory underlying this approach and details on how it has been applied in a variety of applications throughout the country are described in depth elsewhere (Stauffer and Seaman, 1990, 1991; Seaman et al., 1992, 1997).

Results of detailed performance evaluations of the MM5 modeling system in regulatory air quality application studies have been widely reported in the literature (e.g., Emery et al., 1999; Tesche et al., 2000, 2003) and many have involved comparisons with other prognostic models such as RAMS and SAIMM. The MM5 enjoys a far richer application history in regulatory modeling studies compared with RAMS or other models. Furthermore, in evaluations of these models in over 60 recent regional scale air quality application studies since 1995, we have generally found that MM5 model tends to produce somewhat better photochemical model inputs than alternative models. For these and other reasons, MM5 was selected as the meteorological modeling system for the Gorge Study.

2.2.2 MM5 Configuration for Gorge Study Modeling

Based on the sensitivity testing carried out by WSU, WRAP and others, the MM5 (ver 3.63) configuration to be used in the initial Gorge MM5 modeling consist of the following (see Table 2-1 for more details):

- 36 km grid of continental U.S. with 34 vertical layers;
- 12 km grid for Pacific Northwest including all of ID, OR and WA and portions of CA, NV, UT, WY and MT;
- 4 km grid for most of OR and WA and western portion of ID;
- 1.33 km grid on key episode days (as needed) focused on the Gorge;
- For the 12, 4 and 1.33 km runs use two way nesting with no feedback (also called interactive one way nesting);
- Initialization and boundary conditions from Eta analysis fields;
  - Eta 3D and surface analysis data (ds609.2);
  - Not using NCEP global tropospheric SST data (ds083.0) ;
  - Observational enhancement (LITTLE_R)
    - NCEP ADP surface obs (ds464.0)

    - NCEP ADP upper-air obs (ds353.4)
- Initially use Pleim-Xiu (P-X) land soil model (LSM);
- Initially use Pleim-Chang Asymmetric Convective Mixing (ACM) PBL model;
- Kain-Fritsch 2 cumulus parameterization;
- Mixed phase (Reisner 1) cloud microphysics;
- Raptid Radiative Transfer Model (RRTM) radiation;
- No Shallow Convection (ISHALLO=0);
- Standard 3D FDDA analysis nudging; and
- No surface nudging.

2.3 SMOKE Emissions Modeling System

2.3.1 SMOKE Overview

The Sparse Matrix Operator Kernel Emissions (SMOKE) Emissions Processing System Prototype was originally developed at MCNC (Coats, 1995; Houyoux and Vukovich, 1999). As with most ‘emissions models’, SMOKE is principally an *emission processing system* and not a true *emissions modeling system* in which emissions estimates are simulated from ‘first principles’. This means that, with the exception of mobile and biogenic sources, its purpose is to provide an efficient, modern tool for converting emissions inventory data into the formatted emission files required by an air quality simulation model. For mobile sources, SMOKE actually simulates emissions rates based on input mobile-source activity data, emission factors and sometimes output from transportation travel-demand models.

SMOKE was originally designed to allow emissions data processing methods to utilize emergent high-performance-computing (HPC) as applied to sparse-matrix algorithms. Indeed, SMOKE is the fastest emissions processing tool currently available to the air quality modeling community. The sparse matrix approach utilized throughout SMOKE permits both rapid and flexible processing of emissions data. The processing is rapid because SMOKE utilizes a series of matrix calculations instead of less efficient algorithms used in previous systems. The processing is flexible because the processing steps of temporal projection, controls, chemical speciation, temporal allocation, and spatial allocation have been separated into independent operations wherever possible. The results from these steps are merged together at a final stage of processing.

SMOKE supports area, mobile, fire and point source emission processing and also includes biogenic emissions modeling through a rewrite of the Biogenic Emission Inventory System, version 3 (BEIS3) (see, http://www.epa.gov/ttn/chief/software.html#pcbeis). SMOKE has been available since 1996, and it has been used for emissions processing in a number of regional air quality modeling applications. In 1998 and 1999, SMOKE was redesigned and improved with the support of the U.S. Environmental Protection Agency (EPA), for use with EPA's Models-3/CMAQ (http://www.epa.gov/asmdnerl/models3). The primary purposes of the SMOKE redesign were support of: (a) emissions processing with user-selected chemical mechanisms and (b) emissions processing for reactivity assessments.

SMOKE contains a number of major features that make it an attractive component of the Gorge modeling system (Seppanen, 2003). The model supports a variety of input formats from other emissions processing systems and models including the Inventory Data Analyzer (IDA), Emissions Modeling System—2003 (EMS-2003), and the Emissions Preprocessor System (EPS). It supports both gridded and county total land use scheme for biogenic emissions modeling. Although not necessary in the Gorge modeling, SMOKE can accommodate emissions files from up to 10 countries and any pollutant can be processed by the system.

Recent *computational improvements* to SMOKE include: (a) enhanced disk space requirements compared with other emissions processing software, (b) run-time memory allocation, eliminating any need to recompile the programs for different inventories, grids, or chemical mechanisms, and (c) updated I/O API libraries. A number of *science features* have been incorporated into the "current" version of SMOKE (ver. 2.2) including: (a) any chemical mechanism can be used to partition pollutants to model species, as long as the appropriate input data are supplied, (b) integration with the MOBILE6.2 on-road mobile source emissions model including link based processing, (c) support of plume-in-grid (PiG) processing, (d) integration of the BEIS3 emissions factors in SMOKE. A new version of SMOKE (ver.2.2) was released in October 2005 (www.cmascenter.org). However, the Gorge modeling will be based on the WRAP emissions set up that uses older versions.

Notable features of SMOKE from an *applications* standpoint include: (a) improved control strategy input formats and designs, (b) control strategies can include changes in the reactivity of emitted pollutants, a useful capability, for example, when a solvent is changed in an industrial process, (c) no third party software is required to run SMOKE, although some input file preparation may require other software, (d) fewer SMOKE programs than the SMOKE prototype because programs were combined where possible to be used for multiple source categories, (e) integration with Models-3 file formats and settings, (f) improved data file formats, (g) support of various air quality model emissions input formats (e.g., CMAQ, MAQSIP, UAM-IV, UAM-V, REMSAD and CAMx), (h) enhanced quality assurance pre- and post-processing, (h) fully integrated with Models-3, which will provide the SMOKE Tool for SMOKE input file preparation, (i) enhanced treatment of growth and control factors, (j) improved emissions reporting and QA capabilities, and (k) improved temporal allocation.

2.3.2 SMOKE Configuration for Gorge Modeling

As an emissions processing system, SMOKE has far fewer 'science configuration' options compared with the MM5 and CMAQ models. For a thorough characterization of the methods that will be used to exercise the SMOKE system for the Gorge emissions processing, see section 5.2, "Development of Emissions Model Inputs and Resultant Inventories". Table 2-1 summarizes the version of the SMOKE system to be used and the sources of data to be employed in constructing the required modeling inventories.

2.4 CMAQ Modeling System

2.4.1 CMAQ Overview

For more than a decade, EPA has been developing the Models-3 Community Multiscale Air Quality (CMAQ) modeling system with the overarching aim of producing a 'One-Atmosphere' air quality modeling system capable of addressing ozone, particulate matter (PM), visibility and acid deposition within a common platform (Dennis, et al., 1996; Byun et al., 1998a; Byun and Ching, 1999, Pleim et al., 2003). The original justification for the Models-3 development emerged from the challenges posed by the 1990 Clean Air Act Amendments and EPA's desire to develop an advanced modeling framework for 'holistic' environmental modeling utilizing state-of-science representations of atmospheric processes in a high performance computing environment (Ching, et al., 1998). EPA completed the initial stage of development with Models-3 and released the Community Multi-Scale Air Quality model (CMAQ) in mid-1999 as the initial operating science model under the Models-3 framework (Byun et al., 1998b). The most recent rendition is CMAQ version 4.5, publicly released October 2005 and is the version to be used in the Gorge modeling.

CMAQ consists of a core Chemical Transport Model (CTM) and several pre-processors including the Meteorological-Chemistry Interface Processor (MCIP), initial and boundary conditions processors (ICON and BCON) and a photolysis rates processor (JPROC). EPA is continuing to improve and develop new modules for the CMAQ model and typically provides a new release each year. In the past EPA has also provides patches for CMAQ as errors are discovered and corrected. More recently EPA has funded the Community Modeling and Analysis Systems (CMAS) center to support the coordination, update and distribution of the Models-3 system (www.cmascenter.org).

A number of features in CMAQ's theoretical formulation and technical implementation make the model well-suited for PM modeling. In CMAQ, the modal approach has been adapted to dynamically represent the PM size distribution using three log-normal modes (2 fine and 1 coarse). Transfer of mass between the aerosol and gas phases is assumed to be in equilibrium and all secondary aerosol (sulfate, nitrate, SOA) is assumed to be in the fine modes. The thermodynamics of inorganic aerosol composition are treated using the ISORROPIA module. Aerosol composition is coupled to mass transfer between the aerosol and gas phases. For aqueous phase chemistry, the RADM model is currently employed. This scheme includes oxidation of SO_2 to sulfate by ozone, hydrogen peroxide, oxygen catalyzed by metals and radicals. The impact of clouds on the PM size distribution is treated empirically. For wet deposition processes, CMAQ uses the RADM/RPM approach. Particle dry deposition is included as well. CMAQ contains three options for treating secondary organic aerosol (SOA), latest being the Secondary Organic Aerosol Model (SORGAM) that was updated in August 2003 to be an reversible semi-volatile scheme whereby VOCs can be converted to condensable gases that can then form SOA and then evaporate back into condensable gases depending on atmospheric conditions.

The newest features implemented in the latest CMAQ (ver 4.4 released October 2004) are described in the release notes available on the CMAS Center website (www.cmascenter.org). Table 2-3 highlights the major options in CMAQ (ver 4.4) for different processes and compares them with the recently released CAMx (ver 4.10s) model in Table 2-4, which is discussed later in this chapter.

2.4.2 CMAQ Configuration for Gorge Modeling

In this section we identify the main science options we recommend for the Gorge air quality modeling with CMAQ. In particular, we propose to run CMAQ (ver 4.5) with the base configuration as shown in Table 2-3. The model would be set up and exercised on the 36 km grid continental US Inter-RPO modeling domain that is also used by WRAP, CENRAP and VISTAS. For the 12 km episodic modeling, CMAQ will be set up on a 12 km domain cover the states of Oregon, Washington, Idaho and neighbors whose definition is to be determine using one-way nesting. That is, boundary conditions for the 12 km grid simulation are extracted from the 36 km run using the CMAQ BCON processor. Similarly, the boundary conditions (BCs) for the 4 km OR/WA domain will be extracted from the 12 km results, and the BCs for the 1.33 km Gorge grid will come from the 4 km grid results. A total of 19 vertical layers would be implemented, extending up to a region top of 100 mb (approximately 15 km AGL).

The PPM advection solver would be used along with the spatially varying (Smagorinsky) horizontal diffusion approach and K-theory for vertical diffusion. MM5 meteorological output based on the Pleim-Xiu Land-Surface Model (LSM) and initially the ACM planetary boundary layer (PBL) scheme will be used (see Table 2-1) and the recently (October 2005) updated CMAQ Meteorological-Chemistry Interface Processor (MCIP3.0) would process the MM5 data using the "pass through" option. The CB4 gas-phase, RADM aqueous-phase, and AERO4/ISORROPIA aerosol chemistry schemes are recommended for use in the initial CMAQ 2002 modeling. Treatment of reversible secondary organic aerosols would be simulated by the SORGAM implementation in CMAQ (ver 4.5). We would also investigate the need to use the SOAmods update to CMAQ V4.5 that includes secondary organic aerosol (SOA) formation from sesquiterpenes and isoprene.

2.5 CAMx Modeling System

2.5.1 CAMx Overview

The Comprehensive Model with Extensions (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. 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 including Process Analysis (IRR and IPR), Decoupled Direct Method (DDM), and the Ozone Source Apportionment Technology (OSAT). Designed originally to address multiscale ozone issues from the urban- to regional-scale, CAMx has been widely used in recent years by a variety regulatory agencies for 1-hr and 8-hr ozone and PM10 SIP modeling studies as well as by several RPOs for regional haze modeling. Key attributes of the CAMx model include the following:

- Two-way grid nesting that supports multi-levels of fully interactive grid nesting (e.g., 36/12/4/1.33 km);

- CB4 or SAPRC99 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;

- Subgrid-scale Plume-in-Grid (PiG) algorithm to treat the near-source plume dynamics and chemistry from large NOx point source plumes;

- 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 also compatible);

- The Ozone Source Apportionment Technology (OSAT) ozone apportionment technique that identifies the ozone contribution due to geographic source regions and source categories (e.g., mobile, point, biogenic, etc.);

- The PM Source Apportionment Technology (PSAT) to perform PM source apportionment analogous to OSAT.

- The Decoupled Direct Method (DDM) sensitivity method is implemented for emissions and IC/BC to obtain first-order sensitivity coefficients for all gas-phase species.

- Treatment of particulate matter (PM) using either a full-science multisectional or 2-section aerosol thermodynamics algorithms.

Culminating extensive model development efforts at ENVIRON and other participating groups, the CAMx (ver 4.10s) code was released in the autumn of 2004 as a truly “One-Atmosphere’ models that rigorously integrates the gas-phase ozone chemistry with the simulation of primary and secondary fine and course 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:

- Two separate treatments of particulate matter (PM), Mechanism 4 (M4) “one-atmosphere” treatment uses two size sections and science modules comparable to CMAQ (e.g., RADM aqueous-phase chemistry and ISORROPIA equilibrium) and a multi-section “full-science” approach using aerosol modules developed at Carnegie Mellon University (CMU).

- Size distribution is represented using the Multi-component Aerosol Dynamics Model (MADM), which uses a sectional approach to represent the aerosol particle size distribution (Pilinis 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 ISORROPIA (Nenes et al, 1998; 1999) equilibrium approach within MADM, or a fully dynamic or hybrid approach can also be used.

- Secondary organic aerosol thermodynamics are represented using the semi-volatile scheme of Strader and co-workers (1999).

- Aqueous-phase chemical reactions are modeled either using the RADM module (like CMAQ) or the Variable Size-Resolution Model (VRSM) of Fahey and Pandis (2001), which automatically determine 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 4.10+) provides two key options to users interested in simulating PM. For CPU-efficient PM modeling applications, CAMx may be run using Mechanism 4 (M4) with only two size sections (fine and coarse) and the efficient RADM bulk aqueous-phase module (as used in CMAQ). Alternatively, more rigorous aerosol simulations (perhaps for shorter episode) may be addressed using the version that treats N-size sections (N is typically 10) and the rigorous, but computationally-extensive CMU multi-section aqueous-phase chemistry module.

A PM Source Apportionment Technology (PSAT) has recently been added to CAMx and extensively tested and evaluated.

2.5.2 CAMx Configuration for Gorge Modeling

We recommend exercising CAMx (ver 4.30) using similar science options as CMAQ. However, in some instances, the CMAQ and CAMx model development teams chose different options for characterizing physical and chemical processes, or for implementing the governing equations on modern parallel computers. In these cases, we will utilize the science configurations embodied in the current release of CAMx.

Table 2-4 lists the main CAMx configurations recommended for the Gorge modeling. The latest version of CAMx (ver 4.30 or newer) will be employed and the model will be set up and exercised on the same 36, 12, 4 and 1.33 km grids as CMAQ. However, for the 12, 4 and 1.33 km grid episodic simulations, CAMx would be run using two-way grid nesting instead of the one-way nesting that is used by CMAQ. The base configuration of CAMx would use ~19 vertical layers up to 100mb (~15 km AGL) that exactly match those used by CMAQ in the lowest 5,000 m AGL. The PPM advection solver would be used along with the spatially varying (Smagorinsky) horizontal diffusion approach. Vertical diffusion in CAMx would be modeled by K-theory. The MM5 simulation using the Pleim-Xiu Land-Surface Model (LSM) and the ACM Planetary Boundary Layer (PBL) scheme would be used in the CAMx base configuration using the MM5CAMx processor that is similar to the CMAQ MCIP "pass through" option of the MM5 data invoked. CAMx would be exercised with the CB4 gas-phase, RADM aqueous-phase, and CMU/ISORROPIA aerosol chemistry schemes. The SOAP secondary organic aerosol scheme would be used for the base configuration in CAMx.

2.6 Advantages in Operating Multiple Models

EPA's guidance on model selection for $PM_{2.5}$ SIPs and Regional Haze "reasonable progress demonstrations" do 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" (EPA, 2001, pg. 169.) The agency recommends that models used for $PM_{2.5}$ SIPS or RH reasonable progress requirements should meet the requirements for alternative models. The CMAQ, CMAQ-MADRID, CMAQ-AIM and CAMx modeling systems all meet these requirements.

We believe that there is potentially significant value in including multiple modeling systems in the Gorge modeling analysis. Our testing and comparisons of the CMAQ and CAMx models for WRAP, VISTAS and other recent $PM_{2.5}$/regional haze applications demonstrates that the models are capable of producing results of comparable accuracy and reliability and having results from both models has many benefits, such as:

- **Diagnosis:** To serve as an efficient diagnostic tool addressing model performance issues that may arise in the establishment of the episodic base cases. CMAQ and CAMx both include Process Analysis that can help diagnose model performance. CAMx's suite of diagnostic probing tools plus it's 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;

- **Emissions 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 episodic base case simulations, and in the estimate 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.

- **Use of Advanced Modeling Tools:** The two models each have different advanced modeling features that may be if use in the Gorge Study. For example, CMAQ includes a sulfate process tracking that identifies which reactions produced the sulfate (e.g., gas-phase with OH or aqueous-phase with H2O2) that can be useful to help understand the results. CAMx includes PSAT PM source apportionment that can be used to design control strategies or perform PM culpability analysis.

- **Backup Contingency:** To provide a 'backstop' model in the event that unforeseen difficulties with one model occur.

The benefits of employing a pair of complimentary state-of-science air quality models are thus quite significant and well worth the extra effort. Especially considering that the same MM5 output (through MCIP3.0 and MM5CAMx) and SMOKE output and CMAQ IC/BC files (through CMAQ2CAMx emissions and IC/BC converters) can be used to operate CMAQ and CAMx without performing any additional meteorological or emissions modeling.

2.7 Model Limitations

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. Below, we list some of the more important limitations of the various modeling systems to be employed in the Gorge Study.

2.7.1 MM5

MM5 many different physics options that can drastically alter the predicted meteorological fields. MM5 meteorological estimates are particularly sensitive to the choice of Land Soil Model (LSM) and Planetary Boundary Layer (PBL) model. There are numerous limitations in the MM5 with the LSM and PBL treatment being some of the most important. The MM5 Pleim-Xiu/ACM LSM/PBL physic options used by WRAP and the other RPOs frequently predicts very low PBL heights that can appear as “holes” in the spatial distribution of PBL heights that don’t appear physically realistic and may affect air quality modeling. Although the 2002 annual MM5 model performance in the WRAP region mostly met performance benchmarks, there were some concerns raised and, in particular, the overstatement of precipitation amounts has been raised as a major concern (Baker, 2004b). Concerns have also been raised concerning the MM5 performance over the western third of the US (Johnson, 2004). The many limitations in MM5 have spawned the development of a new meteorological model, the Weather Research Forecast (WRF) model.

2.7.2 SMOKE

In WRAP, VISTAS and CENRAP a number of undocumented features of SMOKE necessitated re-runs of the emissions processing software to overcome errors and/or ambiguities in source documentation and QA reporting. It is unclear whether similar conditions will be encountered with the SMOKE version to be used in Gorge Study. Features are continuing to be developed in the SMOKE emissions model. As it is not as mature as some other emission models (e.g., EMS, EPS, etc.) it does not include as many features. We will keep abreast of SMOKE development activities to identify new features that will assist in the Gorge emissions modeling.

2.7.3 CMAQ

Like all air quality models, a major limitation of CMAQ is the emissions, meteorological and IC/BC inputs. 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 the CMAQ nitrate performance suspect with winter overestimations and summer underestimations (Pun, Chen and Seigneur, 2004; Tonnesen and Morris, 2004). The VISTAS and CENRAP preliminary modeling also found the performance for Organic Carbon (OC) to be less than ideal; much of the OC performance problems is due to deficiencies in the CMAQ SOA module that fails to account for several known processes important to SOA (e.g., polymerization). Other science limitations in the current version of CMAQ include simple treatment of sea salt and the use of only three modes to describe the particle size distribution. Lack of any two-way grid nesting limits the ability of the model to properly resolve point source plumes or urban photochemistry and their effects on visibility in the Gorge without a prohibitive number of grid cells. Another limitation of CMAQ is the computational requirements, including the need of excessive disk space.

2.7.4 CAMx

The model inputs are also a major limitation in CAMx and CAMx shares many of the formulation deficiencies of CMAQ. Nitrate formation chemistry is also a major limitation, as evident by the RPO modeling. Although CAMx has some more advanced science modules available, such as the VSRM aqueous-phase and MADM dynamic aerosol modules, these modules may be too computationally expensive to use except in focused sensitivity tests.

2.8 Model Input Requirements

Each of the Gorge Study modeling system components have significant data base requirements. These data needs fall into two categories: those required for model setup and operation, and those required for model evaluation testing. Below, we identify the main input data base requirements for the meteorological, emissions, and air quality models.

2.8.1 MM5

The databases required to set up, exercise, and evaluate the MM5 model for the Gorge modeling episodes consist of various fixed and variable inputs.

- <u>Topography:</u> High resolution (e.g., 30 sec ~15 m) topographic information derived from the Geophysical Data Center global data sets from the National Center for Atmospheric Research (NCAR) terrain databases are available for prescribing terrain elevations throughout the 36, 12, 4 and 1.33 km grid domain.

- <u>Vegetation Type and Land Use:</u> Vegetation type and land use information on the 36 km grid may be developed using the NCAR/PSU 10 min. (~18.5 km) databases while for the finer grids, the United States Geological Survey (USGS) data are available.

- Atmospheric Data: Initial and boundary conditions to the MM5 may be developed from operationally analyzed fields derived from the National Center for Environmental Predictions (NCEP) ETA (40 km resolution) following the procedures outlined by Stauffer and Seaman (1990). These 3-hr synoptic-scale initialization data the horizontal wind components (u and v), temperature (T), and relative humidity (RH) at the standard pressure levels, plus sea-level pressure (SLP) and ground temperature (T_g). Here, T_g represents surface temperature over land and sea-surface temperature over water.

- Water Temperature: Water temperatures required on both 36 km and 12 km grids can be derived from the ETA skin temperature variable. These temperatures are bi-linearly interpolated to each model domain and, where necessary, filtered to smooth out irregularities.

- Clouds and Precipitation: While the non-hydrostatic MM5 treats cloud formation and precipitation directly through explicit resolved-scale and parameterized sub-grid scale processes, the model does not require precipitation or cloud input. The potential for precipitation and cloud formation enters through the thermodynamic and cloud processes formulations in the model. The only precipitation-related input required is the initial mixing ratio field that is developed from the NWS and NMC data sets previously discussed.

- Multi-Scale FDDA: The standard “multi-scale” data assimilation strategy to be used on the 36 km and 12 km grids will objectively analyzed three-dimensional fields produced every 3-hr from the NWS rawinsonde wind, temperature, and mixing ratio data, and similar analyses generated every three hours from the available NWS surface data.

2.8.2 SMOKE

The databases required to set up and operate SMOKE for the Gorge episodes are as follows:

- Area Source emissions in IDA format
- NonRoad source emissions in IDA format
- Stationary Point Source emissions in IDA format
- CEM emissions, day specific for 2002
- Wildfire, prescribed burns and agricultural burning emissions, day specific for 2002
- On-road Motor Vehicle VMT and activity data
- MOBILE6.2 input parameters

Also required for the Gorge modeling are data files specific for:

- Temporal allocation
- Spatial allocation
- Speciation

Chapter 5 discusses the SMOKE data input requirements and data sources in detail.

2.8.3 CMAQ

As described in more detail in Chapter 5, the CMAQ Chemical Transport Model (CTM) requires the following inputs:

- Three-dimensional hourly meteorological fields that will be generated by the CMAQ MCIP3.0 processing of the MM5 output;
- Three-dimensional hourly emissions generated by SMOKE;
- Initial conditions and boundary conditions (IC/BC);
- Topographic information;
- Land use categories; and
- Photolysis rates generated by the CMAQ JPROC processor.

2.8.4 CAMx

CAMx model inputs include (see Chapter 5):

- Three-dimensional hourly meteorological fields generated by MM5CAMx processing of the MM5 output;
- Two-dimensional low-level (surface layer) emissions and elevated point source emissions generated by the CMAQ-to-CAMx emissions processor.
- IC/BC inputs generated by the CMAQ-to-CAMx IC/BC processors;
- Photolysis rates look up table;
- Albedo/Haze/Ozone Column input file;
- Land use and topography

Table 2-1. MM5 meteorological model configuration for Gorge Study modeling.

Science Options	Configuration	Details/Comments
Model Code	MM5 version 3.63	Grell et al., 1994
Horizontal Grid Mesh	36, 12, 4 and 1.33 km	
36 km grid	165 x 129 cells	
12 km grid	145 x 130	
4 km grid	184 x 157	
1.33 km grid	163 x 124	
Vertical Grid Mesh	34 layers	Vertically varying; sigma pressure coord.
Grid Interaction	No Feedback	IFEED=0
Initialization	Eta first guess fields/LittleR	
Boundary Conditions	Eta first guess fields/LittleR	
Microphysics	Reisner I Mixed Ice	Look up table
Cumulus Scheme	Kain-Fritsch 2	On 36 and 12 km Grids; None on 4 and 1.33 km grids; Sensitivity tests?
Planetary Boundary Layer	ACM PBL	Sensitivity tests?
Radiation	RRTM	
Vegetation Data	USGS	24 Category Scheme
Land Surface Model	Pleim-Xiu Land Surface Model (LSM)	Sensitivity tests?
Shallow Convection	None	
Sea Surface Temperature	Eta Skin	Spatially varying
Thermal Roughness	Garratt	
Snow Cover Effects	None	
4D Data Assimilation	Analysis Nudging on 36 and 12	
Obs Nudging		
Surface Nudging	None	
Integration Time Step	Variable	Grid scale dependent
Simulation Periods	Gorge episodes	1.33 km for key day only
Platform	Linux Cluster	MPI multi-processing

Table 2-2. SMOKE emissions model configuration for Gorge modeling.

Emissions Component	Configuration	Details/Comments
Emissions Model	SMOKE ver 2.1	
Horizontal Grid Mesh	36/12/4/1.33 km	
36 km grid	148 x 112 cells	Use WRAP emissions
12 km grid	TBD	Use WRAP emissions
4 km grid	TBD	Use SWCAA/ODEQ emissions
1.33 km grid	TBD	Use SWCAA/ODEQ emissions
Area Source Emissions	SWCAA/ODEQ for OR & WA	Prepared as part of Gorge Study
	2002 WRAP for other states	Generated from EPA NEI02 v.1 and RPO interaction
	Mexico/Canada Emissions:	Same as used in WRAP
On-Road Mobile Sources	SWCAA/ODEQ for OR & WA	Prepared as part of Gorge Study
	2002 WRAP for other states	Generated from EPA NEI02 v.1 and RPO interaction
	Mexico/Canada Emissions:	Same as used in WRAP
Point Sources	SWCAA/ODEQ for OR & WA	Prepared as part of Gorge Study
	2002 WRAP for other states	Generated from EPA NEI02 v.1 and RPO interaction
	Mexico/Canada Emissions:	Same as used in WRAP
Off-Road Mobile Sources	SWCAA/ODEQ for OR & WA	Prepared as part of Gorge Study
	2002 WRAP for other states	Generated from EPA NEI02 v.1 and RPO interaction
	Mexico/Canada Emissions:	Same as used in WRAP
Biogenic Sources	SMOKE BEIS-3	BELD3 vegetative database
Temporal Adjustments	Seasonal, day, hour	Based on latest collected information and CEM-based profiles
Chemical Speciation	Revised CB4 Chemical Speciation	Updated January 2004
Gridding	Revised EPA Spatial Surrogates Used for coarse grids, new surrogates for fine grids	
Growth and Controls	WRAP 2018 EI	
Quality Assurance	QA Tools in SMOKE 2.0	
Simulation Periods	Gorge episodes	1.33 km grid for just key days(s)

Table 2-3. CMAQ air quality model configuration for Gorge modeling.

Science Options	Configuration	Details/Comments
Model Code	CMAQ (ver 4.5)	Available at: www.cmascenter.org
Horizontal Grid Mesh	36/12/4/1.33 km	36 km covering continental U.S; 12,4,1.33 km TBD
36 km grid	148 x 112 cells	RPO National Grid
12 km grid	TBD	
4 km grid	TBD	
1.33 k grid	TBD	
Vertical Grid Mesh	19 Layers	First 17 layers sync'd w/ MM5
Grid Interaction	One-way nesting	
Initial Conditions	~10 days full spin-up	Spin up on 36 km grid for full 10 days
Boundary Conditions	GEOS-CHEM monthly avg, diurnally varying	From 2002 GEOS-CHEM simulation
Emissions		
Baseline Emissions Processing	See SMOKE (Ver 2.1) model configuration	MM5 Meteorology input to SMOKE, CMAQ
Sub-grid-scale Plumes	No Plume-in-Grid (PinG)	Sensitivity tests
Chemistry		
Gas Phase Chemistry	CBM-IV	
Aerosol Chemistry	AE4/ISORROPIA	Includes active Sea Salt
Secondary Organic Aerosols	Secondary Organic Aerosol Model (SORGAM)	Schell et al., (2001)
Cloud Chemistry	RADM-type aqueous chemistry	Includes subgrid cloud processes
N2O5 Reaction Probability	0.01 – 0.001	
Meteorological Processor	MCIP ver 3.0	Includes updates
Horizontal Transport		
Eddy Diffusivity Scheme	K-theory with Kh grid size dependence	Multiscale Smagorinsky (1963) approach
Vertical Transport		
Eddy Diffusivity Scheme	K-theory	
Diffusivity Lower Limit	Variable Kzmin = 0.1 to 2.0 (urban)	Run MCIP3.0 with PURB option
Deposition Scheme	M3dry	Directly linked to Pleim-Xiu LSM parameters
Numerics		
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) solver	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	
Simulation Periods	Gorge episodes	1.33 km grid just for key day(s)
Integration Time Step	TBD	15 minute coupling time step

Table 2-4. CAMx air quality model configuration for Gorge modeling.

Science Options	Configuration	Details
Model Code	CAMx (ver 4.20 or 4.30)	Available at: www.camx.com
Horizontal Grid Mesh	36, 12, 4 and 1.33 km	36 km covering continental U.S; 12 km TBD
36 km grid	148 x 112 cells	
12 km grid	TBD	
4 km grid	TBD	
1.33 km grid	TBD	
Vertical Grid Mesh	19 Layers	17 Layers sync'd w/ MM5
Grid Interaction	Two-way nesting	
Initial Conditions	~10 days full spin-up	36 km full 10 days
Boundary Conditions	GEOS-CHEM monthly avg diurnally varying	2002 GEOS-CHEM simulation
Emissions		
Baseline Emissions Processing	See SMOKE model configuration	MM5 Meteorology input to SMOKE, CAMx
Sub-grid-scale Plumes	No Plume-in-Grid (PinG)	
Chemistry		
Gas Phase Chemistry	CBM-IV	with Isoprene updates
Aerosol Chemistry	ISORROPIA equilibrium	Dynamic and hybrid also available
Secondary Organic Aerosols	SOAP	
Cloud Chemistry	RADM-type aqueous chemistry	CMU multi-section aqueous chemistry available
N2O5 Reaction Probability	None	
Meteorological Processor	MM5CAMx	
Horizontal Transport		
Eddy Diffusivity Scheme	K-theory with Kh grid size dependence	
Vertical Transport		
Eddy Diffusivity Scheme	K-Theory	
Diffusivity Lower Limit	Kzmin = 1.0	Run MM5CAMx with Kz-min=1.0
Deposition Scheme	Wesely	
Numerics		
Gas Phase Chemistry Solver	CMC Fast Solver	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	
Simulation Periods	Gorge episodes	1.33 km for key episode day(s)
Integration Time Step	Wind speed dependent	

3.0 EPISODE SELECTION

This chapter provides discussion of the selection of modeling episodes for the Gorge Study modeling. The Gorge Study modeling is being performed to provide increased understanding of the sources and causes of visibility impairment in the Columbia River Gorge. However, the Gorge is not a Class I area or a nonattainment area so there is no formal emissions control plan that needs to be developed and included in State Implementation Plan (SIP) to demonstrate compliance with an air quality standard or visibility goal within a specific time frame. However, the modeling procedures that are used to demonstrate $PM_{2.5}$ attainment or progress for achieving visibility improvement goals are similar to those to be used in the Gorge Study. Consequently, we generally follow EPA's modeling guidance for $PM_{2.5}$ attainment and regional haze modeling, only adapting them to the specific requirements of the Gorge study.

3.1 Overview of EPA Guidance

EPA's current draft guidance on $PM_{2.5}$/Regional Haze modeling (EPA, 2001) identifies specific goals to consider when selecting one or more episodes for use in demonstrating $PM_{2.5}$ attainment or reasonable progress in attaining the regional haze NAAQS. However, since there is much in common with the goals for selecting episodes for annual and episodic $PM_{2.5}$ attainment demonstrations as well as regional haze, EPA's guidance addresses all three in a common document. These concepts are also appropriate for application to the Gorge visibility modeling, only the Gorge modeling will have to account for more fine scale features than may be needed for $PM_{2.5}$ attainment and regional haze modeling. More recently, EPA has published an updated summary of $PM_{2.5}$ and Regional Haze Modeling Guidance (Timin, 2002) that serves, in some respects, as in interim placeholder until the final guidance is issued as part of the $PM_{2.5}$/regional haze NAAQS implementation process that is expected during 2006.

EPA recommends that episode selection derive from three principal criteria:

- A variety of meteorological conditions should be covered that includes different types and categories;
- To the extent possible, the modeling data base should include days for which extensive data bases (i.e. beyond routine aerometric and emissions monitoring) are available; and
- Sufficient days should be available such that relative reduction factors (RRFs) can be based on several (i.e., $\geq$ 15) days

For regional haze modeling, the guidance goes further by suggesting that the preferred approach is to model a full, *representative* year (EPA, 2001, pg. 188). Moreover, the required RRF values should be based on model results averaged over the 20% worst and 20% best visibility days determined for each Class I are based on monitoring data from the 2000 – 2004 baseline period. More recent EPA guidance (Timin, 2002) suggests that states should model at least 10 worst and 10 best visibility days at each Class 1 area. In terms of Gorge modeling, since the focus is on adverse visibility days then this recommendation can be interpreted that episodes should be selected that encompass different types of adverse visibility days including summer and winter, upriver and downriver and stagnant and transport conditions.

EPA also lists several 'other considerations' to bear in mind when choosing potential PM/regional haze episodes including:

(a) choose periods which have already been modeled;
(b) choose periods which are drawn from the years upon which the current design values are based;
(c) include weekend days among those chosen; and
(d) choose modeling periods that meet as many episode selection criteria as possible in the maximum number of nonattainment or Class I areas as possible.

Clearly, EPA guidance supports selecting Gorge modeling episodes from the enhanced measurement periods during 2003-2005, selecting both summer and winter episodes, and selecting adverse visibility days that encompass the different meteorological types as identified by the cluster analysis from the gradient haze study.

3.2 Columbia River Gorge National Scenic Area Enhanced Monitoring Study

The SWCAA, ODEQ and the US Forest Service routinely measure meteorological parameters and particulate matter (PM) concentrations at various continuous monitoring sites in southwest WA and northwest OR. In addition to the permanent sites at Wishram and Mt Zion, when include IMPROVE Protocol measurements, there were additional ozone, NOx, SO_2, sulfate, nitrate, nephelometer and meteorological monitoring sites located in southwest WA in 2003 to 2005 collected as part of the Gorge intensive monitoring studies. The locations of monitors in and around the Gorge are identified in Figure 3-1 with the parameters and equipment used identified in Table 3-1.

The Haze Gradient Study collected visibility measurements using nephelometers at nine sites in the Gorge area (Green et al., 2006). Figure 3-2 displays the locations of the Haze Gradient Study monitoring sites. Particle light scattering (bsp) was measured using a heated air stream such that the relative humidity (RH) was no more than 50%. At higher RH sulfate and nitrate particles grow and can more effectively scatter light, using the heated sample allows for the intercomparison of the bsp measurements across monitors at different RH so that gradients of visibility impairment in the Gorge can be analyzed. At all nine sites except the Memaloose State Park surface meteorological measurements of wind speed and direction, temperature and RH were also included. There were two intensive measurement periods for the Haze Gradient Study:

- July 1, 2003 – February 28, 2005; and
- August 14, 2003 – February 28, 2005

It is highly desirable to select modeling episodes from these intensive periods.

Columbia River Gorge NSA
Air Quality Study Locations

Figure 3-1. Locations of monitoring sites operated during the Gorge Study monitoring program.

Figure 3-2a. Location of western sites (Sauvie Island, Steigerwald, Mt. Zion, and Strunk Road) [Source: Green, et al., 2006].

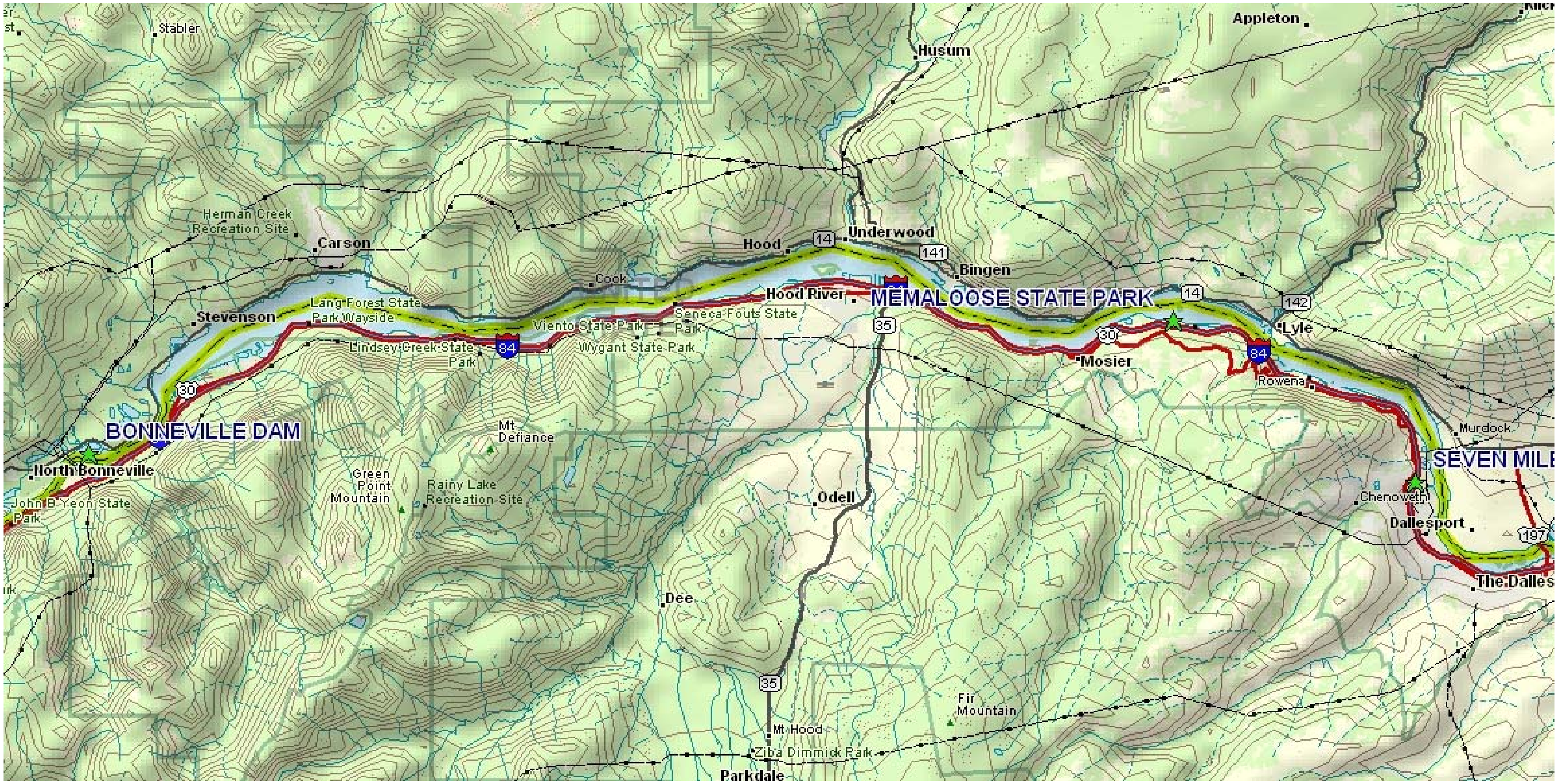


Figure 3-2b. Locations of Bonneville, Memaloose State Park, and Seven Mile Hill monitoring sites [Source: Green et al., 2006].

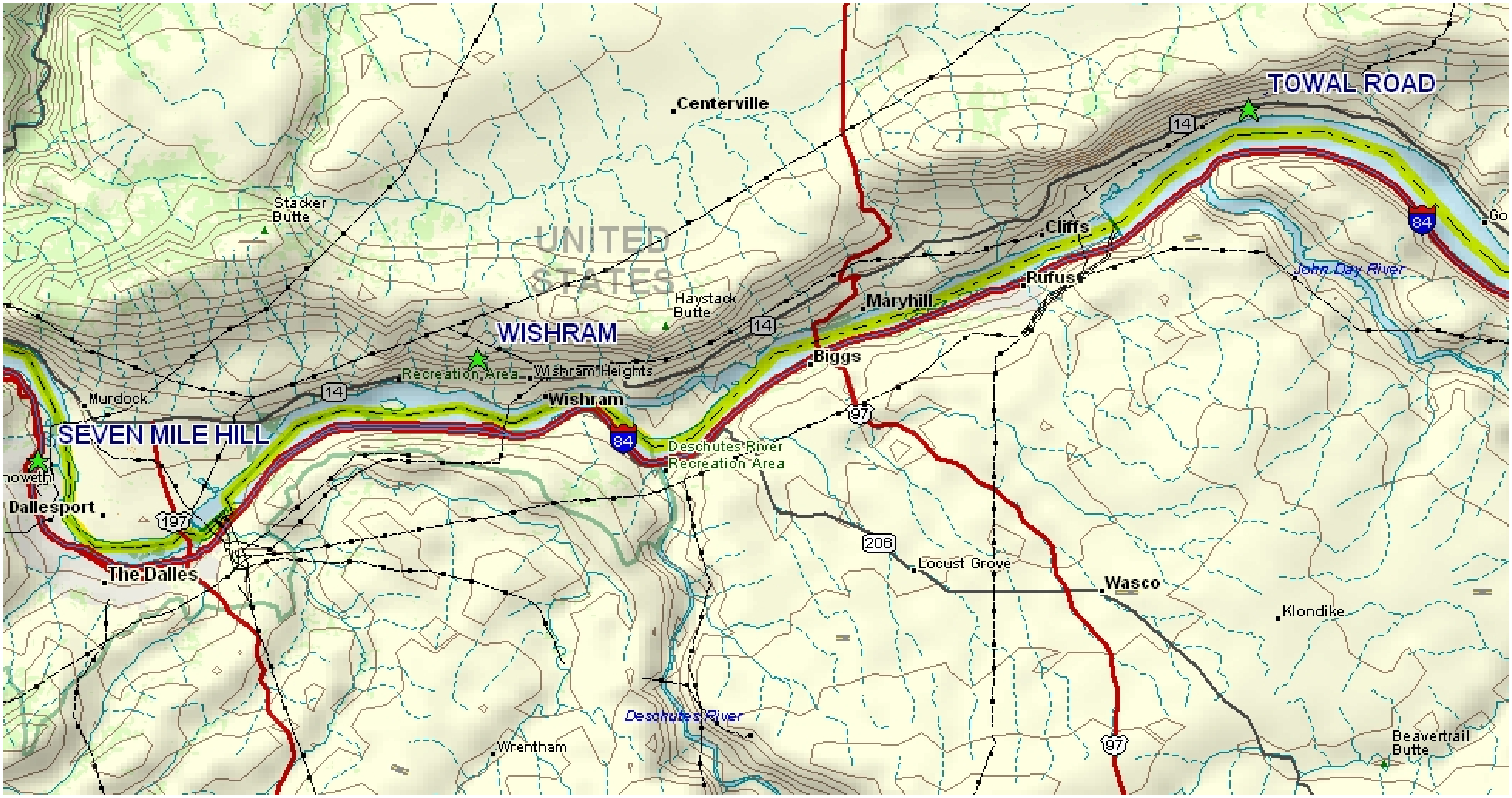


Figure 3-2c. Location of eastern monitoring sites (Seven Mile Hill, Wishram, and Towal Road) [Source: Green et al., 2006].

Table 3-1. Monitors and equipment in close proximity to Columbia River Gorge Scenic Area.

LONGVIEW	dry neph	Radiance M903
Olympic School	data logger	ESC 8816
1324 30th Ave, Longview, WA		
lat 46 8' 23.160"		
long -122 57' 40.260"		
elev 17 ft msl		
SAUVIE ISLAND	ozone analyzer	Dasibi 1003-AH
Rt 1 Box 442 SS Beach, Portland, Or	dry neph	Radiance M903
lat 45 - 46" 6.62 "	dry neph	Radiance M903
long -122 46 ' 19.48" elev 18 ft msl	WS/WD	Climatronics
Near Scappoose, OR	AT	Climatronics
approx 7 mi N of I-5 Bridge	RH	
on Sauvie Island in Columbia River	PM2.5	
VANCOUVER	Vis camera - digital	HRDC-1 Olympus
Smith Tower - Mid Columbia Manor	computer enclosure	
515 Washington, Vancouver, WA	computer	Gateway
lat 45 37' 32.08"		
long -122 40' 18.912"		
elev 200 ft msl		
BPA, Vancouver	met	
Ross Substation	chart recorder	Yokogawa 3 channel
5411 NE Hwy 99, Vancouver, WA	data logger	ESC 8800
lat 45 39' 46.33"		
long -122 39 6.48"		
elev 255 ft msl		
ATLAS & COX, Vancouver	CO	
2111 E Fourth Plain Blvd, Vancouver, WA	chart recorder	L & N
lat 45 38' 18.48"	data logger	ESC 8800
long -122 38' 53.100"		
elev 184 ft msl		
YACOLT SCHOOL	*PM2.5 FRM**	R & P 2025
406 W Yacolt Rd, Yacolt, WA	dry neph	Radiance M903
lat 45 52' 1.380"	data logger	ESC 8800
long -122 24' 44.880"		
elev 765 ft msl		
MCLOUGHLIN MIDDLE SCHOOL	dry neph	Radiance M903
5802 MacArthur, Blvd	data logger	ESC 8800
Vancouver, WA		
lat 45 37' 28.62"		
long -122 36' 44.100"		
elev 302 ft msl		
MOUNTAIN VIEW HIGH SCHOOL	ozone analyzer	Dasibi 1008-AH
1500 SE Blairmont Dr	ozone transfer std.	Dasibi 1008-AH
Vancouver, WA	data logger	ESC 8816
lat 45 36' 37.320"	chart recorder	Yokogawa 1 channel
long -122 31' 4.440"		
elev 305 ft msl		
MOOSE LODGE	PM 2.5 FRM	R & P 2000
8205 NE Fourth Plain Blvd	PM-10 FRM	
Vancouver, WA	TEOM	R & P 1400a
lat 45 38' 54.420"	Data logger	ESC 8816
long -122 35' 15.300"		
elev 242 ft msl		

Table 3-1. (Cont.) Monitors and equipment in close proximity to Columbia River Gorge Scenic Area.

PORTLAND – MILWAUKEE	ozone analyzer	Dasibi 1003-AH
10955 SE 25th St, Milwaukie, Oregon		
lat 45 26" 35.44"		
long -122 38' 16.95"		
elev 95 ft msl		
PORTLAND - SE LAFAYETTE	ozone analyzer	Dasibi 1003-AH
5824 SE Lafayette, Portland, OR	dry neph	Radiance M903
lat 45 - 29" - 47.83"	met gear	Met One
long -122 36' - 10.52"	PM2.5 FRM	R&P 2025
elev 246 ft msl	data logger	Odessa 3260
	PM10	
	CO2	
	NO2	
	VOC/Aldehyde	
	PUFF	
	Solar Radiation	
PORTLAND - CARUS	ozone analyzer	Dasibi 1003-AH
13575 Spangler Road, Oregon City, OR	dry neph	MRI 1550B
lat 45 - 15' 33.28"	WS/WD sensors	Climatronics
long -122 - 35' 13.33"	AT	Climatronics
elev 568.75 ft msl	data logger	Odessa 3260
STEIGERWALD	dry neph	Radiance M903
2 mi E of Washougal, WA	met gear	
on HWY 14	chart recorder	Yokogawa 4 channel
	data logger	ESC 8800
lat 45 - 34' 10.68"		
long -122 - 17' 54.600"		
elev 42'		
STRUNK ROAD	dry neph	Radiance M903
~5 mi E of Washougal, WA	met gear	
on Strunk Road at Cape Horn	chart recorder	Yokogawa 4 channel
lat 45 - 35' 08.220"	data logger	ESC 8800
long -122 - 11' 51.660"		
elev 1246 ft msl		
MT ZION	dry neph	Radiance M903
162 Oregon View Lane	WD/WS sensors	Climatronics
Washougal, WA 98671	Temp sensor	RM Young
	RH sensor	Rotronic
lat 45 34' 4.44"	ambient neph	OPTEC
long -122 - 12' 44.04"	IMPROVE	4 Modules
elev 739 ft msl	aethelometer	Anderson AE-16
	chart recorder / met	Yokogawa 3 channel
	chart recorder / rh	Yokogawa 1 channel
	data logger / neph	ESC 8816
	room temp sensor	
	Precip Collector	Aerochem/301
	Weigh rain guage	Belfort
VISTA HOUSE	camera	
~ MP 25 on I-84, Oregon		
lat 45 32' 20.18"		
long -122 14' 48.66"		
elev 800 ft msl		

Table 3-1. (Cont.) Monitors and equipment in close proximity to Columbia River Gorge Scenic Area.

BONNEVILLE DAM	dry neph	Radiance M903
~ MP 40 on I-84, OR/WA	met gear	
	chart recorder	L & N
	data logger	ESC 8800
(winter/summer 03/04 and winter 04/05 study)	IAS IMPROVE like	IAS
(winter/summer 03/04 and winter 04/05 study)	DRUM sampler	UC Davis
installed 10/6/04	SODAR	Aerovironment model 2000
Cascade Island:		
lat 45 - 38' 47.10"		
long -121 - 56' 35.22"		
elev 76 ft msl		
MT HOOD - Multipor Ski Lift	dry neph	Radiance M903
Government Camp, OR	IMPROVE	
	WS/WD sensors	Climatronics
lat 45 17' 18.0 "		
long -121 47' 25.0"		
elev 5074 ft msl		
MEMALOOSE STATE PARK	dry neph	Radiance M903
MP 68 on I-84, Oregon		
lat 45 41' 51.96"	data logger	ESC8800
long -121 20' 39.000"		
elev 137 ft msl		
SEVEN MILE HILL	dry neph	Radiance M903
Bob Mc Fadden	met gear	RM Young
MP 89 on I-84 2472 Badger View Dr	data looger	ESC 8800
The Dalles, OR		
lat 45 38' 7.680"		
long -121 12' 36.600"		
elev 1845 ft msl		
THE DALLES	PM2.5 FRM	R&P 2025
1112 Cherry Heights, The Dalles, OR	dry neph	Radiance M903
lat 45 35' 54.360 "		
long -121 12' 36.60"		
elev 327 ft msl		
WISHRAM	dry neph	OPTEC
Avery near Wishram Hts	WS/WD sensors	RM Young
Wishram, WA 98673	Temp Sensor	RM Young
~MP 92 on I-84	RH sensor	Rotronic
on Washington side	ambient neph	Radiance M903
~ MP 92 on US Hwy 14, WA	IMPROVE samplers	(4 Modules)
	aethelometer #1	Anderson AE-16
lat 45 - 40' 10.14"	aethelometer #2	OPTEC
long -120 - 59' 53.540"	ozone analyzer	Dasibi 1008-PC
elev 1182 ft msl	ozone t. std.	Dasibi 1008-PC
	chart recorder / met	Yokogawa 3 channel
	chart recorder / rh	Yokogawa 1 channel
	chart recorder / ozone	Yokogawa
	chart recorder / neph	Yokogawa 1 channel
	data logger	ESC 8816
	vis camera - digital	Kodak DC260
	desktop computer	Dell (photo uplink)
(winter 03/04 and 04/05 study)	DRUM sampler	UC Davis custom

Table 3-1. (Cont.) Monitors and equipment in close proximity to Columbia River Gorge Scenic Area.

TOWAL ROAD	SODAR	AeroVironment
~ MP 120 on US Hwy 14	dry neph	Radiance M903
~15 Mi E of HWY 97	met gear	
elev 496 ft msl	chart recorder	Yokogawa 4 channel
lat 45 - 45' 13.867"	data logger	ESC 8800
long -120 - 37' 37.380"	desktop computer/SODAR	Gateway
(winter 03/04 and 04/05 study)	IAS sampler	IAS
MOBILE TRAILER 6X10	trailer	Wells Cargo 6 X 10
	OC/EC	Sunset Labs RT-3005
	OC/EC laptop computer	Toshiba LT II
	sulfates	R&P 8400S Pulse Generator
		R&P 8400S Pulse Analyzer
(Wishram - winter	nitrates	R&P 8400N Pulse Generator
Mt Zion - Summer)		R&P 8400N Pulse Analyzer
	zero air gas generator	Teledyne - Adv. Air Pollution
	SO2	Thermo 43C
Robbins/Bradford Island 11/1/03 to 7/1/04	NOx	Thermo 42C
lat 45 - 38' 32.580"	cal dilution system	Environics 6100
long -121 - 57' 11.04"	chart recorder	Yokogawa 3 channel
elev 85 ft msl		
	data logger	ESC 8800
	air conditioner	Coleman
MOBILE TRAILER 8X12	Trailer	Wells Cargo 8X12
	OC/EC	Sunset Labs Mod 3
	OC/EC laptop computer	Compaq Presario 2100
	sulfates	R&P 8400S Pulse Generator
		R&P 8400S Pulse Analyzer
(Bonneville Dam)	nitrates	R&P 8400N Pulse Generator
Robbins/Bradford Is. OR Winter 03/04		R&P 8400N Pulse Analyzer
Cascade Is. WA Summer 04 & Winter 04/05	zero air gas generator	Teledyne - Adv. Air Pollution
	SO2	Thermo 43C
	NOx	Thermo 42C
	cal dilution system	Environics 9100
	chart recorder	Yokogawa 3 channel
	data logger	ESC 8800
	air conditioner	Coleman TSL

Table 3-1. (Concl.) Monitors and equipment in close proximity to Columbia River Gorge Scenic Area.

PENDLETON - McKAY CREEK	PM2.5	
3745 SW Marshall Pl, Pendleton, OR	PM10	
lat 45 39' 10.38"	Nephelometer	
long -118 49' 20.04"	WS/WD	
elev 1061 ft msl	AT	
Washougal Water Treatment Plant	SODAR	AeroVironment
(when not in use at Towal Rd)		
lat 45 - 34' 18.960"		
long -122 - 19' 23.820"		
elev 29 ft msl		

3.3 Selection of Episodes for Gorge Air Quality Study Modeling

There were two major components to the intensive monitoring program under the Gorge Air Quality Study. The first major component was the Haze Gradient Study, which was comprised of a series of 9 nephelometers located throughout the Gorge Scenic Area. These locations also included surface meteorological monitoring instruments with the exception of the Memaloose location. The second major monitoring component was comprised of aerosol and gaseous pollutant monitoring including sulfates, nitrates, oxides of nitrogen, sulfur dioxide, organic carbon/elemental carbon, particulate matter samplers, high time resolution particulate matter samplers, aethalometers and two SODARs for limited upper air meteorological data.

These two components were developed separately as funding became available. The Haze Gradient Study via nephelometers was funded first with limited resources from EPA. Additional Congressional funding was provided later which provided the capability to add the gaseous monitoring instruments. Results from the Haze Gradient Study were used to identify episodes that would be evaluated in greater detail via the gaseous pollutants. These same episodes were envisioned to serve as the basis for the modeling events. The Gorge Study Technical Team envisioned from 2 to 4 episodes per intensive monitoring period would likely be identified. In addition to the intensive monitoring studies being coordinated by SWCAA and ODEQ, the US Forest Service undertook a separate Fog and Cloud Water Study at the east end of the Scenic Area in the 2003/2004 winter season.

At a Technical Team meeting on June 14, 2005, Dr. Mark Green with the Desert Research Institute (DRI) summarized nephelometer data received to date for the Scenic Area. The purpose of this summary was to identify event dates that would be used to analyze filter samples from the IMPROVE-like samplers deployed during the intensive monitoring periods. These samplers ran on a one day in three schedule consistent with the IMPROVE samplers maintained by the US Forest Service at Mt Zion and Wishram. Approximately 50 event dates were identified. Some events were large and some were much smaller. These data were analyzed further by DRI using a cluster analysis to identify trends or unique values for these episodes. Based on this initial evaluation, the following episodes were suggested as potential episodes to model.

- November 1 to December 1, 2003 – Towal Rd/Wishram peaks and Sauvie peaks
- January 5 to January 25, 2004 – Memaloose/Wishram/Towal Rd peaks
- February 8 to February 28, 2004 – Towal Rd/Wishram peaks
- July 22 to August 21, 2004 – all sites summertime

- August 26 to September 5, 2004 – Sauvie/Sauvie/Zion peaks
- September 20 to October 8, 2004 – Bonneville/Sauvie/Zion/Strunk peaks
- November 5 to December 5, 2004 – Towal/Wishram/7Mile/Memaloose peaks
- January 15 to March 1, 2005 – many sites

On December 15, 2005 the Gorge Technical Team held a conference call to go over and prioritize the episodes based on the preliminary results from the Haze Gradient Study. The Haze Gradient Study identified six candidate periods for modeling:

- November 2004
- February 2005
- February 2004
- July 2004
- August 2004
- September 2004

Daily particle scattering (bsp) and continuous bsp, SO4 and NO3 for these candidate episodes are shown in Figures 3-3 through 3-8.

3.3.1 November 3-18, 2004 Episode

During the November 2004 episode the highest light scattering (bsp) of the candidate episodes was observed with values exceeding 200 Mm^{-1} observed at the Wishram and Towal Road sites in the eastern side of the Gorge on November 10, 2004 with elevated bsp in excess of 100 Mm^{-1} observed at five other sites in the Gorge (Figure 3-3). Between November 7 and November 13, bsp was observed at over 100 $Mm\text{-}^{1}$ at more than one site in the Gorge. The elevated bsp is due to light scattering from the combination of SO4, NO3 and OC with the extreme spikes being due to NO3 which exhibits more diurnal variability than SO4 and OC. The November 2004 episode starts off fairly clean on November 3, 2004 with all sites have bsp in the 30-50 Mm^{-1} range and builds up to the peak in excess of 200 Mm^{-1} at some sites on November 10th then dropping down to relatively clean values (~20 Mm-1) on November 18. Key episode days during this period include:

- November 8, 2004
- November 10, 2004
- November 11, 2004
- November 12, 2004
- November 13, 2004

The IMPROVE samples were collected on November 5, 8, 11, 14 and 17 of this period.

3.3.2 February 7-28, 2005

There were two key periods when elevated light scattering was observed in the Gorge during the February 2005 episode, February 13, 2005 and February 24-27, 2005 (Figure 3-4). During both of these periods the highest values occurred in the east side of the Gorge at the Towal Road and 7 mile sites. During both elevated periods light scattering exceeded 80 Mm^{-1}. At the Bonneville Dam site, SO4 was higher than NO3, whereas at the Wishram site NO3 was higher than SO4. The SO4 and NO3 instruments were not always working correctly during this episode. The IMPROVE data for 2005 are not yet available, which is an important component needed for modeling. Key episode days during this period are:

- February 11, 2005
- February 25, 2005
- February 26, 2005
- February 27, 2005

3.3.3 February 10-19, 2004

Elevated light scattering in excess of 60 Mm^{-1} occurred at several sites during the February 11-15, 2004 period, with values in excess of 100 Mm^{-1} occurring at the Towal Road and Memaloose sites on the eastern side of the Gorge on February 14, 2004 (Figure 3-5). The scattering at Bonneville Dam tracks the NO3 better than SO4. At Wishram the continuous SO4 data is missing after February 13. The NFS fog water sampling study was in operation during this episode. IMPROVE monitoring dates during this period are February 9, 12, 15 and 18. Key episode days are:

- February 13, 2004
- February 14, 2004
- February 15, 2004

3.3.4 July 23-31, 2004

Light scattering is not as high during the summer periods with values exceeding 30 MM^{-1} on July 24 and July 27-29, 2004 (Figure 3-6). Because NO3 is low during this summer period, light scattering is due to SO4 and OC. During the July 27-29, 2004 period, bsp is in mainly the 40-60 Mm^{-1} range for sites in the Gorge. The IMPROVE monitors were operating on July 23, 26, and 29 during this candidate episode period. Key modeling days are:

- July 24, 2004
- July 27, 2004
- July 28, 2004
- July 29, 2004

3.3.5 August 10-22, 2004

Most Gorge sites experienced elevated scattering in the 30-50 Mm^{-1} range during August 11-16, 2004 with a secondary peak August 18-19, 2004 (Figure 3-7). The continuous SO4 measurements at Bonneville Dam track the light scattering well. The IMPROVE monitors were collecting samples on August 10, 13, 16, 19 and 22 during this period. Key episode days are:

- August 11, 2004
- August 12, 2004
- August 13, 2004
- August 14, 2004
- August 15, 2004
- August 16, 2004
- August 18, 2004
- August 19, 2004

3.3.6 September 1-6 and 24-28, 2004

Light scattering in excess of 100 Mm^{-1} occurred at several sites on September 3, 2004 with elevated extinction in excess of 50 Mm^{-1} also occurring on September 24-27, 2004 (Figure 3-8). The scattering tracks closely with the continuous OC measurements suggesting that fires may be the cause of the visibility impairment events as there were known fires in the region. Consequently, this episode is dropped from consideration.

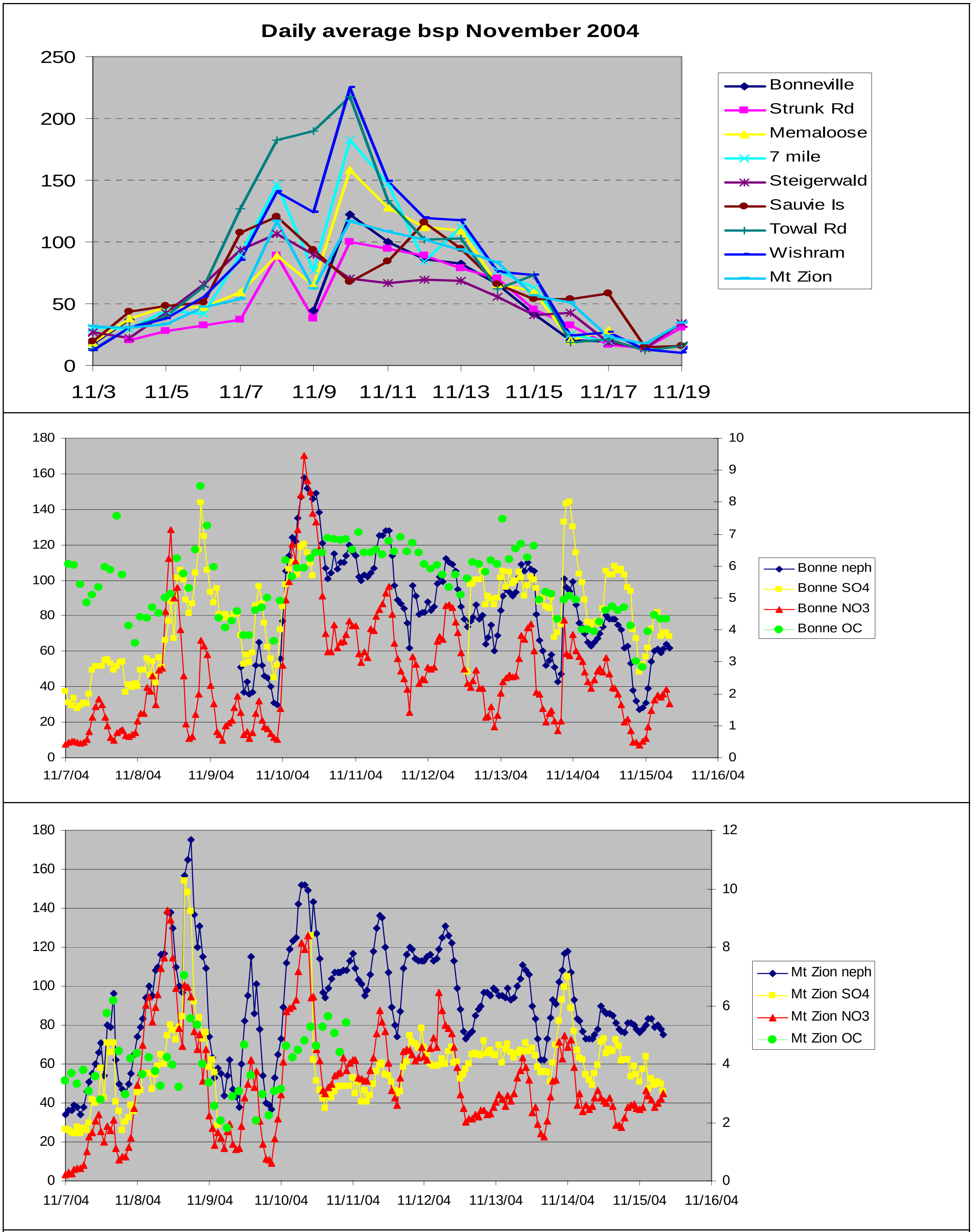


Figure 3-3a. Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (middle) and Mt. Zion (bottom) sites for November 2004.

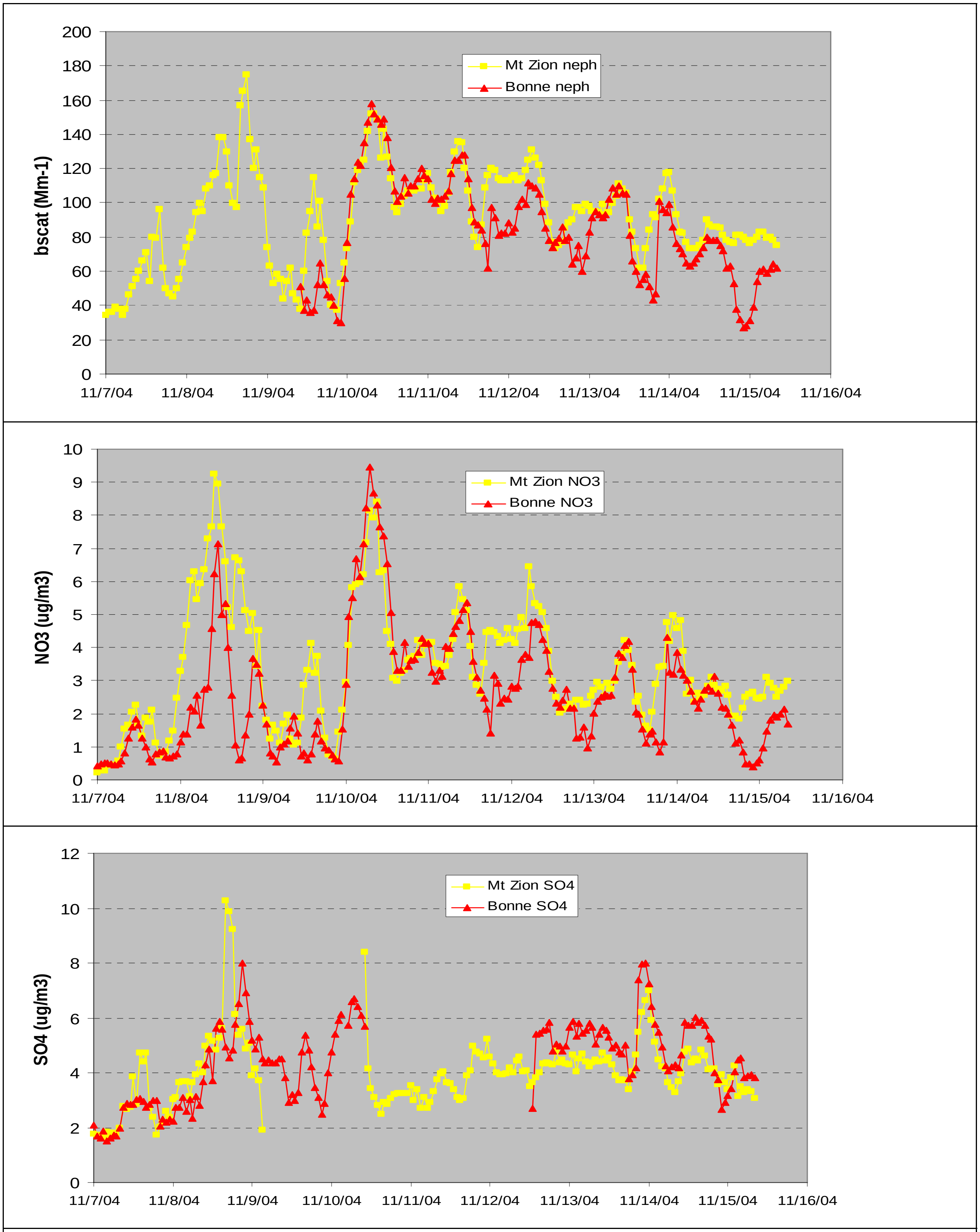


Figure 3-3b. Continuous particle light scattering (bsp) (top), nitrate (NO3) (middle) and sulfate (SO4) (bottom) at the Bonneville Dam and Mt. Zion sites during November 2004.

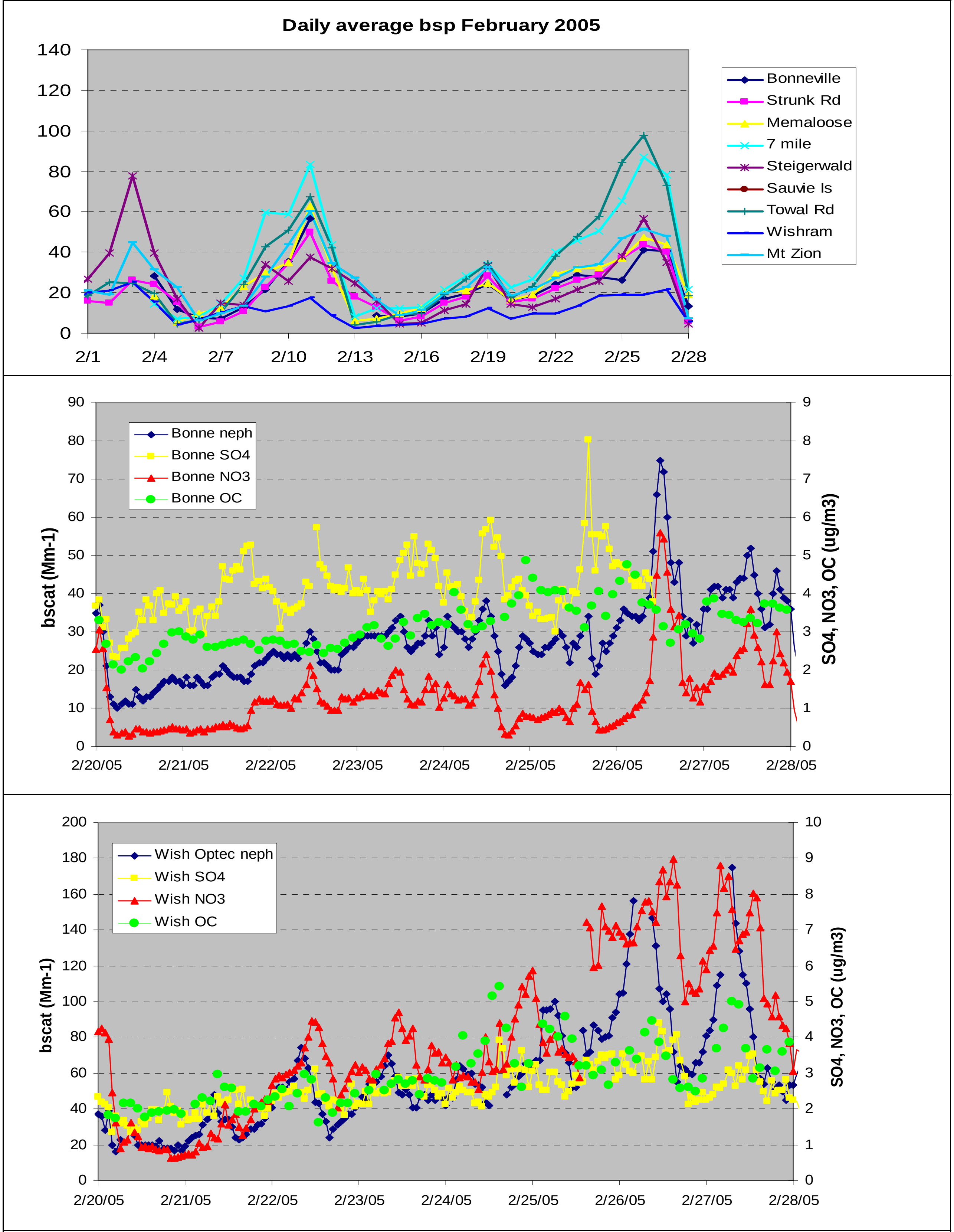


Figure 3-4a. Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (middle) and Wishram (bottom) sites for February 2005.

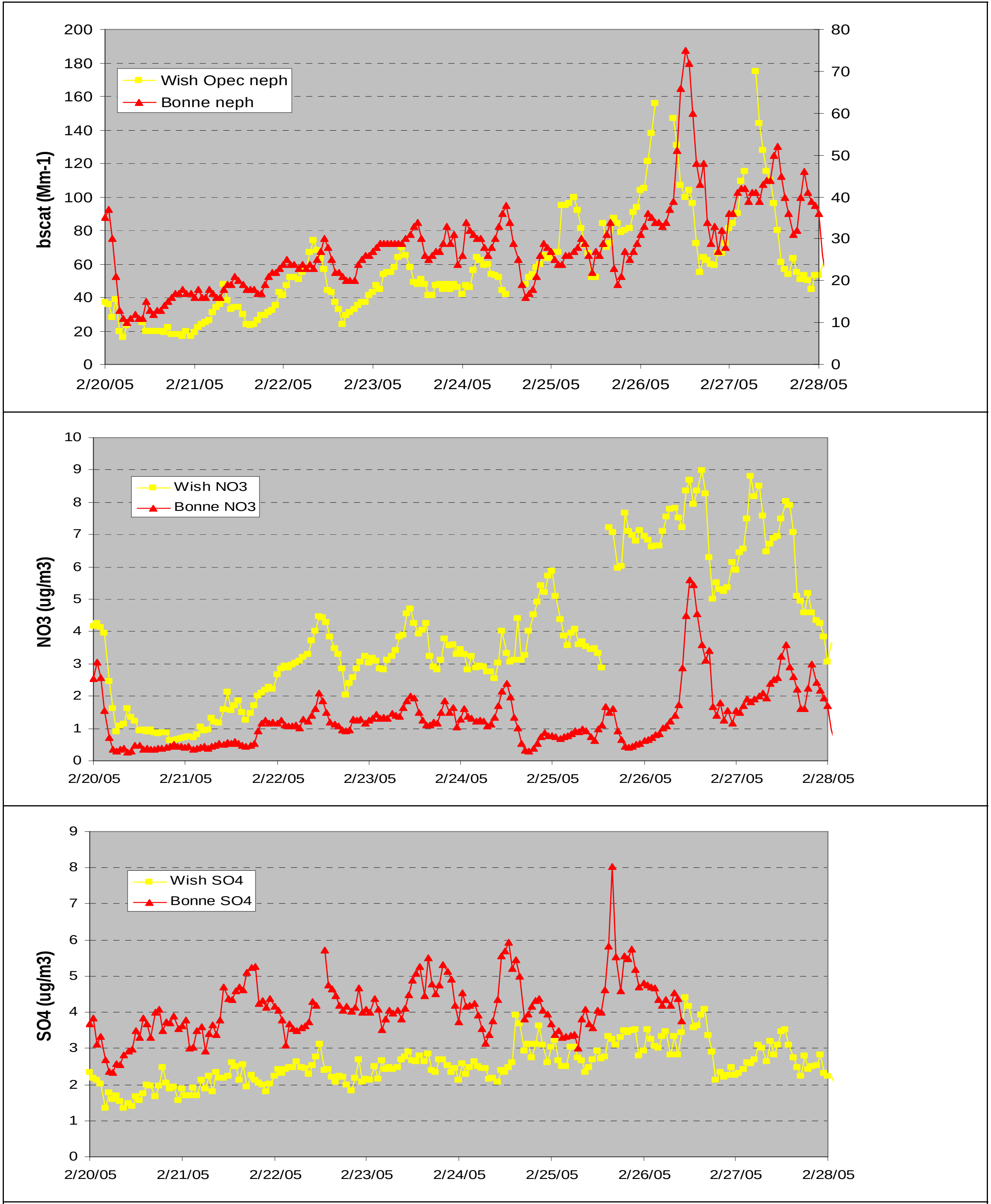


Figure 3-4b. Continuous particle light scattering (bsp) (top), nitrate (NO3) (middle) and sulfate (SO4) (bottom) at the Bonneville Dam and Wishram sites during February 2005.

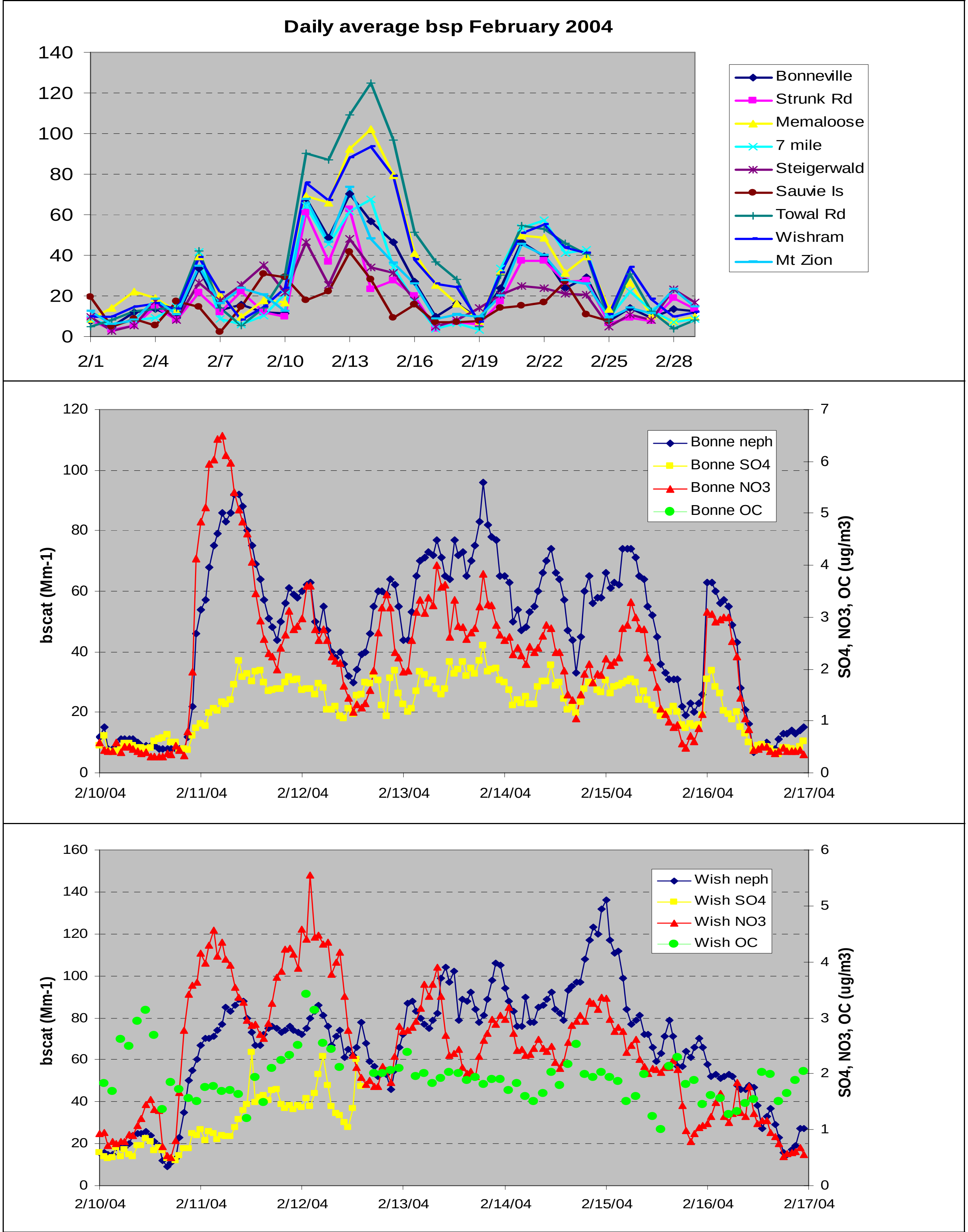


Figure 3-5a. Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (middle) and Wishram (bottom) sites for February 2004.

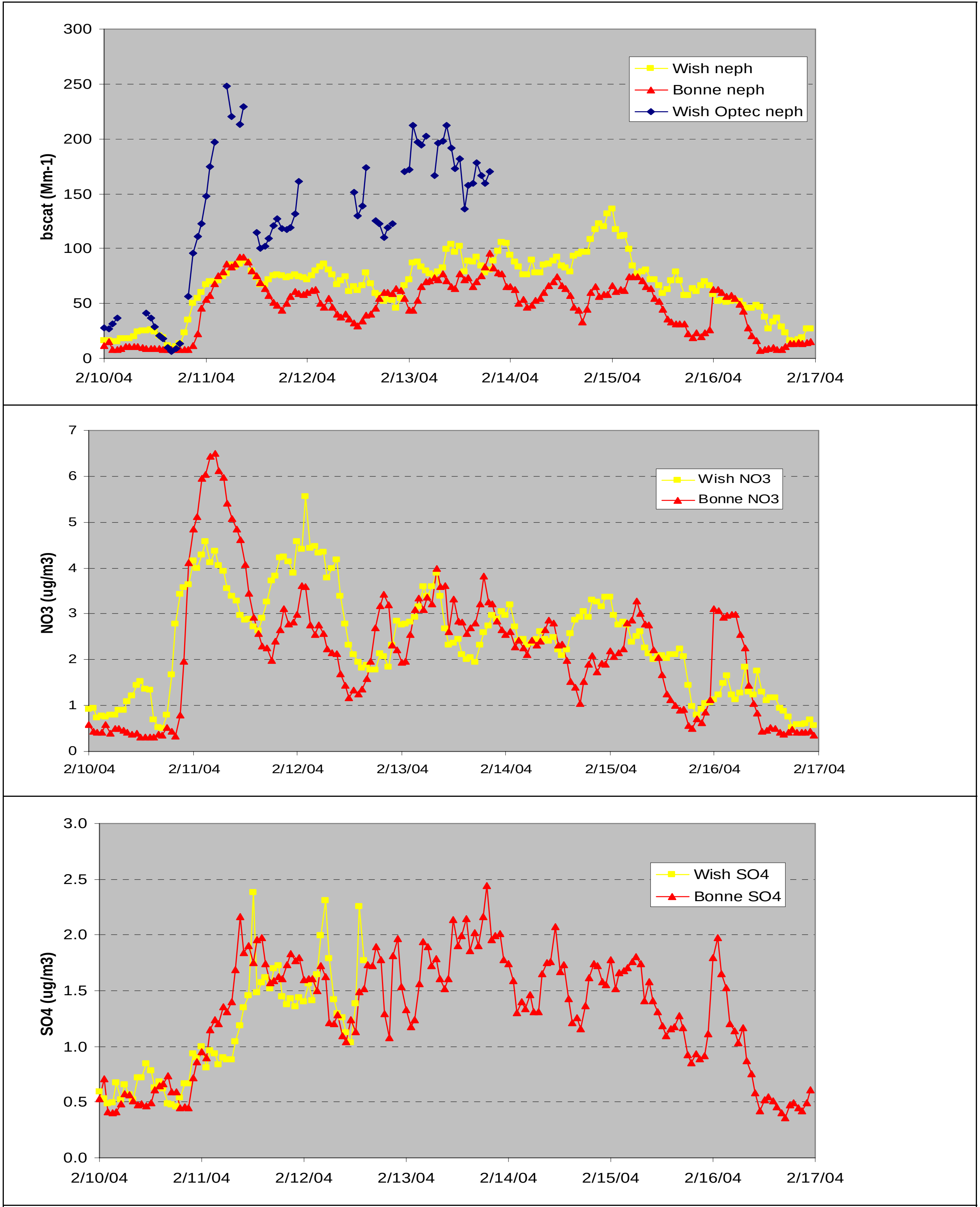


Figure 3-5b. Continuous particle light scattering (bsp) (top), nitrate (NO3) (middle) and sulfate (SO4) (bottom) at the Bonneville Dam and Wishram sites during February 2004.

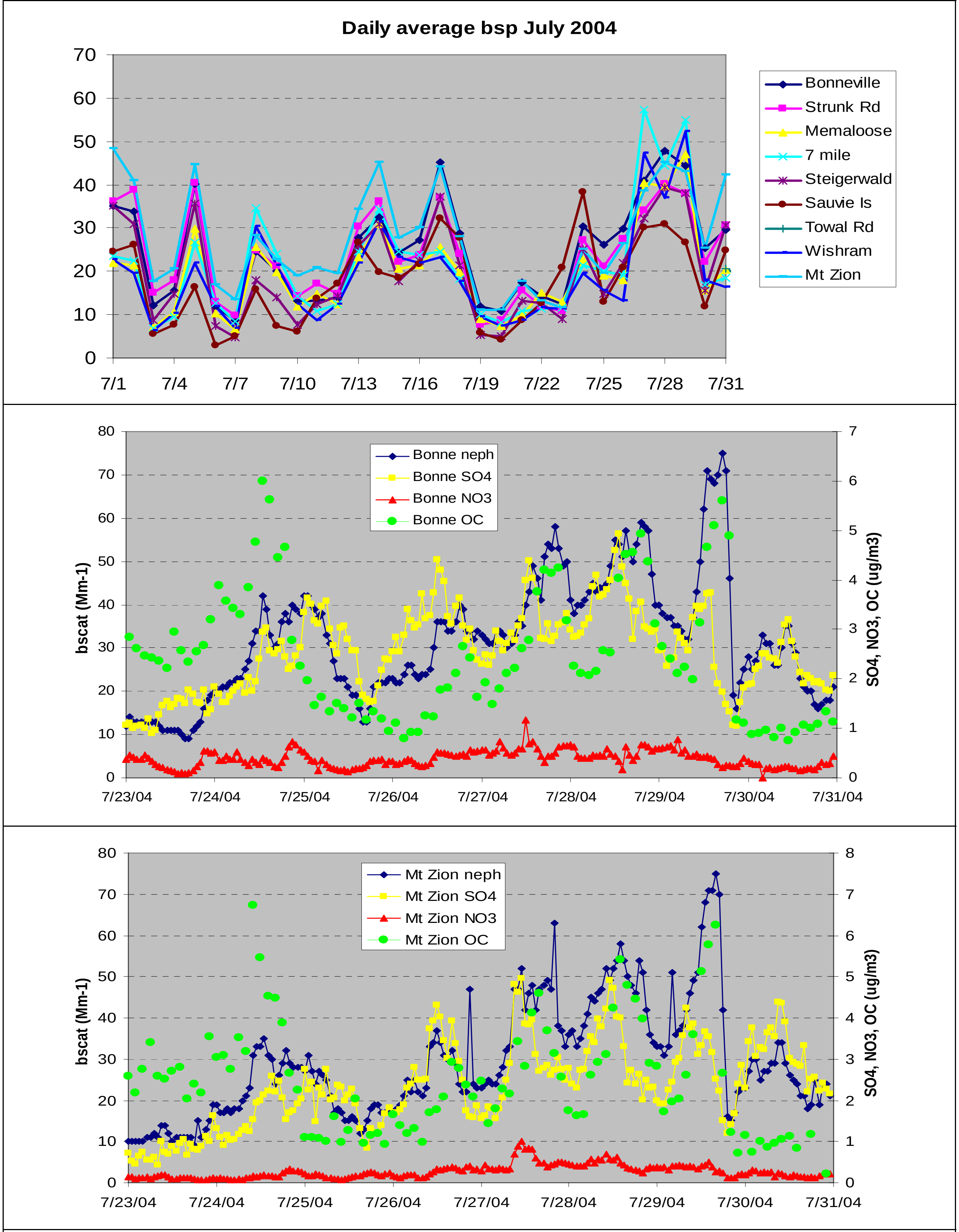


Figure 3-6a. Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (middle) and Mt. Zion (bottom) sites for July 2004.

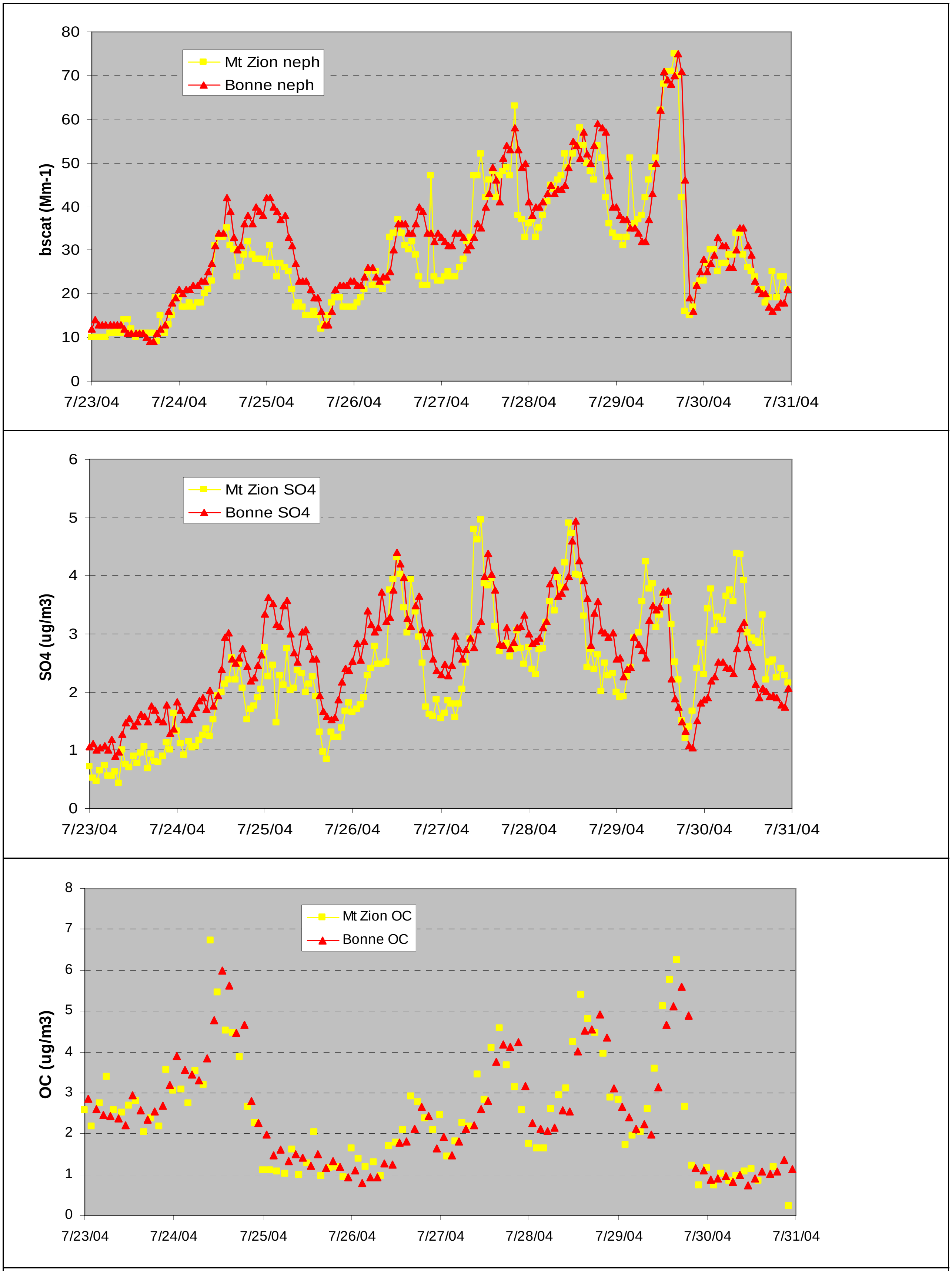


Figure 3-6b. Continuous particle light scattering (bsp) (top), sulfate (SO4) (middle) and Organic Carbon (OC) (bottom) at the Bonneville Dam and Mt. Zion sites during July 2004.

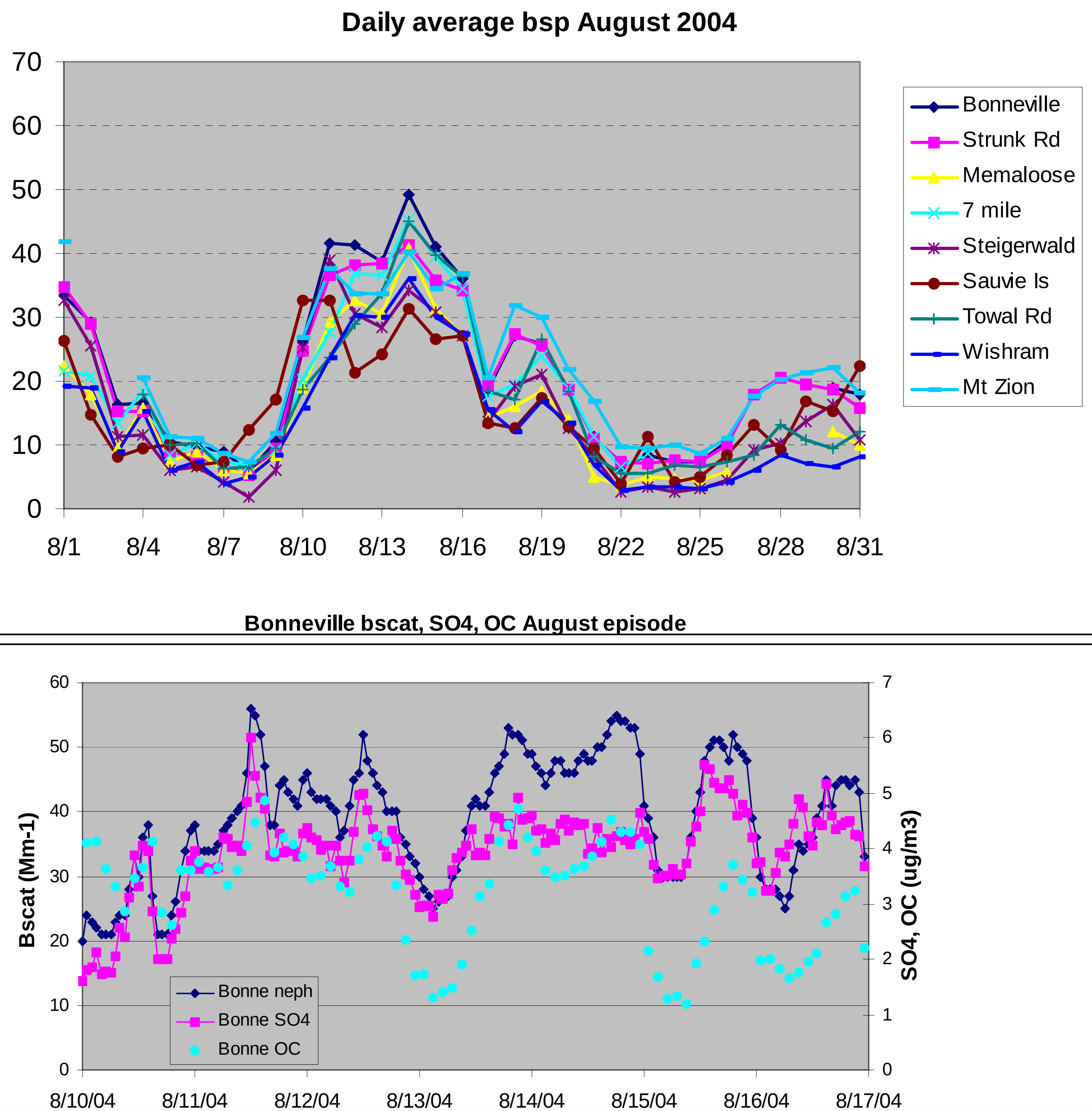


Figure 3-7. Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (bottom) sites for August 2004.

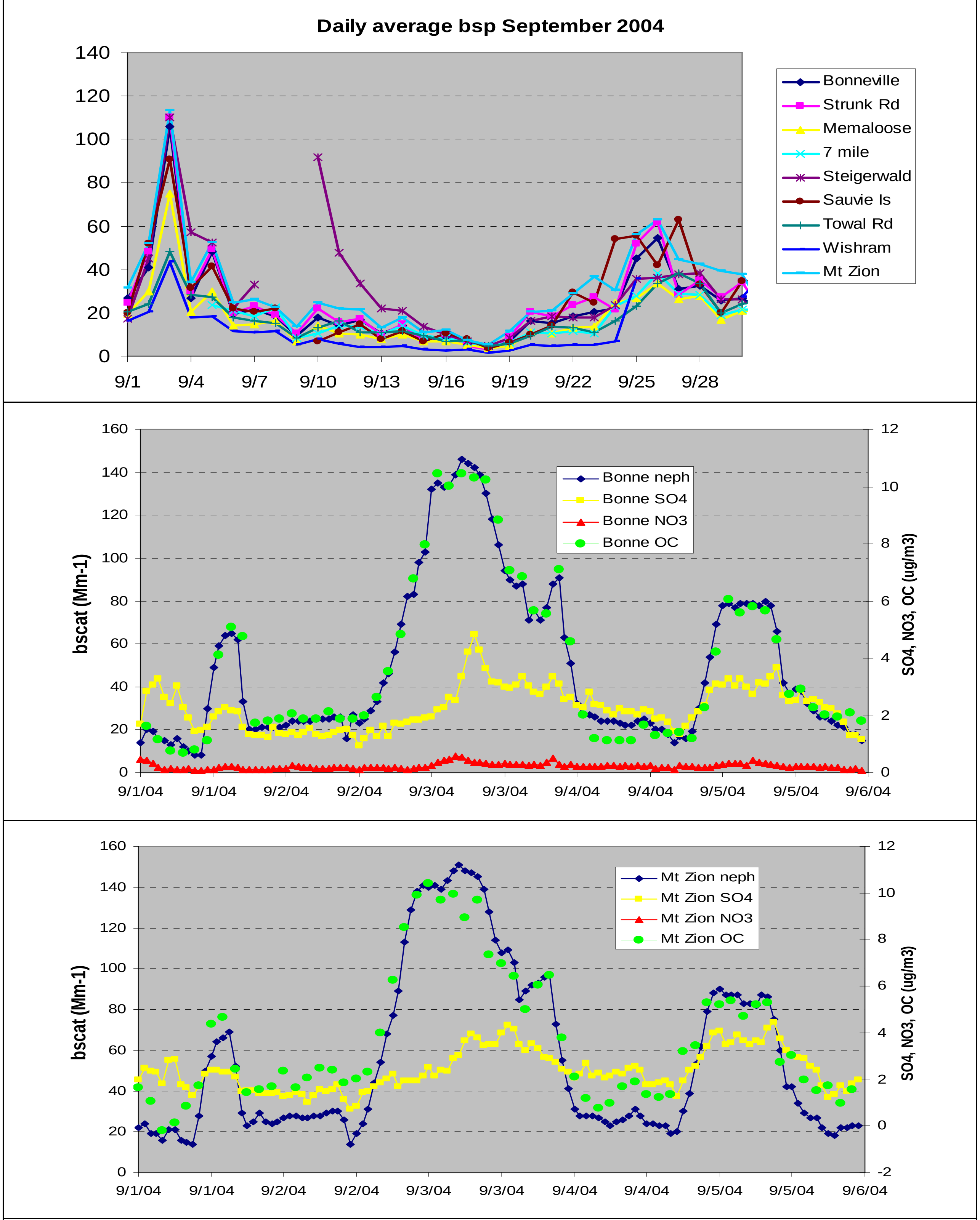


Figure 3-8. Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (middle) and Wishram (bottom) sites for September 2004.

3.3.7 Episode Selection and Prioritization

Current resources for modeling limit the number of episodes to be looked at. At this point we are limited to modeling two episodes. Although visibility impairment appears to be greater in the Gorge in the winter than summer, it is important that both seasons be analyzed. The summer seasons are also when there are the most visitors to the Gorge with more scenic vista viewing occurring.

The Haze Gradient Study classified each monitoring day into five clusters based on the meteorological characterization (Green et al., 2006). These clusters are briefly defined in Table 3-2.

Table 3-2. Classification of clusters by meteorology and seasonality (Source: Green et al., 2006).

Cluster	Wind Pattern	Seasonality
1. Light Up Gorge	Light up gorge, increasing with distance into gorge	Peak in transition months April and October, more common in winter than summer
2. Moderate Up Gorge	Moderate up gorge, increasing with distance into gorge, large diurnal variation in speed	Late summer- early fall Peak in August, most common cluster August to October
3. Strong Up Gorge	Strong up gorge, increasing with distance into gorge	Peak in July, most common cluster May-July
4. Light Down Gorge	Light down gorge, except diurnally changing direction at eastern sites, up gorge Sauvie Island	Mainly Autumn and Spring (most common cluster November), uncommon summer
5. Winter Down Gorge	Down gorge, light in eastern end, increasing through gorge, light down at Sauvie Island	Predominantly winter – most common cluster December-February, no occurrences May-September

Table 3-3 lists the classification of the meteorological conditions by cluster type for the key episode days for the five candidate modeling episodes.

Table 3-3. Classification of key episode days during the five candidate episode periods.

	Number of Key Days for Each Cluster					Number IMPROVE
	1	2	3	4	5	
November 2004				1	4	2
February 2005				2	2	NA
February 2004					3	1
July 2004	1	2	1			1
August 2004	4	2	2			3

Based on this analysis, EPA guidance and results from the Haze Gradient Report we recommend the following episode modeling priority:

1. November 2004
2. August 2004
3. February 2004
4. July 2004
5. February 2005

Thus, the initial Gorge Study Modeling recommends that we focus on the November 2004 and August 2004 episodes.

4.0 MODELING DOMAINS AND DATA AVAILABILITY

This chapter summarizes the model domain definitions for the Columbia River Gorge Scenic Areal modeling including the model domain, resolution, map projections and nesting schemes for high resolution sub-domains.

4.1 Horizontal Modeling Domain

The 36 km continental US horizontal domain for each of the models will be identical to those used by WRAP, CENRAP and VISTAS. The CMAQ and CAMx air quality modeling domain is nested in the MM5 domain. The selection of the MM5 domain is described by Johnson (2004). Figure 4-1 shows the MM5 horizontal domain as the outer most, blue grid. Also shown in Figure 4-1 is the CMAQ and CAMx 36 km domain nested in the MM5 domain. To achieve finer spatial resolution in the Gorge Region we will also use a nested higher resolution grids with a 12, 4 and 1.33 km grid resolution.

Both MM5 and CMAQ/CAMx will employ the Regional Planning Organization (RPO) unified grid definition for the 36 km continental domain for the Gorge modeling. The RPO unified grid consists of a Lambert-Conformal map projection using the map projections parameters listed in Table 4-1.

Table 4-1. RPO Unified grid definition.

Parameter	Value
projection	Lambert-Conformal
alpha	33 degrees
beta	45 degrees
x center	97 degrees
y center	40 degrees

The MM5 36 km grid include 164 cells in the east-west dimension and by 128 cells in the north-south dimension. The CMAQ/CAMx 36 km grid include 148 cells in the east-west dimension and 112 cells in the north-south dimension. Because the MM5 model is also nested in the Eta model, there is a possibility of boundary effects near the MM5 boundary that occur as the Eta meteorological variables are being simulated by MM5 and must come into dynamic balance with MM5's algorithms. Thus, a larger MM5 domain was selected to provide a buffer of 8 to 9 grid cells around each boundary of the CMAQ/CAMx 36 km domain. This is designed to eliminate any errors in the meteorology from boundary effects in the MM5 simulation at the interface of the MM5 and Eta models. The buffer region used here exceeds the EPA suggestion of at least 5 grid cell buffer at each boundary.

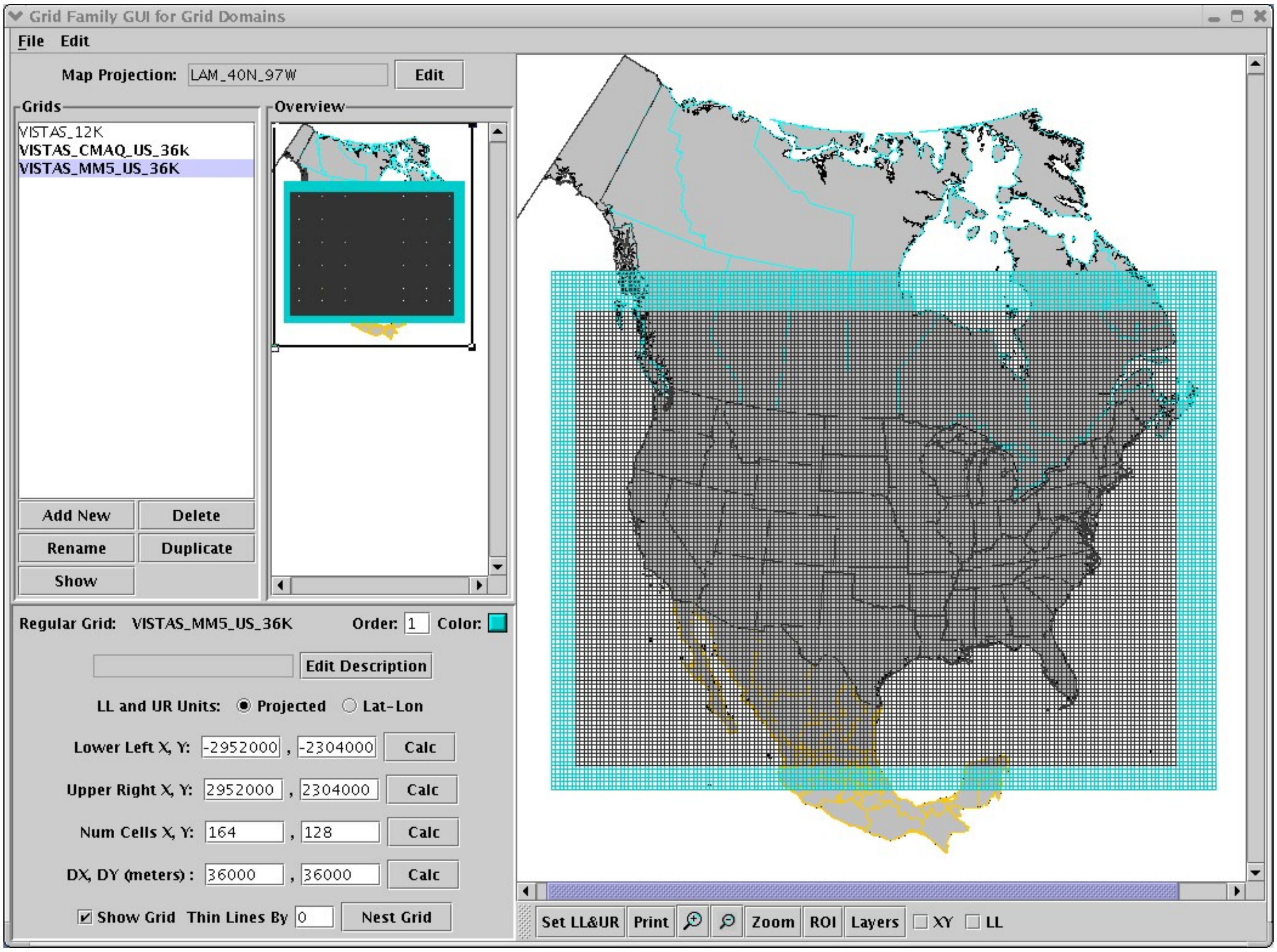
Table 4-2 lists the number of rows and columns and the definition of the X and Y origin (i.e., the southwest corner) for the 36 km for both MM5 and CMAQ/CAMx. Note that the CMAQ/CAMx grid is rotated 90 degrees relative to the MM5 grid, so rows and columns are reversed. In Table 4-2 "Dot" refers to the grid mesh defined at the vertices of the grid cells while "cross" refers to the grid mesh defined by the grid cell centers. Thus, the dimension of the dot mesh is equal to the cross mesh plus one. Finally, we note that the grid definition for the SMOKE emissions model, CMAQ Meteorology Chemistry Interface Processor (MCIP), CMAQ Chemical Transport Model (CCTM), MM5CAMx processor and CAMx model are identical.

Table 4-2. Grid definitions for MM5 and CMAQ/CAMx.

Model	Columns dot(cross)	Rows dot(cross)	Xorigin	Yorigin
MM5 36km	129 (128)	165 (164)	-2952000	-2304000
CMAQ/CAMx 36km	149 (148)	113 (112)	-2736000	-2088000

4.2 Vertical Modeling Domain

The CMAQ and CAMx vertical structure is primarily defined by the vertical grid used in the MM5 modeling. The MM5 model employed a terrain following coordinate system defined by pressure, using 34 layers that extend from the surface to the 100 mb. Table 4-3 list the layer definitions for both MM5 and for CMAQ and CAMx. We will use the exactly same vertical layer structure in CAMx as in CMAQ, except CAMx requires an extra layer at the top. A layer averaging scheme is adopted for CMAQ/CAMx to reduce the computational cost of the CMAQ and CAMx simulations. The effects of layer averaging were evaluated by WRAP and VISTAS and found to have a relatively minor effect on the model performance metrics when both the 34 layer and a 19 layer CMAQ model simulations were compared to ambient monitoring data (Morris et al., 2004a).



Map Projection: LAM_40N_97W

Grids:
VISTAS_12K
VISTAS_CMAQ_US_36k
VISTAS_MM5_US_36K

Regular Grid: VISTAS_MM5_US_36K Order: 1 Color:

LL and UR Units: ● Projected ○ Lat-Lon

Lower Left X, Y: -2952000 , -2304000

Upper Right X, Y: 2952000 , 2304000

Num Cells X, Y: 164 , 128

DX, DY (meters) : 36000 , 36000

☑ Show Grid Thin Lines By 0

Figure 4-1. Nesting of 36-km CMAQ/CAMx grid in the MM5 36-km grid.

Table 4-3. Vertical layer definition for MM5 simulations (left most columns), and approach for reducing CMAQ/CAMx layers by collapsing multiple MM5 layers (right columns).

MM5					**CMAQ**	**19L**			
Layer	Sigma	Pres(mb)	Height(m	Depth(m)	Layer	Sigma	Pres(mb)	Height(m)	Depth(m
34	**0.000**	**100**	**14662**	**1841**	**19**	**0.000**	**100**	**14662**	**6536**
33	0.050	145	12822	1466		0.050	145		
32	0.100	190	11356	1228		0.100	190		
31	0.150	235	10127	1062		0.150	235		
30	0.200	280	9066	939		0.200	280		
29	**0.250**	**325**	**8127**	**843**	**18**	**0.250**	**325**	**8127**	**2966**
28	0.300	370	7284	767		0.300	370		
27	0.350	415	6517	704		0.350	415		
26	0.400	460	5812	652		0.400	460		
25	**0.450**	**505**	**5160**	**607**	**17**	**0.450**	**505**	**5160**	**1712**
24	0.500	550	4553	569		0.500	550		
23	0.550	595	3984	536		0.550	595		
22	**0.600**	**640**	**3448**	**506**	**16**	**0.600**	**640**	**3448**	**986**
21	0.650	685	2942	480		0.650	685		
20	**0.700**	**730**	**2462**	**367**	**15**	**0.700**	**730**	**2462**	**633**
19	0.740	766	2095	266		0.740	766		
18	**0.770**	**793**	**1828**	**259**	**14**	**0.770**	**793**	**1828**	**428**
17	0.800	820	1569	169		0.800	820		
16	**0.820**	**838**	**1400**	**166**	**13**	**0.820**	**838**	**1400**	**329**
15	0.840	856	1235	163		0.840	856		
14	**0.860**	**874**	**1071**	**160**	**12**	**0.860**	**874**	**1071**	**160**
13	0.880	892	911	158	**11**	**0.880**	**892**	**911**	**158**
12	**0.900**	**910**	**753**	**78**	**10**	**0.900**	**910**	**753**	**155**
11	0.910	919	675	77		0.910	919		
10	**0.920**	**928**	**598**	**77**	**9**	**0.920**	**928**	**598**	**153**
9	0.930	937	521	76		0.930	937		
8	**0.940**	**946**	**445**	**76**	**8**	**0.940**	**946**	**445**	**76**
7	**0.950**	**955**	**369**	**75**	**7**	**0.950**	**955**	**369**	**75**
6	**0.960**	**964**	**294**	**74**	**6**	**0.960**	**964**	**294**	**74**
5	**0.970**	**973**	**220**	**74**	**5**	**0.970**	**973**	**220**	**74**
4	**0.980**	**982**	**146**	**37**	**4**	**0.980**	**982**	**146**	**37**
3	**0.985**	**986.5**	**109**	**37**	**3**	**0.985**	**986.5**	**109**	**37**
2	**0.990**	**991**	**73**	**36**	**2**	**0.990**	**991**	**73**	**36**
1	**0.995**	**995.5**	**36**	**36**	**1**	**0.995**	**995.5**	**36**	**36**
0	**1.000**	**1000**	**0 0**	**0**	**0**	**1.000**	**1000**	**0 0**	

4.3 Higher Resolution Modeling Domains

A 12 km higher resolution modeling domain will be nested in the continental US Inter-RPO 36 km domain and cover all of Oregon, Washington and Oregon and portions of neighboring States and Canada. Nested within the 12 km domain will be a 4 km grid that covers most of Washington and Oregon and into western Idaho. Finally, for key episode day(s) a 1.33 km grid nest will be used covering the Gorge area. Figure 4-1 displays the proposed MM5 36/12/3/1.33 km nested grid modeling domains. The SMOKE emissions and CMAQ/CAMx air quality modeling domains will be slightly smaller and offset by several (at least 5) buffer grid cells from the MM5 boundaries to limit the uncertainties associated with MM5 predictions near its boundaries.

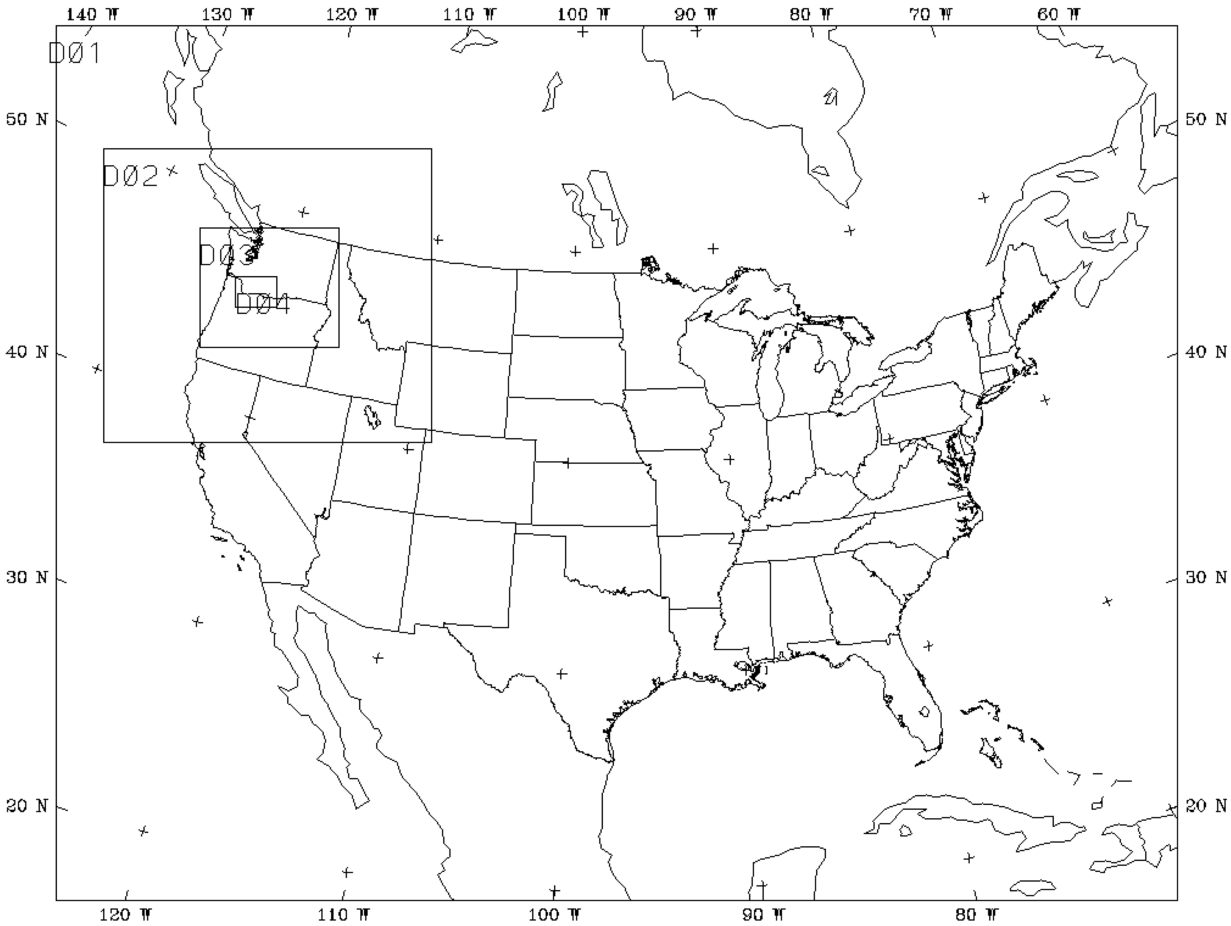


Figure 4-1a. Proposed 36 km (D01), 12 km (D02), 4 km (D03) and 1.33 km (D04) nested-grid modeling domains for MM5 meteorological modeling.

Figure 4-1b. Proposed 12 km (D02), 4 km (D03) and 1.33 km (D04) nested-grid modeling domains for MM5 meteorological modeling.

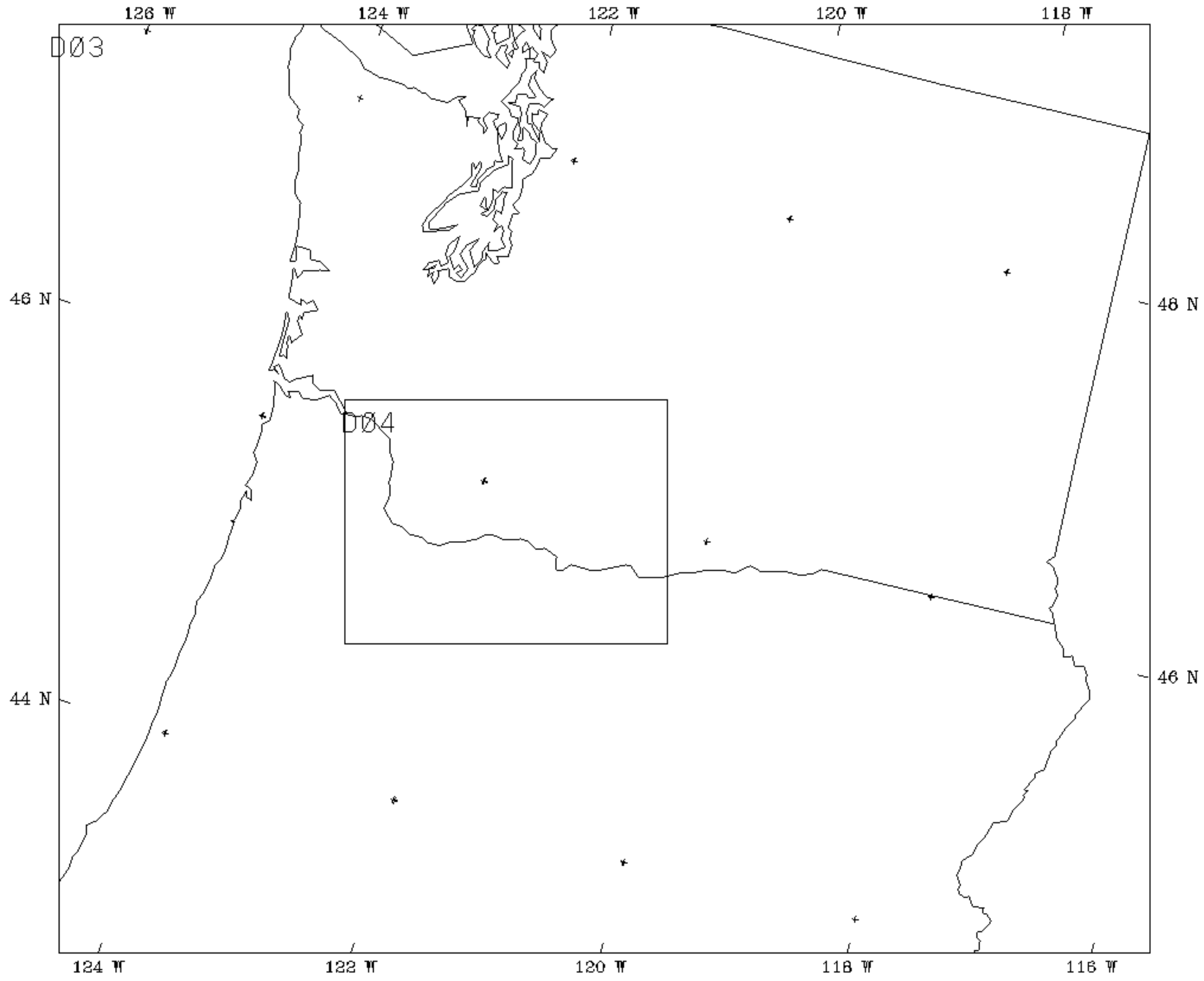


Figure 4-1c. Proposed 4 km (D03) and 1.33 km (D04) nested-grid modeling domains for MM5 meteorological modeling.

4.4 Data Availability

The CMAQ and CAMx modeling systems require emissions, meteorological, initial and boundary condition (IC/BC) and ozone column data for defining the inputs.

4.4.1 Emissions Data

The base year emissions inventory for the Gorge episodic modeling will be founded on revised 2002 emissions developed by WRAP. These data will be augmented by emissions for several counties in Oregon and Washington that will be provided by SWCAA/ODEQ. Figure 4-2 lists the counties that SWCAA/ODEQ are collecting refined emission estimates for the Gorge study.

As necessary, all emissions will be converted to Inventory Data Analyzer (IDA) formatted versions and the data will be processed for air quality modeling using the Sparse Matrix Operating Kernel Emissions (SMOKE) model. Included in these runs will be the temporal and speciation profiles and cross-reference data provided with the SMOKE model augmented with any recommended and approved emission profile data provided by the emissions inventory contractor, obtained from EPA, or prepared by the Study Team prior to initial emissions modeling. Spatial allocation of the emissions will be based on profiles and spatial allocation factors developed by the Study Team.

For the 36 km grid, we proposed to use the WRAP seasonal 2002 anthropogenic emissions without any projections. For biogenic sources, the SMOKE-BEIS-3 module would be run with the new MM5 data to generate day-specific 36 km biogenic emissions for the Gorge modeling episodes. For the 12/4/1.33 km grids, where necessary the 2002 emissions would be projected to 2004. Biogenic emissions would be generated using SMOKE-BEIS-3. The SMOKE-MOBILE6 module would be use for on-road mobile sources.

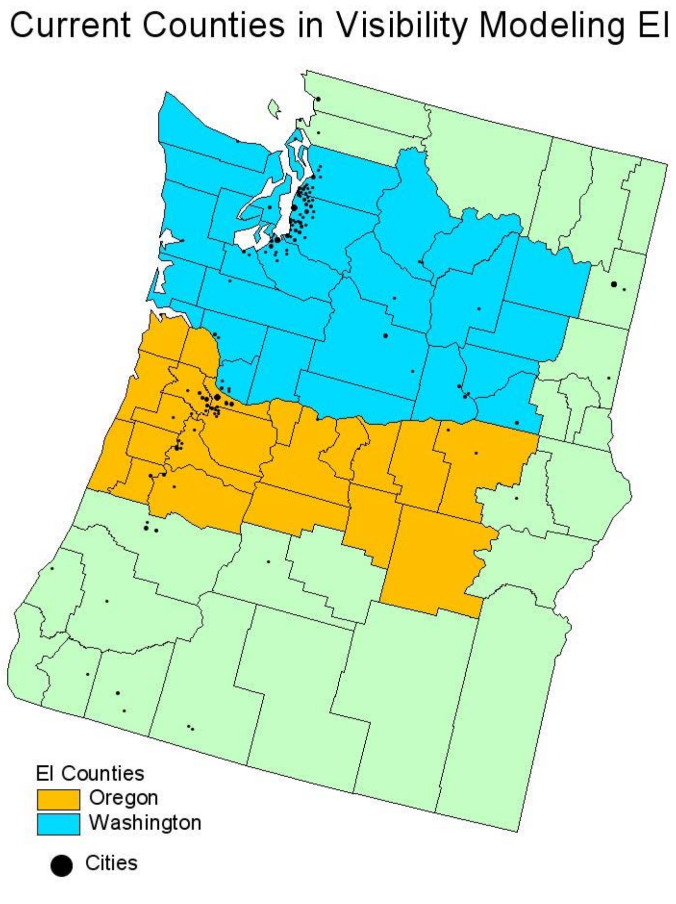


Figure 4-2. Counties where ODEQ and SWCAA are assembling emissions for Gorge Study modeling (Spokane is also included).

4.4.2 Air Quality

Data from routine ambient monitoring networks as well as the intensive Gorge measurement program for both gas and aerosol species are used in the model performance evaluation. Table 4-4 summarizes routine ambient monitoring networks, the Gorge intensive monitoring was described in Chapter 3. Figure 4-3 displays the locations for the routine ambient monitoring sites for all networks but the AQS network, which contains so many sites they would obscure the other networks.

Table 4-4. Overview of routine ambient data monitoring networks.

Monitoring Network	Chemical Species Measured	Sampling Period	Data Availability/Source
The Interagency Monitoring of Protected Visual Environments (**IMPROVE**)	Speciated PM25 and PM10 (see species mappings)	1 in 3 days; 24 hr average	http://vista.cira.colostate.edu/improve/Data/IMPROVE/improve_data.htm
Clean Air Status and Trends Network (**CASTNET**)	Speciated PM25, Ozone (see species mappings)	Approximately 1-week average	http://www.epa.gov/castnet/data.html
National Atmospheric Deposition Program (**NADP**)	Wet deposition (hydrogen (acidity as pH), sulfate, nitrate, ammonium, chloride, and base cations (such as calcium, magnesium, potassium and sodium)), Mercury	1-week average	http://nadp.sws.uiuc.edu/
Air Quality System (**AQS**) Aka Aerometric Information Retrieval System (**AIRS**)	CO, NO2, O3, SO2, PM25, PM10, Pb	Typically hourly average	http://www.epa.gov/air/data/
Speciation Trends Network (**STN**)	Speciated PM	24-hour average	http://www.epa.gov/ttn/amtic/amticpm.html
Southeastern Aerosol Research and Characterization (**SEARCH**) (Southeastern US only)	24-hr PM25 (FRM Mass, OC, BC, SO4, NO3, NH4, Elem.); 24-hr PM coarse (SO4, NO3, NH4, elements); Hourly PM2.5 (Mass, SO4, NO3, NH4, EC, TC); Hourly gases (O3, NO, NO2, NOy, HNO3, SO2, CO)	Hourly or 24-hour average, depending on parameter.	Electric Power Research Institute (EPRI), Southern Company, and other companies. http://www.atmospheric-research.com
EPA Particulate Matter Supersites	Speciated PM25		http://www.epa.gov/ttn/amtic/supersites.html
Photochemical Assessment Monitoring Stations (**PAMS**)	Varies for each of 4 station types.		http://www.epa.gov/ttn/amtic/pamsmain.html
National Park Service Gaseous Pollutant Monitoring Network	Acid deposition (Dry; SO4, NO3, HNO3, NH4, SO2), O3, meteorological data	Hourly	http://www2.nature.nps.gov/ard/gas/netdata1.htm

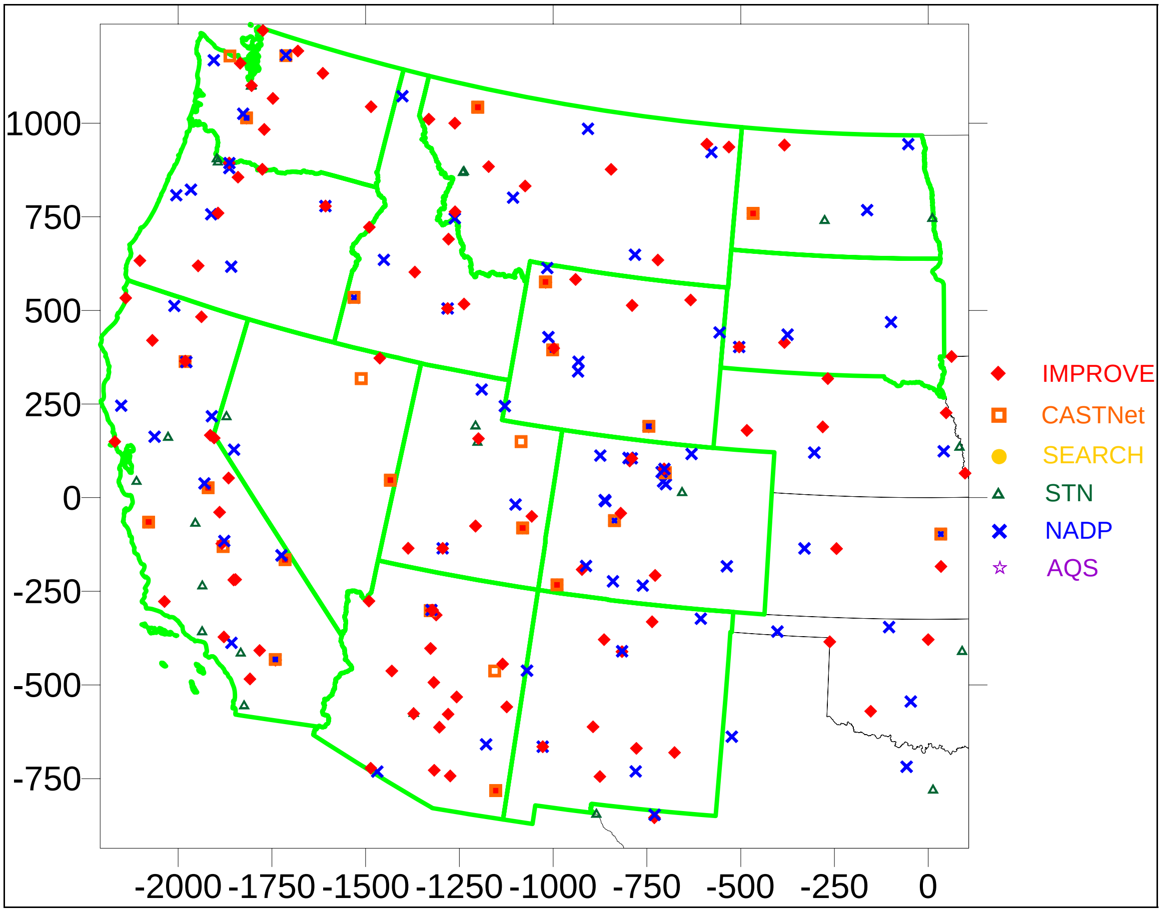


Figure 4-3. Locations of IMPROVE, CASTNet, SEARCH, STN and NADP monitoring sites in and near the western U.S.

4.4.3 Ozone Column Data

Additional data used in the air quality modeling include the Total Ozone Mapping Spectrometer (TOMS). TOMS data is available for 24-hour average and is obtained from http://toms.gsfc.nasa.gov/eptoms/ep.html. The TOMS data is used in the CMAQ (JPROC) and CAMx (TUV) radiation model to calculate photolysis rates.

4.4.4 Meteorological Data

Meteorological data are being generated using the MM5 prognostic meteorological model as described in Chapter 2.

4.4.5 Initial and Boundary Conditions Data

The CMAQ default Initial Concentrations (ICs) will be used for both CMAQ and CAMx along with a ~10 day spin up period on the 36 km grid to eliminate any significant influence of the ICs.

The CMAQ and CAMx Boundary Conditions (BCs) will be based on monthly average results from a 2002 GEOS-CHEM global climate model simulation. The 2002 GEOS-CHEM model output has been processed to define day-specific high time resolved (i.e., 3-hourly) CMAQ and CAMx BCs for 2002 that are used in the RPOs 2002 annual modeling. These data will be averaged to obtain monthly average diurnally varying boundary conditions that will be used to define the concentrations along the edges of the 36 km domain.

5.0 MODEL INPUT PREPARATION PROCEDURES

In this section we describe the procedures to be used to develop the CMAQ and CAMx model inputs for the Gorge 2004 modeling episodes. The development of the CMAQ and CAMx meteorological and emissions inputs are discussed first followed by the science options to be used by CMAQ and CAMx. The procedures for developing the initial and boundary conditions and photolysis rates inputs are then discussed along with the model application procedures.

5.1 Meteorological Inputs to Emissions and Air Quality Models

The emissions and air quality models require certain meteorological input data including wind fields, estimates of turbulent eddy dispersion, humidity, temperature, clouds, and actinic flux. Spatially gridded and hourly varying meteorological data are needed to estimate biogenic, mobile source emissions, and plume-rise for large, elevated point sources. Meteorological data are needed to drive chemical transport models for solving atmospheric diffusion and chemistry equations for model species. Because observed data are not available for the full gridded model domain, numerical meteorological models are used to provide these inputs.

The National Center for Atmospheric Research (NCAR)/Pennsylvania State University (PSU) Fifth-Generation Mesoscale Model (MM5) (v3.63) will be used to simulate meteorology at a 36-km resolution for the Gorge episodes plus ~10 day spin-up period. For the last two days of the spin-up period the 12 km grid will also be used. For all Gorge episode days the 36/12/4 km grid structure will be used. On key episode day(s) to be determined, a 1.33 km grid will be specified over the Gorge area. The modeling results in the Gorge using the 4 km and 1.33 km grid will be analyzed. If significant improvement in model performance is seen using the 1.33 km grid then this issue will be discussed with the SWCAA and Gorge Technical Team. However, there are currently insufficient resources to model all episode days at 1.33 km.

The MM5 is a three-dimensional prognostic meteorological model that is used not only for meteorology studies but also for air quality studies. Some of the physics used in the simulation include nonhydrostatic dynamics; four-dimensional data assimilation of wind, temperature, and mixing ratio; explicit treatment of moisture; cumulus cloud parameterization; vertical mixing of momentum in the mixed layer; PBL process parameterization; atmospheric radiation; sea ice treatment; and snow cover (see Chapter 2 for more details).

5.1.1 MCIP Reformatting Methodology

The Models-3 Community Multiscale Air Quality (CMAQ) modeling system is designed to simulate multiscale (urban and regional) and multi-pollutant (oxidants, acid deposition, and particles) air quality problems. But before running the CMAQ Chemical Transport Model (CCTM), the MM5 generated meteorological data must be pre-processed and converted to Models-3 consistent data structures. MCIP version 3.0 will be used to preprocess the MM5 meteorological output. The “pass through” option in MCIP will be used in the Gorge Study modeling. One of MCIP’s functions is to translate meteorological parameters from the output of the Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR)

Mesoscale Modeling System Generation 5 (MM5) to the Models-3 input/output applications program interface (I/O API format) which is required for operation of Models-3 CMAQ processors. Some other necessary parameters not available from the meteorological model are estimated with appropriate diagnostic algorithms in the program. The key functions of MCIP include:

1. Reading in meteorological model output files
2. Extraction of meteorological data for CTM window domain
3. Interpolation of coarse meteorological model output for finer grid
4. Collapsing of meteorological profile data if coarser vertical resolution data is requested
5. Computation or passing through surface and PBL parameters
6. Diagnosing of cloud parameters
7. Computation of species-specific dry deposition velocities
8. Generation of coordinate dependent meteorological data for the generalized coordinate CCTM simulation
9. Output meteorological data in Models-3 I/O API format

The MCIP processor transforms the data into I/O API format while also calculating several new data fields (e.g. low, middle, and high cloud fractions) that are not readily available in the raw MM5 output. It also interpolates temperature and wind speed to observation height (1.5m and 10m, respectively). The MCIP processor culls a minimum of six cells about the domain periphery to minimize edge effects in the MM5 simulation. MCIP can be used to further reduce the rows or columns in the MM5 data so that the domain definition for the MCIP output files precisely matches the domain used in the air quality modeling. MCIP also allows MM5 layers to be "collapsed" (i.e., some layers can be aggregated). When feasible it is desirable to use the same layer structure in the air quality model as in the MM5 to prevent errors associated with aggregating layer data and to maintain consistency between data produced by the meteorological model and those used by the chemistry-transport model. However, due to computational costs associated with using large number of vertical layers, vertical layer collapsing is typically used to reduce the total number of layers used by the CCTM. In the Gorge Study modeling we will collapse from 34 layers in MM5 output into 19 layers for the CMAQ air quality simulations. The first 8 layers of CMAQ, up to approximately 450 m AGL, will match the MM5 vertical layer structure exactly. The region top for CMAQ is the same as used by MM5, 100mb (approximately 15 km AGL). The 36 km analysis domain contains 148 columns, 112 rows, and 19 layers. The definition of the horizontal extend of the 12 km domain is to be determined, but 19 layers will be used. More details on the CMAQ modeling domain definitions are provided in Chapter 4 with the vertical layer structure of MM5 and MCIP/CMAQ shown in Table 4-3.

5.1.2 Products of the CMAQ Meteorological Input Development Process

The meteorological input development process produces three two-dimensional and four three-dimensional daily meteorological and geophysical output data in the Models-3 I/O API format. These CCTM-ready meteorological input files are used in both emissions processing and the CCTM simulations. The met fields are 36 km and 12 km horizontal resolution on a Lambert Conformal Projection (LCP) coordinate system with 19 vertical sigma layers extending from the surface to the 100 mb pressure level. The data files include three-dimensional gridded fields of u- and v-wind components, vertical velocity, temperatures, Jacobian, Jacobian weighted air density, total air density, water vapor, cloud water content, rain water content, ice and snow mixing ratio, layer heights, and vertical exchange coefficients. Two-dimensional gridded fields of latitude and longitude, squared map-scaled factor, surface temperatures and pressures, 1.5 and 10 meter temperature, planetary boundary heights, rainfall, total cloud fraction, snow cover, deposition velocities, u* and w*, surface roughness length, as well as dominant land use category are also developed.

Table 5-1 shows the configuration to be used in MCIP version 3.0 for processing the 2002 MM5 output to produce CCTM-ready meteorology input files.

Table 5-1. MCIP V3.0 configuration used In the Gorge modeling.

Module or Option	Values or Setting	Additional Information
PBL value computation option	1	Use PBL value from input meteorology
Radiation fields	1	Use radiation fields from input meteorology
Dry deposition option	2	Use Models-3 (Pleim) dry deposition routine
Output interval	60	Unit is in minutes
Vertical layer structure	19 layers	See Chapter 4

5.1.3 MM5 Reformatting Methodology

MM5CAMx serves the same purpose as MCIP in the CAMx modeling system. MM5CAMx will be exercised using the same layer structure as MCIP, with the addition of a layer aloft that is needed to assure mass consistency in CAMx. Two sets of vertical turbulent diffusivity files will be generated:

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

MM5CAMx will be operated initially with a 0.1 m^2/s minimum K_V (Kz_min) value, however the CAMx-ready K_V files may be updated to a 1.0 m^2/s Kz_min to be consistent with CMAQ.

5.1.4 Treatment of Minimum K_V

The minimum K_V value (Kz_min) is an area of ongoing investigation by the CMAQ and CAMx developers. EPA initially recommended a 1.0 m^2/s Kz_min for CMAQ modeling, but in their latest release of CMAQ (V4.5) EPA has an option for using Kz_min values of 0.1 to 2.0 m^2/s depending on the amount of urban land use present. We propose to use this option in the Gorge modeling for CMAQ and do something similar for CAMx.

5.2 Development of Emissions Model Inputs and Resultant Inventories

The current base year emissions inventory for the National Emissions Inventory (NEI) is 2002. WE will use the current 2002 emissions and SMOKE set up developed for the WRAP study as the starting point for the Gorge emissions modeling. For the 36 km grid, the WRAP anthropogenic emissions will be used "as is" and the biogenic emissions will be updated.

For the 12/4/1.33 km grids, the 2002 emissions would be projected to 2004 and the SMOKE emissions modeling system would be used to generate the hourly speciated spatially varying emission inputs needed by CMAQ and CAMx.

The WRAP projected 2004 emissions would be replaced by 2004 emissions data provided by SWCAA/ODEQ for several counties in Washington and Oregon (Figure 4-2).

These emissions will then be converted to Inventory Data Analyzer (IDA) formatted versions and the data will be processed for air quality modeling using the Sparse Matrix Operating Kernel Emissions (SMOKE) model. Included in these runs will be the temporal, spatial, and speciation profiles and cross-reference data currently provided with SMOKE augmented with any recommended and approved emission profile data provided by SWCAA, ODEQ, WAECY or others. The processing will be adjusted for each run to account for the specific air quality model (AQM) input required by CMAQ.

5.2.1 Emissions Modeling Methodology

Emissions inventory development for photochemical modeling must address several source categories including: (a) stationary point sources, (b) area sources, (c) on-road mobile sources, (d) non-road mobile sources, and (e) biogenic sources. For this analysis, these estimates must be developed to support the episode that is being modeled (i.e., the historical base year when the episode actually occurred; 2004).

Development of an emissions inventory customized for the Gorge region requires a merging of: (a) the most recent *pertinent* regional inventory and (b) available high-resolution, locale-specific emissions estimated by local, state, and regional agencies in the Gorge region. Local air regulatory and transportation planning agencies are generally the best sources of domain specific activity and control factors to use in developing the base year emissions. Often, these local emissions data sets come from a variety of sources, frequently in different formats.

5.2.2 Set-up of SMOKE Over the Gorge Modeling Domain

SMOKE will be configured to generate point, area, nonroad, highway, and biogenic source emissions for the Gorge 12, 4 and, as necessary, 1.33 km grids. In addition, certain subcategories, such as fires and EGUs will be maintained in separate source category files in order to allow maximum flexibility in producing alternate strategies. Settings for each of the source categories are discussed in relevant sections below. With the exception of biogenic and highway mobile source emissions that are generated using the, respectively, BEIS and MOBILE6 modules in SMOKE, pre-computed annual emissions will be processed using the month, day, and hour specific temporal profiles of the SMOKE model. Day-specific emissions will be generated for biogenic and on-road mobile sources using the SMOKE-BEIS-3 and SMOKE-MOBILE6 modules and the 2004 MM5 meteorological data generated as part of the study.

Population will be used as a gridding default for all source categories when the assigned surrogate would cause SMOKE to drop emissions. This can be a case when the county-level emission inventories are prepared using surrogates other than those available for modeling purposes. Special attention will be made to develop high resolution surrogate distributions in the WA/OR region and within the Gorge itself. We will examine the emissions modeling set up for the Portland ozone modeling and use high resolution data as available. The 36 km domain for the air quality modeling will be based on the EPA's 36-km national CMAQ domain, illustrated in Figure 5-1 below (details on the modeling domains are provided in Chapter 4).

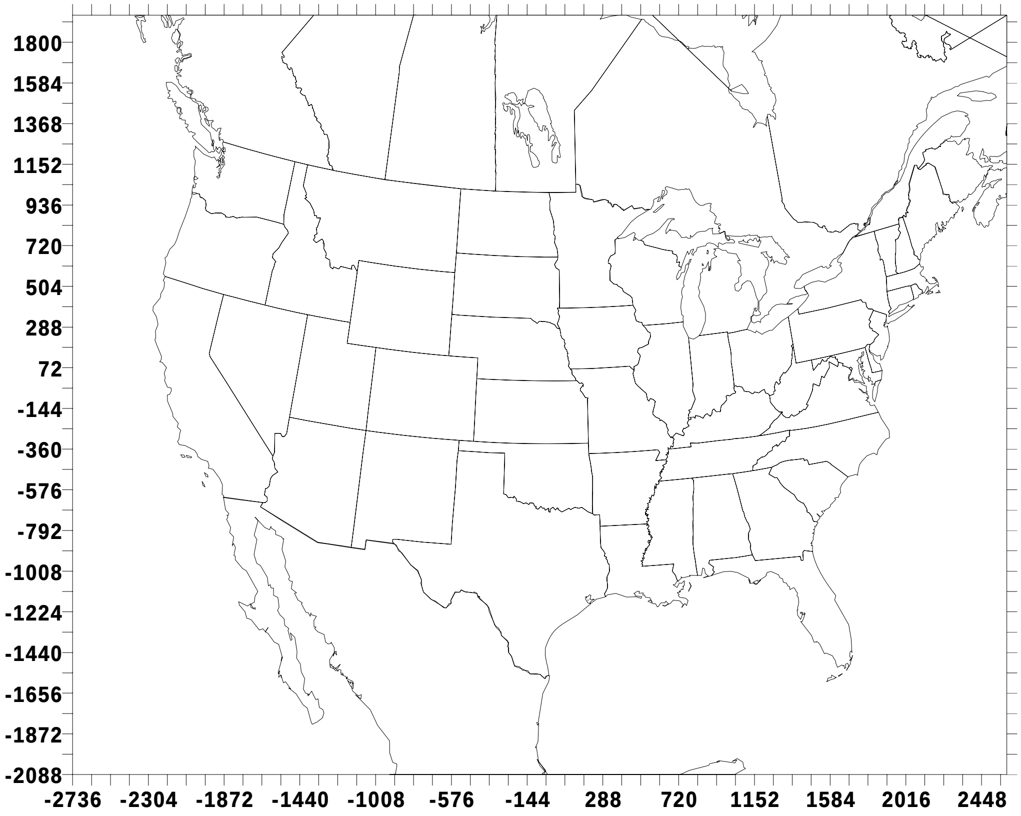


Figure 5-1. EPA 36-km National CMAQ domain.

The parameters for the SMOKE runs are as follows:

Episodes: Proposed November 2004 and August 2004 Gorge Episodes.

Future Years: 2018.

Output Time Zone: Greenwich Mean Time (zone 0)

Projection: Lambert Conformal with Alpha=33, Beta=45, Gamma=-97, and center at (Lon -97, Lat 40).

Domain:

- 36 km Grid: Origin at (-2736, -2088) kilometers with 148 rows by 112 columns and 36-km square grid cells.
- 12/4/1.33 km Grid: To be determined, but offset from MM5 domains discussed in Chapter 4

Layer Structure: The CMAQ and CAMx layer structure will include ~19 layers, with specific layer positions defined in the meteorology files (see Chapter 4).

CMAQ/CAMx Model Species: The CMAQ/CAMx initial configuration will be for the CB-IV chemical mechanism with PM. The model species in the emission input files will be: CO, NO, NO2, ALD2, ETH, FORM, ISOP, NR, OLE, PAR, TERPB, TOL, XYL, NH3, SO2, SULF, PEC, PMFINE, PNO3, POA, PSO4, and PMC.

Meteorology Data: Daily (25-hour). SMOKE requires the following five types of MCIP outputs: (1) Grid cross 2-d, (2) Grid cross 3-d, (3) Met cross 2-d, (4) Met cross 3-d, and (5), Met dot 3-d. These files need to match the grid projection and overlap with the emissions modeling region but can be larger in the horizontal directions than the modeling region shown in Figure 5-1. Therefore, the data files for the 36 Kilometer grid domain will be at least 90 columns by 132 rows.

Elevated Sources: All sources will be treated by SMOKE as potentially elevated. No plume-in-grid sources will be modeled. Wildfire and some prescribed fire emissions will be handled as point sources as available.

Biogenic emissions will be modeled for each episode day, using the daily meteorology. Point sources, including CEM and fire emissions will be modeled for each episode day to take advantage of the available day-specific emissions (if available) and meteorology. Area sources, including non-road mobile and dust emissions, with the exception of windblown dust emissions, do not utilize meteorological data, and are temporally allocated by monthly, daily and hourly profiles.

5.2.3 Development of Point Source Emissions

Stack parameters are often more important to the reliability of the air quality modeling results than the emissions rates themselves. Stack parameter data are frequently incorrect, especially in some of the current regional modeling inventories and careful QA is required to assure that the point source emissions are properly located both horizontally and vertically on the modeling grid. SMOKE has a number of built-in QA procedures designed to catch missing or out-of-range stack parameters. These procedures will be invoked in the processing of the point source data.

Depending on the emissions input files from WRAP or SWCAA/ODEQ, for the initial baseline modeling, we will be separating the point source emissions into EGU and non-EGU categories. The non-EGU category will not be using any day or hour-specific emissions. All non-EGU point source emissions will be temporally allocated to month, day, and hours using annual emissions and source category code (SCC) based allocation factors. These factors will be based on the cross-reference and profile data supplied with the SMOKE.

For EGU sources with EPA reported CEM data, or with hourly emissions provided by stakeholders, actual hourly data will be used. For those sources where EPA CEM data are utilized, NOx, SO2, and heat input-based hour-specific profiles will be developed and applied to NOx, SO2, and all other emissions, respectively. This will ensure that the annual emission values are maintained, but distributed using hourly to annual profiles. For sources providing hour-specific data and where they were approved by the State in which they operated, those data were substituted for EPA CEM-based emissions and distributions.

To temporally allocate the remaining EGU point sources, the NOx, SO2, and heat input data were collected from the 2004 Continuous Emissions Monitoring (CEM) datasets, and used to develop unit-level temporal distributions. The hour, day of week, and monthly specific temporal profiles will be used in conjunction with the EI supplied emissions data to calculate hourly EGU emissions by unit.

All point sources will be spatially allocated in the domain based on the stationary source geographic coordinates. If a point source is missing its latitude/longitude coordinates, the source will be placed in the center of its respective county.

5.2.4 Development of Area and Non-Road Source Emissions

All non-road mobile and area source emissions, except ammonia emissions (see below), will be temporally allocated to month, day of the week, and hours using annual emissions and source category code (SCC) based allocation factors. These factors will be based on the cross-reference and profile data supplied with the SMOKE. Area and non-road sources will be spatially allocated in the domain based on SCC-based spatial allocation factor files. If an area or non-road source SCC does not have an existing cross-reference profile assigned to it, the county-level emissions will be allocated by population density in the respective county.

If needed, a crustal PM transport factor will be applied to fugitive dust emission sources that have been identified in U.S. EPA modeling to have only a portion of its mass transportable from the source of the emission generation. The EPA's studies indicate that 60 to 90 percent of PM emissions from fugitive dust sources do not reach an elevated level necessary to be transported or modeled in an episodic simulation. This issue will be evaluated as part of the Gorge Modeling.

Ammonia Emissions

Ammonia emissions will be generated using the ammonia emission inventory modeling system recently developed for WRAP. The model treats all major sources of ammonia emissions (livestock, fertilizer application, natural soils, domestics sources and wild animals). The remaining ammonia emissions source categories are based on the latest 2002 inventories used for the WRAP. The WRAP ammonia model will be run using the latest 2004 36/12/4/1.33 km MM5 meteorological data. The model generates hourly gridded emissions data using gridded meteorological data to apply various adjustments to emission factors and temporal allocation factors. Therefore, SMOKE is not required for the generation of these emissions estimates, although these emissions are processed through SMOKE in order to merge these source categories with the remaining area source emission estimates to obtain gridded model-ready data files.

5.2.5 Development of On-Road Mobile Source Emissions

The MOBILE6 module of SMOKE will be used to develop the base year on-road mobile source emissions estimates for CO, NOx, PM, and VOC emissions. The MOBILE6 parameters, vehicle fleet descriptions, and VMT estimates will be combined with gridded, episode-specific temperature data to calculate the gridded, temporalized emission estimates. Of note, whereas the on-network emissions estimates are spatially allocated based on link location and subsequently summed to the grid cell level, the off-network emissions estimates are spatially allocated based on a combination of the FHWA version 2.0 highway networks and population. The MOBILE6 emissions factors are based on episode-specific temperatures predicted by the meteorological model. Further, the MOBILE6 emissions factors model accounts for the following:

- Weekly average minimum/maximum temperatures;
- Facility speeds;
- Locale-specific inspection/maintenance (I/M) control programs, if any;
- Adjustments for running losses;
- Splitting of evaporative and exhaust emissions into separate source categories; AND
- VMT, fleet turnover, and changes in fuel composition and Reid vapor pressure (RVP).

The primary input to MOBILE6 is the MOBILE shell file. The MOBILE shell contains the various options (e.g. type of inspection and maintenance program in effect, type of oxygenated fuel program in effect, alternative vehicle mix profiles, RVP of in-use fuel, operating mode) that direct the calculation of the MOBILE6 emissions factors.

5.2.6 Development of Biogenic Source Emissions

A revised version of a commonly used biogenic emissions model, the Biogenic Emissions Inventory System (BEIS), has recently been developed and tested by EPA over two separate modeling domains/episodes. This version of the model (BEIS-3, v1.2) contains several changes over BEIS-2, including the following:

- Vegetation input data -- are now based on a 1-km Biogenic Emissions Landuse Database (BELD3) vegetation data base,
- Emission factors – many updates including some recent NARSTO modifications,
- Environmental algorithm -- includes a sunlit/shaded leaf solar radiation model.

For this particular application of BEIS-3, version 1.2 as currently incorporated in the SMOKE processor will be used.

The BELD-3 landuse data on a Lambert conformal grid at 1-km resolution have already been developed, are available, and will be used to estimate biogenic emissions in this study. The BEIS model also requires as input hourly, gridded temperature and solar radiation data to estimate biogenic emissions, and these data will be derived from the MM5 2004 36/12/4/1.33 km predictions.

5.2.7 Wildfires, Prescribed Burns, Agricultural Burns. Wind Blown Dust and Sea Salt Source Emissions

If the SWCAA/ODEQ provides any emissions from fires they will be processed separately and merged with the final model-ready emissions.

5.2.8 Speciation and Reformatting of Emissions

SMOKE will be run to speciate the emissions estimates according to the requirements of the Carbon Bond Mechanism version four (CBM-IV, CB-IV or CB4). The SMOKE model will also reformat the emissions estimates for use in CMAQ modeling. For each model-ready emissions inventory, SMOKE will produce at a minimum five (5) separate air quality model-ready files:

- low-level point source;
- area source;
- elevated point source;
- mobile source; and
- biogenics.

Other source categories, such as EGU and fire emissions may also be handled as separate air quality model-ready files.

5.2.9 Development of Modeling Inventories

The emissions inventories developed for the Gorge Study modeling can be grouped into two distinct types: (1) Base Year (2004) inventories; and (2) Future Year inventories. For the 2018 emissions we will process the WRAP 2018 emission inventories for the Gorge grid structure and modeling episodes.

5.2.10 Products of the Emissions Inventory Development Process

In addition to the CMAQ-ready and CAMx-ready input files generated for each hour of the days modeled in the two 2004 modeling episodes, a number of quality assurance (QA) files will be prepared and used to check for gross errors in the emissions inputs. Importing the model-ready emissions into PAVE and looking at both the spatial and temporal distribution of the emission provides insight into the quality and accuracy of the emissions inputs.

- Visualizing the model-ready emissions with the scale of the plots set to a very low value, we can determine whether there are areas omitted from the raw inventory or if emissions sources are erroneously located in water cells.

- Spot-check the holiday emissions files to confirm that they are temporally allocated like Sundays.

- Producing pie charts emission summaries that highlight the contribution of each emissions source component (e.g. nonroad mobile).

- Normalizing the emissions by population for each state will illustrate where the inventories may be deficient and provide a reality check of the inventories.

- Spot-check vertical allocation of point sources using PAVE.

We will use state inventory summaries prepared prior to the emissions processing to compare against SMOKE output report totals generated after each major step of the emissions generation process.

To check the chemical speciation of the emissions to CB-IV terms and the vertical allocation of the emissions, we will compare reports generated with SMOKE reports to target these specific areas of the processing. For speciation, we will compare the inventory import state totals versus the same state totals with the speciation matrix applied.

For checking the vertical allocation of the emissions, we will create reports by source, hour, and layer for Oregon and Washington. We will create these reports for a representative weekday in each of the episodes for each of these states.

The quantitative QA analyses often reveal significant deficiencies in the input data or the model setup. It may become necessary to tailor these procedures to track down the source of each major problem. As such, we can only outline the basic quantitative QA steps that we will perform in an attempt to reveal the underlying problems with the inventories or processing. Following are some of the reports that may be generated to review the processed emissions:

- State and county totals from inventory for each source category
- State and county totals after spatial allocation for each source category
- State and county totals by day after temporal allocation for each source category for representative days
- State and county totals by model species after chemical speciation for each source category
- State and county model-ready totals (after spatial allocation, temporal allocation, and chemical speciation) for each source category and for all source categories combined
- If elevated source selection is chosen by user, the report indicating which sources have been selected as elevated and plume-in-grid will be included
- Totals by source category code (SCC) from the inventory for area, mobile, and point sources
- Totals by state and SCC from the inventory for area, mobile, and point sources
- Totals by county and SCC from the inventory for area, mobile, and point sources
- Totals by SCC and spatial surrogates code for area and mobile sources
- Totals by speciation profile code for area, mobile, and point sources
- Totals by speciation profile code and SCC for area, mobile, and point sources
- Totals by diurnal temporal profile code for area, mobile, and point sources
- Totals by diurnal temporal profile code and SCC for area, mobile, and point sources
- PAVE plots of gridded inventory pollutants for all pollutants for area, mobile, and point sources

5.3 CMAQ Modeling Methodology

5.3.1 CMAQ Science Configuration

This section described the model configuration and science options to be used in the Gorge Study modeling effort. The recommendations are based on testing and model evaluations of several models or model configurations carried out in BRAVO (Pitchford, 2004), CENRAP

(Pun, Chen and Seigneur, 2004; Tonnesen and Morris, 2004), VISTAS (Morris et al., 2004), MRPO (Baker, 2004) and WRAP (Tonnesen, 2003) modeling studies. Table 5-2 summarizes the proposed configuration for CMAQ. The latest version of CMAQ is currently Version 4.5 that was released October 2005 and is currently proposed for use in the Gorge modeling. However, if EPA releases an updated version of CMAQ in time, the Gorge Study would likely switch to the latest version at that time.

In the CMAQ base configuration we will run the 36 km for the ~10 spin-up days prior to the two 2004 Gorge episodes with the 12 km grid introduced for the last two spin-up days. For all of the Gorge episode days a 4 km grid would also be used, with some key episode day(s) also being modeled with the 1.33 km grid. Day-specific 2004 emissions would be used with the 12/4/1.33 km grid, but the WRAP 2002 emissions would be used for the 36 km grid. CMAQ uses one-way grid nesting where the boundary conditions for the 12 km grid simulation are extracted from the 36 km run using the CMAQ BCON processor. Similarly, boundary conditions for the 4 km and 1.33 km grids are extracted from their 12 km and 4 km parent grids using the CMAQ BCON processor, respectively. The base configuration of CMAQ will use 19 vertical layers up to a region top of 100 mb (approximately 15 km AGL) (see Table 4-3).

The PPM advection solver would be used along with the spatially varying (Smagorinsky) horizontal diffusion approach. K-theory will be used for vertical diffusion. The CMAQ MCIP3.0 meteorological processor would be run using the percent urban (PURB) option for specifying a minimum eddy diffusion constant (Kz_min) that would range from 0.1 to 2.0 m^2/s depending of the fraction of urban land use category present.

The MCIP3.0 will be used to process the MM5 data using the “pass through” option.

The AERO3/ISORROPIA aerosol chemistry scheme will be used for inorganic aerosol thermodynamics.

The CB-IV gas-phase chemical mechanism is selected for the Gorge modeling.

Table 5-2. Proposed Gorge Study model configuration for the CMAQ.

Model Option	CMAQ
Model Version	Version 4.5 (October 2005)
Horizontal Resolution	36/12 14/1.33 km
No. Vertical Layers	NZ = 19
Horizontal Advection	PPM
Vertical Advection	PPM
Horizontal Diffusion	Spatially Varying
Vertical Diffusion	K_V (Eddy Diffusion)
MM5 Configuration	Pleim-Xiu/ACM
MM5 Processing	MCIP 3.0 Pass Through
Gas-Phase Chemistry	CB4
Gas-Phase Chemistry Solver	EBI
Secondary Organic Aerosol	SORGAM
Aqueous-Phase Chemistry	RADM
Aerosol Chemistry	AE4/ISORROPIA
Dry Deposition	Pleim-Xiu
Plume-in-Grid	Off
Initial Concentrations	CMAQ Default
Boundary Conditions	Monthly Avg GEOS-CHEM
Emissions	WRAP 2002 augmented by SWCAA/ODEQ data for WA and OR

5.3.2 Spin-Up Initialization

For the two 2004 Gorge episodes, CMAQ will be initialized with a 10 day spin up period on the 36 km grid with the 12km grid introduced for the last two spin up days.

5.3.3 Boundary Conditions

Harvard University was contracted by the RPOs to perform a 2002 GEOS-CHEM global climate model simulation. VISTAS has processed the 2002 GEOS-CHEM model output and generated day-specific 3-hourly boundary conditions (BCs) for the 36 km Inter-RPO grid in the CMAQ BCON format. These data will be processed to obtain monthly average hourly varying boundary condition inputs that will be used with the two Gorge 2004 episodes

5.3.4 Photolysis Rates

Several chemical reactions in the atmosphere are initiated by the photodissociation of various trace gases. To accurately represent the complex chemical transformations in the atmosphere, accurate estimates of these photodissociation rates must be made. The Models-3 CMAQ system includes the JPROC processor, which calculates a table of clear-sky photolysis rates (or J-values) for a specific date. JPROC uses default values for total aerosol loading and provides the option to use default column O3 data or to use TOMS data for total column O3. We will use day-specific TOMS ozone data for the Gorge episodic modeling.

JPROC produces a "look-up" table provides the photolysis rates as a function of latitude, altitude, and time (in terms of the number of hours of deviation from local noon, or hour angle). In the current CMAQ implementation, the J-values are calculated for six latitudinal bands (10º, 20º, 30º, 40º, 50º, and 60º N), seven altitudes (0 km, 1 km, 2 km, 3 km, 4 km, 5 km, and 10 km), and hourly values up to ±8 hours of deviation from local noon. During model calculations, photolysis rates for each model grid cell are estimated by first interpolating the clear-sky photolysis rates from the look-up table using the grid cell latitude, altitude, and hour angle, followed by applying a cloud correction factor.

The photolysis rates input file must be prepared as separate look-up tables for each simulation day. The modeling team has already prepared scripts to automate the production of photolysis rate files for each day of the episodic simulation. Photolysis files are ASCII files, and these will be visually checked for selected days to verify that photolysis are within the expected ranges.

5.4 CAMx Modeling Methodology

This section described the model configuration and science options to be used in the Gorge Study CAMx modeling effort. Table 5-3 summarizes the proposed configuration for CAMx. The latest version of CAMx is currently Version 4.30 and is currently proposed for use in the Gorge Study modeling. However, a more appropriate updated version of CAMx is available, the Gorge Study would likely switch to the latest version.

5.4.1 CAMx Science Components

Because CAMx supports two-way nesting and CMAQ does not, the model configuration will be slightly different. In the CAMx base configuration we will run the 36 km for the first 8 days of the 10 day spin up period and then run the 36/12 km grids for the last two days of the spin-up period. For the episode days the 36/12/4 km grid structure will be run using two-way nesting. On specific days CAMx will be run using a 36/12/4/1.33 km two-way nesting. The base configuration of CAMx will use 20 vertical layers up to a region top of 100 mb (approximately 15 km AGL). CAMx will include one extra layer at the very top of the modeling domain.

The PPM advection solver would be used along with the spatially varying (Smagorinsky) horizontal diffusion approach. K-theory will be used for vertical diffusion. Two sets of CAMx vertical diffusivity inputs will be generated using MM5CAMx: (1) one using the O’Brien scheme; and (2) the other using the Kv scheme in CMAQ. We will initially run MM5CAMx specifying a minimum eddy diffusion constant (Kz_min) of 0.1 m^2/s. As part of the CAMx modeling system there is a utility that produces enhanced minimum Kz (Kz_min) values near the surface to account for increased mixing due to roughness and the urban heat island. The selection of the Kz_min approach will be based on the latest thinking and sensitivity tests.

The CAMx 4.30 Mechanism 4 (M4) Course/Fine approach will be used for the Gorge Study modeling that assumes all secondary PM is fine.

The CB-IV gas-phase chemical mechanism is selected for the Gorge Study modeling. The RADM aqueous-phase chemistry and SOAP SOA module will also be used.

Table 5-3. Proposed Gorge Study model configuration for the CAMx.

Model Option	CMAQ
Model Version	Version 4.30 (2006)
Horizontal Resolution	36/12 km
No. Vertical Layers	NZ = 20
Horizontal Advection	PPM
Vertical Advection	PPM
Horizontal Diffusion	Spatially Varying
Vertical Diffusion	K_V (OB70 and CMAQ)
MM5 Configuration	Pleim-Xiu/ACM
MM5 Processing	MM5CAMx
Gas-Phase Chemistry	CB4
Gas-Phase Chemistry Solver	CMC
Secondary Organic Aerosol	SOAP
Aqueous-Phase Chemistry	RADM
Aerosol Chemistry	ISORROPIA
Dry Deposition	Wesley
Plume-in-Grid	Off
Initial Concentrations	CMAQ Default
Boundary Conditions	Monthly Average Diurnally Varying GEOS-CHEM
Emissions	WRAP 2002 augmented by SWCAA/ODEQ data for WA and OR

5.4.2 Spin-Up Initialization

For the 2004 episodic CAMx modeling, the model will be exercised for the two Gorge 2004 episodes using a 10 day initialization period on the 36 km grid with the last two days on the 36/12km grids the same as CMAQ.

5.4.3 Boundary Conditions

CAMx boundary conditions would be monthly average diurnally varying based on the 2002 GEOS-CHEM global climate model simulation. The CMAQ-to-CAMx BC processor would be used to processor the CMAQ BCON files for input into CAMx.

5.4.4 Photolysis Rates

The TUV photolysis rates processor would be used to generate the photolysis rates input file for CAMx. TOMS ozone data would be used to develop the CAMx Albedo/Haze/Ozone input file for the two 2004 Gorge episodes.

6.0 QUALITY ASSURANCE PROJECT PLAN

In this section we discuss the quality assurance procedures that will be used in the Gorge Study modeling. These procedures constitute our Quality Assurance Project Plan (QAPP) for the study,

6.1 Quality Assurance Objectives

In December 2002, the USEPA publish extensive guidance on developing a Quality Assurance Project Plan (QAPP) for modeling studies (EPA, 2002). The objective of a QAPP is to ensure that a modeling study is scientifically sound, robust, and defensible. The new EPA guidance suggests that a QAPP should include the following elements:

- a systematic planning process including identification of assessments and related performance criteria;
- peer reviewed theory and equations;
- a carefully designed life-cycle development process that minimizes errors;
- clear documentation of assumptions, theory, and parameterization that is detailed enough so others can fully understand the model output;
- input data and parameters that are accurate and appropriate for the problem;
- output data that can be used to help inform decision making; and
- documentation of any changes from the original quality assurance plan.

Moreover, the EPA guidance specifies that different levels of QAPP may be required depending on the intended application of the model, with a modeling study designed for regulatory purposes requiring the highest level of quality assurance.

The QAPP also provides a valuable resource for project management. It can be used to document data sources and assumptions used in the modeling study, and it can be used to guide project personnel through the data processing and model application process to ensure that choices are consistent with the project objectives.

The guidance document also addresses model development, coding and selection of models, and model performance requirements. For the Gorge Study modeling we are using existing EPA sponsored models (SMOKE and CMAQ), a model developed by ENVIRON (CAMx) and the MM5 model developed by NCAR/PSU and have no current plans for model development activities. Thus, our QAPP focuses primarily on documenting data sources and QA of data processing performed by the model team. In addition, because no official EPA guidance currently exists for visibility model performance, a major objective of our QAPP will be to propose and define model performance evaluation procedures. QA objectives for specific aspects of the project are discussed below, and these will be incorporated into a QAPP that conforms to the EPA guidance document for modeling studies.

6.2 Emissions Model Inputs and Outputs

Emissions Quality Assurance (QA) and Quality Control (QC) are the single most critical step in performing air quality modeling studies. Because emissions processing is tedious, time consuming and involves complex manipulation of many different types of large data sets, errors are frequently made in emissions processing and, if rigorous QA measures are not in place, these errors may remain undetected.

As part of the Gorge Study modeling effort, an "Emissions Gatekeeper" function will be implemented. The Study Team envisions the role of this Gatekeeper as one to perform quality assurance activities on the following emission inventory (EI) data:

(1) EI data obtained from the WRAP 2002 emissions inventory for the continental U.S. Canada and Mexico; and
(2) The emission inventory obtained from SWCAA and ODEQ developed as part of the Gorge Study for counties in Washington and Oregon.

Specifically, the Emissions Gatekeeper will review the content and format of the provided emission inventories ensuring an appropriate appraisal of the emissions data and estimates with particular focus on the states of Washington and Oregon. Other tasks will include any additional translation from mass emissions files into the emissions modeling input file structure necessary for modeling. The Study Team will supplement these activities with QA checks on the intermediate and model output files using internal and public domain visualization and diagnostic packages.

We propose a multi-step emissions QA/QC approach that involves several staff to QA/QC the emissions as they are processed. This includes the initial emissions QA/QC by the Emissions Gatekeeper described above, as well as QA/QC by the Emissions Modeler during the processing of emissions and then additional QA/QC by the air quality modeler of the processed model ready emission files. This multistep process with three separate groups involved in the QA/QC of the emissions is much more likely to catch any errors prior to the air quality model simulations.

6.2.1 Emissions Modeling QA/QC

Input Screening Error Checking Algorithms: Although the SMOKE emissions model will be used for emissions processing, some of additional input error checking algorithms will be used to screen the data and identify potential emission input errors. Additionally, EPA has issued a revised stack QA and augmentation procedures memorandum that will be used to identify and augment any outlying stacks.

SMOKE error messages: SMOKE provides various cautionary or warning messages during the emissions processing. We will redirect the SMOKE output to log files and review the log files for serious error messages. An archive of the log files will be maintained so that the error messages can be reviewed at a later date if necessary.

SMOKE emissions summaries: We will use QA functions built into the SMOKE processing system to provide summaries of processed emissions as daily totals according to species, source category and county and state boundaries. These summaries will then be compared with summary data prepared for the pre-processed emissions, e.g., state and county totals for emissions from the augmented emissions data.

6.2.2 QA of the Model-Ready Emissions Impacts

The goal of the post-processed emissions summary QA is to detect possible errors in the final, model-ready binary emissions files by preparing summary plots that characterize spatial and temporal patterns in the emissions data. This step is designed to catch errors that may be missed in the internal SMOKE QA procedures. We will use a QA/QC post-processing program that read the CMAQ-ready I/O API emissions file formats for each of the major source categories (mobile, area, point, biogenic, fire) and produce the following plots.

Spatial Summary: We will sum the emissions for all layers and for all 24 hours that is used to prepare a PAVE plot showing the daily total emissions spatial distribution. For a 20 day simulation this produces approximately 20 days x 20 species x 5 emissions categories = 2,000 plots. In our base case simulations these plots will be presented as tons per day. The objective of this step is to identify errors in spatial distribution of emissions.

Vertical Profile: For point sources the emissions total for each layer will be summed and plotted to show the vertical distribution of emissions. These plots show the emissions on the x-axis for each model layer on the y-axis. The objective of this step is to identify possible errors in vertical distribution of emissions.

Short Term Temporal Summary: The total domain emissions for each hour will be accumulated and time series plots prepared that display the diurnal variation in total hourly emissions. The objective of this step is to identify errors in temporal profiles.

Long Term Temporal Summary: The total domain emissions for each day will be accumulated and displayed as time series plots that show the daily total emissions across the domain as a function of time. The objective of this step is to identify particular days for which emissions appear to be inconsistent with other days for no reason (e.g., not a weekend) and compare against the general trend.

Control Strategy Spatial Displays: Spatial summary plots of the daily total emissions differences between a control strategy and base case emissions scenarios will be generated. These plots can be used to immediately identify a problem in a control strategy.

6.3 Meteorological Model Outputs

As part of the Gorge Study modeling QA effort, a “Meteorological Gatekeeper” function will be implemented. The task of the Gatekeeper is to provide an independent review and quality assurance of the meteorological modeling and related data sets developed by the Study Team. This Gatekeeper QA review serves two specific purposes: (a) to ensure that any potential problems with the data sets (should they exist) are identified and corrected in a timely manner, and (b) to provide the study team with information to support ongoing CMAQ and CAMx model performance testing and sensitivity analyses. In the case of meteorology, the Gatekeeper's independent QA analysis of the MM5 meteorological data sets serves to provide direct assistance to the emissions and air quality modeling team as it undertakes to ratify the SMOKE model outputs and to diagnose the CMAQ and CAMx model performance and sensitivity analyses.

In addition to having personal responsibility for the quality and chain of custody of the meteorological data sets developed by the Study Team, the Meteorological Gatekeeper will be responsible for ensuring and maintaining the integrity of the data files. In performing the Meteorological Gatekeeper quality assurance activity, one of the first steps is to conduct an independent operational evaluation on the MM5 model results at 36 km, 12 km, 4 km and 1.33 km grid scale. This evaluation covers surface and aloft wind direction, temperature, mixing ratio, precipitation, and planetary boundary layer (PBL) depths on a continental scale (36 km) and subregional scale (12 km) basis. The MM5 evaluation procedures will be similar as those employed by WRAP, only focused on the Gorge Study area (see: http://pah.cert.ucr.edu/aqm/308/mm5.shtml). The Gatekeeper will also perform supplemental, ad hoc analysis of pertinent MM5 fields (e.g., PBL depths) where that might be useful to the emissions and air quality modeling teams. Another task of the Gatekeeper will be to exercise the Meteorological Chemistry Interface Processor (MCIP) version 3.0 and MM5CAMx processor to produce binary input files for the CMAQ and CAMx air quality models, respectively.

In summary, the quality assurance plan for the meteorological data will include the following elements:

- Upon generating the MM5 output files, we will verify the integrity of the file transfer (e.g., no missing and/or corrupted files);

- We will process the 2004 MM5 data using the MCIP3.0 and MM5CAMx processors to generate 2004 model-ready meteorological inputs for CMAQ and CAMx, respectively.

- We will create horizontal and vertical plots of temperature, pressure, precipitation, modeled flow patterns, PBL heights, etc. to assess whether the MCIP output fields are reasonable; and

- The Gorge Study 2004 MM5 episodic simulation will be evaluated using the same surface observations, subdomains and procedures as used to evaluate the WRAP 2002 MM5 simulation as an independent QA and evaluation of the database.

6.4 Air Quality Model Inputs and Outputs

Key aspects of QA for the CMAQ and CAMx input and output data include the following:

- Verification that correct configuration and science options are used in compiling and running each model of the in the CMAQ modeling system, where these include the MCIP, JPROC, ICON, BCON and the CCTM.
- Verification that correct configuration and science options are used in compiling and running each model of the in the CAMx modeling system, where these include the MM5CAMx, TUV, CMAQ-to-CAMx IC, BC and emissions processors and other processors.
- Verification that correct input data sets are used when running each model.
- Evaluation of CMAQ and CAMx results to verify that model output is reasonable and consistent with general expectations.
- Processing of ambient monitoring data for use in the model performance evaluation.
- Evaluation of the CMAQ and CAMx results against concurrent observations.
- Backup and archiving of critical model input data.

The most critical element in the QA plan for CMAQ and CAMx simulations is the QA/QC of the meteorological and emissions input files. The major QA issue specifically associated with the air quality model simulations is verification that the correct science options were specified in the model itself and that the correct input files were used when running the model. For the CMAQ and CAMx modeling we employ a system of naming conventions using environment variables in the compile and run scripts that guarantee that correct inputs and science options are used. We also employ a redundant naming system so that the name of key science options or inputs are included in the name of CMAQ and CAMx executable program, in the name of the CMAQ and CAMx output files, and in the name of the directory in which the files are located. This is accomplished by using the environment variables in the scripts to specify the names and locations of key input files. For example, if a model simulation is performed using the CB4 mechanism, all compile and run scripts contain the variable definition “$MECH = CB4”, and this variable is hard coded into the script for the executable name, the output file name, and the output directory name. This procedure produces long file/directory names but it effectively prevents mistakes or makes mistakes readily apparent if they do occur.

A second key QA procedure is to never “recycle” run scripts, i.e., we always preserve the original runs scripts and directory structure that were used in performing a model simulation. For example, if we perform simulation with the SAPRC mechanism, instead of editing the original scripts to specify “$MECH = SAPRC” we will create a parallel directory structure with a new set of scripts to perform the SAPRC simulations. This provides a permanent archive of the scripts that were used in performing model simulations. In addition, output from the model simulation will be directed to a log file that provides a record of input file names, warning messages etc that will be archived.

We will also perform a post-processing QA of the CMAQ and CAMx output files similar to that described for the emissions processing. We will generate animated gif files using PAVE that can be viewed to search for unexpected patterns in the CMAQ and CAMx output files. In the case of model sensitivity studies, the animated gifs will be prepared as difference plots for the sensitivity case minus the base case. Often, errors in the emissions inputs can be discovered by viewing the animated GIFs. Finally, we will produce 24 hour average plots for each day of the CMAQ simulations. This provides a summary that can be useful for more quickly comparing various model simulations.

7.0 MODEL PERFORMANCE EVALUATION

7.1 Overview

This chapter describes a range of model testing methodologies *potentially* available to the Gorge Study air quality modeling Study Team in its efforts to adequately evaluate the performance of the CMAQ and CAMx air quality modeling systems for the two 2004 modeling episodes. Since one cannot know at this juncture the specific performance problems that may arise in the initial 2004 CMAQ and CMAQ base case simulations, we set forth in this chapter a broad range of methods and techniques that *may* be brought to bear in examining CMAQ and CAMx model performance. We identify the core operational evaluation procedures, recommended in EPA (2001) guidance that will be performed in the model performance evaluation. We also describe a broad range of additional performance testing methods that may be worth considering, if necessary. Implementation of one or several of these various techniques would have to be performed under separate funding. However, our base effort model performance evaluation is intended to provide a robust assessment of the operational ability of the CMAQ and CAMx models to predict fine particulate and visibility at sites in and around the Columbia River Gorge National Scenic Area.

At a minimum, the evaluation of the CMAQ and CAMx modeling systems for the Gorge Study episodic 2004 simulations will be consistent with EPA's draft guidance on PM model testing enhanced to take advantage of the special study data collected as part of the Gorge Study monitoring program. This guidance essentially calls for an operational evaluation of the model focusing on a specific set of gas phase and aerosol chemical species and a suite of statistical metrics for quantifying model response over the annual cycle. The emphasis is on assessing: (a) How accurately the model predicts observed concentrations? and, (b) How accurately does the model predict responses of predicted air quality to changes in inputs? States are encouraged to utilize the evaluation procedures set forth in the earlier 1991 guidance document (EPA, 1991) for gas phase species and the newer (2001) guidance of PM species. Thus, in carrying out the initial operational evaluation and the subsequent final evaluation, we will implement the suggested EPA performance testing methodologies for the key gas phase and aerosol species. Since these methods are explicitly presented in EPA's guidance document, there is no need to repeat them here.

Subject to the availability of time and currently unallocated resources, the Gorge Study evaluation will also attempt to employ other testing methods beyond those in the EPA guidance document. However, the level of this effort without additional resources will depend on how smoothly the integration of other data (e.g., emissions and meteorological) are introduced into the Gorge Study modeling. For example, if emissions are not in an adequate form usable for SMOKE emissions modeling, then current budget resources may have to be reallocated from model performance to fixing the emissions. This discussion is not intended to circumvent a full evaluation of the modeling systems, rather to recognize the very real resource limitations and if resources are diverted to other activities without additional funding, then work is dropped on the back end that usually includes limitations on the model performance evaluation.

7.2 Context for the Gorge Study Model Evaluation

We begin the discussion of the Gorge Study modeling evaluation methodology by reviewing how the CMAQ and CAMx model output is used to estimate visibility impairment. When designing a model performance evaluation, it is important to understand how the modeling results will ultimately be used. EPA has published two versions of draft guidance for fine particulate and regional haze modeling (EPA, 2000; 2001), utilizing a Fine Particulate Guidance Workgroup to provide technical input in the development of both documents[1]. More recently, EPA has 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 might contain.

The CMAQ and CAMx models do not directly estimate visibility, instead they estimate PM and gaseous species concentrations from which visibility can be estimated. The most frequent equation to convert PM species concentrations to light extinction is the IMPROVE reconstructed mass equation:

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

where:

b_{ext} is the estimated extinction coefficient (Mm^{-1});
$[SO_4]$ is the sulfate concentration assumed to be ammonium sulfate;
$[NO_3]$ is the particulate nitrate concentration assumed to be ammonium nitrate;
[OC] is the organic carbon concentration;
[EC] is the elemental carbon concentration;
[IP] is the inorganic primary fine particulate (< 2.5 μ) concentration excluding primary sulfates and nitrates;
[CM] is the coarse particulate (> 2.5 μ and <10 μ) concentration;
$b_{rayleigh}$ is the light-scattering due to 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 that is assumed to be 1.0.

The IMPROVE Steering Committee have proposed a new IMPROVE equation that includes new f(RH) curves, accounts for NO2 and Sea Salt and contains other updates.

The Gorge Study 2004 CMAQ and CAMx model testing will concentrate on an operational evaluation of those model predictions that are most necessary for estimating visibility (e.g., SO_4, NO_3, OC, EC, IP and CM and direct measurements of light scattering and absorption). 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 regional haze

---

[1] Members of the Gorge Study modeling team participated on the EPA fine particulate modeling work group over the two-year span of its activities.

predictions. This evaluation will be focused on the Gorge and surrounding areas, and will also carried out across subdomains (e.g., WRAP, MRPO, VISTAS and MANE-VU).

Another key component of the evaluation will be comparisons against the Gorge Study nephelomter measurements of light scattering. In this case the IMPROVE and new IMPROVE equations can be used with appropriate (RH) values, only without including EC and NO2 in the extinction equation.

7.3 Multi-Layered Model Testing Process

EPA's "Draft Guidance for Demonstrating Attainment of Air Quality Goals for $PM_{2.5}$ and Regional Haze" (EPA, 2001) affirms the recommendations of numerous modeling scientists over the past decade (see, for example, Dennis et al., 1990; Tesche et al., 1990, 1994; Seigneur et al., 1998, 2000; Russell and Dennis, 2000; Arnold et al., 2003; Boylan et al., 2003; Tonnesen, 2003) that a comprehensive, multi-layered approach to model performance testing should be performed, consisting of the four components: operational, diagnostic, mechanistic (or scientific) and probabilistic. As applied to regional PM/visibility models, this multi-layered framework may be viewed conceptually as follows:

> **Operational Evaluation**: Tests the ability of the model to estimate PM concentrations (both fine and coarse) and the components at PM_{10} and $PM_{2.5}$ including the quantities used to characterize visibility (i.e., sulfate, nitrate, ammonium, organic carbon, elemental carbon, $PM_{2.5}$, and PM_{10}). This evaluation examines whether the measurements are properly represented by the model predictions but does not necessarily ensure that the model is getting "the right answer for the right reason";

> **Diagnostic Evaluation:** Tests the ability of the model to predict visibility and extinction, PM chemical composition including PM precursors (e.g., SOx, NOx, and NH_3) and associated oxidants (e.g., ozone and nitric acid); PM size distribution; temporal variation; spatial variation; mass fluxes; and components of light extinction (i.e., scattering and absorption);

> **Mechanistic Evaluation:** Tests the ability of the model to predict the response of PM and visibility to changes in variables such as emissions and meteorology; and

> **Probabilistic Evaluation:** Takes into account the uncertainties associated with the model predictions and observations of PM and visibility.

Within the constraints of the Gorge Study modeling schedule and budget resources, effort will attempt to include elements of each of these components. The operational evaluation will obviously receive the greatest attention since this is the primarily thrust of EPA's 2001 PM guidance. However, we will consider, where feasible and appropriate, diagnostic and mechanistic tests (e.g., use of probing tools, indicator species and ratios, aloft model evaluations, urban vs. rural performance analyses), and traditional sensitivity simulations to explore uncertainty. The scope of these additional diagnostic and mechanistic tests will be shaped by available time and resources.

7.4 Development of Consistent Evaluation Data Sets

7.4.1 Surface Measurements

The ground-level model evaluation database will be developed using several routine and research-grade databases. The first is the routine gas-phase concentration measurements for ozone, NO, NO_2 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., with particular emphasis in the central U.S. These include the: (a) Interagency Monitoring of Protected Visual Environments (IMPROVE), (b) Clean Air Status and Trends Network (CASTNET), (c) Southeastern Aerosol Research and Characterization (SEARCH), (d) EPA $PM_{2.5}$ and PM_{10} Mass Networks (EPA-FRM), (e) EPA Speciation Trends Network (STN); (f) National Acid Deposition Network (NADP) and (g) EPA Supersites (EPA-SPEC) networks. Typically, these networks provide ozone, other gas phase precursors and product species, PM, and visibility measurements.

As an example, the IMPROVE network gives daily (24-hour) average mass concentrations every 3 days for SO_4, NO_3, organic carbon (OC), elemental carbon (EC), soil (IP), CM, $PM_{2.5}$ and PM_{10}. These data are available at 2 sites in the Gorge as well as several sites at nearby Class I areas in Oregon and Washington. In addition, hourly values of light extinction and deciview are available at several of these sites. The data collected as part of the Gorge-Study intensive monitoring program will be a key component of the model performance evaluation data. These data were discussed in Chapter 3 so are not repeated here. We will use data from these and the other observational databases listed in Table 7-1, supplemented with the routine AIRS/AQS data, as appropriate, for CMAQ and CAMx model performance testing.

Another important consideration is that different PM monitoring networks may use different measurement approaches that "measure" different amounts of the same species that are also different from the modeled species. For example, the IMPROVE network only speciates $PM_{2.5}$ so any sulfate or nitrate in the coarse mode ($PM_{2.5-10}$) is included in the CM species. The CMAQ and CAMx models will be evaluated separately for each network. Finally, the mapping of the modeled species to the monitored data will also have to be performed in a consistent fashion.

Table 7-1. Ground-level ambient data monitoring networks and stations available in the United States.

Monitoring Network	Chemical Species Measured	Sampling Frequency; Duration	Approximate Number of Monitors
IMPROVE	Speciated $PM_{2.5}$ and PM_{10}	1 in 3 days; 24 hr	11
CASTNET	Speciated $PM_{2.5}$, Ozone	Hourly, Weekly; 1 hr, Week	3
SEARCH	24.hr PM25 (FRM Mass, OC, BC, SO4, NO3, NH4, Elem.); 24-hr PM coarse (SO4, NO3, NH4, elements); Hourly PM2.5 (Mass, SO4, NO3, NH4, EC, TC); and Hourly gases (O3, NO, NO2, NOy, HNO3, SO2, CO)	Daily, Hourly;	0
NADP	WSO4, WNO3, WNH4	Weekly	23
EPA-FRM	Only total fine mass ($PM_{2.5}$)	1 in 3 days; 24 hr	**(?)**
EPA-STN	Speciated $PM_{2.5}$	Varies; Varies	12
AIRS/AQS	CO, NO, NO_2, NO_x, O_3	Hourly; Hourly	25

Monitoring Network	Chemical Species Measured	Sampling Frequency; Duration	Approximate Number of Monitors
EPA-SPEC	Various as part of St. Louis Super Site	Various	1+
GORGE	PM, gaseous, bsp	Various	~20

7.5 Model Evaluation Tools

This section introduces the various statistical measures, graphical tools, and related analytical procedures that have proven useful over the years in evaluating grid-based chemical transport models. Many of the methodologies mentioned below are being utilized to one degree or another in WRAP, CENRAP and VISTAS. Where appropriate, they will also be used in the Gorge 2004 evaluation of the CMAQ and CAMx modeling systems. However, while we plan on calculating a rich variety of statistical performance metrics, only a very limited subset of these measures will actually be relied upon to form judgments concerning model acceptability and in the final reporting because some of them are redundant.

7.5.1 Statistical Performance Metrics

EPA's 2001 PM and regional haze guidance suggests a suite of metrics for use in evaluating model performance. The standard set of statistical performance measures suggested by EPA for evaluating fine particulate models includes: (a) normalized bias; (b) normalized gross (unsigned) error; (c) fractional bias; (d) fractional gross error; and (e) fractional bias in standard deviations. These measures are subsumed within the list of metrics that are calculated on a routine basis using standard model evaluation tools (these are identified in Table 7-2). These statistical measures will be generated for each model simulation performed for each analysis region. From past regional PM model evaluations we have found the fractional bias and fractional error to be the most useful summary measures and we will focus mainly upon them in the Gorge Study modeling, but not to the exclusion of others that are found to yield discriminating power. For ozone and other gas phase species (NO, NO_2, SO_2) we will include use the traditional statistical measures (EPA, 1991, 1999).

Typically, the statistical metrics are calculated at each monitoring site across the full computational domain for all simulation days. In the Gorge Study CMAQ/CAMx evaluation, we will stratify the performance statistics across relevant space and time scales. As part of the operational evaluation, the gas-phase and aerosol statistical measures shown in Table 7-2 will be computed for subdomains as appropriate. Temporally, we will compute the statistical measures for the appropriate averaging times: 1 hr for ozone, and gas-phase precursors such as NO, NO_2, CO, SO_2; 8-hr for ozone, 24 hr for sulfate, nitrate, PM and other aerosol species, and continuous PM species for the special study measurements taken as part of the Gorge Study. These results will then be averaged over days and time of day for display, further analysis, and reporting. Should it become necessary as part of model performance diagnosis, we will consider aggregating the statistics in other ways, e.g., (a) day vs. night, (b) weekday vs. weekend, (c) precipitation vs. non-precipitation days, and (d) Haze Gradient Study cluster classification in order to help elucidate model performance problems. Absent performance difficulties, these supplemental time/space analyses would only be considered if additional resources are made available.

As part of the operational evaluation, the metrics defined in Table 7-2 will be calculated for each gas phase species and each fine particulate species in the extinction equation as well as separately for SO_4, NO_3, ammonium (NH_4), EC, OC, bsp, etc on subdomains in and around the Gorge. In any diagnostic evaluations that are performed, we will examine the model's ability to estimate the gaseous species listed above from EPA's guidance (EPA, 2001). However, in reality ambient gaseous species in 2004 are principally available for ozone, NO_2, SO_2, and CO.

Table 7-2. Core statistical measures to be used in the Gorge Study 2004 episode air quality model evaluation with ground-level data (see ENVIRON, 2003b,d for details).

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 %

Statistical Measure	Shorthand Notation	Mathematical Expression	Notes
Mean Absolute Gross Error (***MAGE***)	**Mean_Abs_G_Err**	$\frac{1}{N}\sum_{i=1}^{N}\left\|P_i - O_i\right\|$	
Mean Normalized Gross Error (***MNGE***)	**Mean_Norm_G_Err**	$\frac{1}{N}\sum_{i=1}^{N}\frac{\left\|P_i - O_i\right\|}{O_i}$	Reported as %
Mean Bias (***MB***)	**Mean_Bias**	$\frac{1}{N}\sum_{i=1}^{N}\left(P_i - O_i\right)$	Reported as concentration (e.g., μg/m^3)
Mean Normalized Bias (***MNB***)	**Mean_Norm_Bias**	$\frac{1}{N}\sum_{i=1}^{N}\frac{\left(P_i - O_i\right)}{O_i}$	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).

7.5.2 Graphical Representations

The Gorge Study CMAQ and CAMx operational air quality model evaluation will utilize numerous graphical displays to facilitate quantitative and qualitative comparisons between CMAQ/CAMx predictions and measurements. Together with the statistical metrics listed in Table 7-2, the graphical procedures are intended to help: (a) identify obviously flawed model simulations, (b) guide the implementation of performance improvements in the 2004 model input files in a logical, defensible manner, and (c) to help elucidate the similarities and differences between the alternative CMAQ/CAMx simulations. These graphical tools are intended to depict the model's ability to predict the observed fine particulate and gaseous species concentrations.

The core graphical displays to be considered for use in the Gorge Study modeling include the following:

- Scatter plots of predicted and observed concentrations;
- Time series plots at monitoring locations;
- Spatial maps of ground-level gas-phase and particulate concentration maps (i.e., tile plots);
- Bias and error stratified by concentration (Bugle Plots);
- Bias and error stratified by time (e.g., Soccer Plots); and
- Separate displays of above by monitoring network, subregions and time.

These graphical displays will be generated, were appropriate for the full 2004 episodes as well as for individual days.

7.5.3 Probing Tools and Allied Methods

The CMAQ/CAMx operational model evaluation will employ routine operational evaluation methods and standard statistical metrics (Table 7-2) and graphical displays to support the assessment of whether the models are shown to perform with sufficient accuracy and reliably for its intended purpose. Ideally, this operational evaluation will confirm that the modeling systems are performing consistent with its scientific formulation, technical implementation, and at a level that is at least as reliable as other current state-of-science methods. Should unforeseen model performance problems arise in the 2004 episodic Base Case model simulations, it may be necessary to draw into the evaluation supplemental diagnostic tools to aid in model testing. These diagnostic techniques are loosely referred to as “probing tools”. The actual need for their use, if any, can only be determined once the initial 2002 CMAQ/CAMx operational evaluation is completed. Should such diagnostic methods actually be needed, their usage will require additional resources. Below, we identify the types of probing tools that could be brought to bear to enhance the currently planned Gorge Study operational evaluation of the CMAQ and CAMx models.

Current ‘One-Atmosphere” models, such as CMAQ and CAMx, have been outfitted with a number of “probing tools” that have proven to be very useful in testing and improving model performance and in evaluating emissions control strategies. Among the probing tools available in one or both models are: (a) ozone source apportionment technology (OSAT) and PM source apportionment technology (PSAT) algorithms, (b) process analysis (PA), and (c) the decoupled direct method (DDM) sensitivity analysis. The Gorge Study may choose to evaluate these tools as part of modeling exercise.

Source Apportionment Technology: CAMx contains a suite of “source attribution” methods. One such method is Ozone Source Apportionment Technology (OSAT). OSAT tracks ozone formation based on how groups of ozone precursors contributed to ozone formation. Thus, OSAT decides whether ozone formation is NOx or VOC limited in each grid cell at each time step, and bases ozone attributions on the relative amounts of the limiting precursor from different sources that are present in that grid cell at that time step. These incremental ozone attributions are integrated throughout the model run. The method is generally applicable and has been widely used to aid model diagnosis in the performance testing phase and to guide control strategy formulations as well. A new PM Source Apportionment Technology (PSAT) has been implemented in CAMx funded by the MRPO that has been fully tested and evaluated. A Tagged Species Source Apportionment (TSSA) approach has also been implemented in CMAQ and is undergoing further testing.

Decoupled Direct Method (DDM): Various forms of the Decoupled Direct Method (DDM) have been installed in CMAQ and CAMx, based on the original work of Dunker and co-workers (Dunker, 1981; 1984; Dunker et al., 2002) and researchers at Georgia Institute of Technology (GIT). In general, the DDM method: (a) calculates first order sensitivities dC/dP where C is a concentration output and P an input parameter[2], (b) promotes accuracy by using consistent numerical methods and the same time steps for concentrations and sensitivities, (c) optimizes the code for efficiency, but not at expense of accuracy, and (d) calculates sensitivities with respect to parameters representing pollutant sources – emissions, BCs and ICs. Finally, the DDM provides a flexible and powerful user interface for defining various sensitivities including:

- Emissions resolved by geographic area.
- Emissions resolved by source category.
- BCs optionally resolved by boundary edge (N, S, E, W, Top).
- All sensitivities available relative to sources of individual species (NO, PAR, etc.) or species group (VOC, NOx or ALL).
- Simultaneously calculate sensitivities to many initial condition, boundary condition and emissions parameters.

In recent comparisons between CAMx DDM sensitivities and brute-force sensitivities (calculated from +/- 20% perturbations) Dunker et al., (2002a,b) reported that sensitivities of ozone with respect to area source NOx and VOC emissions were calculated and results indicated that the agreement between DDM and brute force sensitivities is excellent. DDM implementation into CMAQ is reported by Kumar (2003).

Process Analysis (PA): Photochemical air quality model simulations are usually evaluated primarily in terms of their ability to simulate observed O_3 data. There is an increasing awareness that chemical mechanisms, and air quality models must also be evaluated in terms of their ability to simulate the fundamental chemical processes that control O_3 formation and the sensitivity of O_3 to emissions reductions (Arnold et al., 1998). Process analysis is a method for explaining model simulations by adding algorithms to the AQM to store the integrated rates of species changes due to individual chemical reactions and other sink and source processes (Jeffries and Tonnesen, 1994; Tonnesen, 1995). By integrating these rates over time and outputting them at hourly intervals, process analysis provides diagnostic outputs that can be used to explain a model simulation in terms of the budgets of free radicals, production and loss of odd oxygen and O_3, and conversion of NOx to inert forms, as well as the effects of transport and other sink and source terms. Of particular importance to the Gorge Study modeling, process analysis can also improve model diagnosis and

---

[2] Recent research by Prof. Russell and coworkers at GIT has led to the extension of the CMAQ DDM method to include second order sensitivity coefficients (see, Hakami et al., 2003).

performance evaluation efforts by identifying processes that are ‘out of balance’ (Tesche and Jeffries, 2002), by identifying situations for which the model formulation and/or implementation should not be expected to apply and by suggesting how ambient data can be used to evaluate model accuracy for key terms in the chemical processing of VOC and NOx (e.g., Imre et al., 1998).

Process Analysis (PA) is implemented in both CMAQ and CAMx and each model supports three complementary aspects of the method: (a) the integrated process rate (IPR), (b) integrated reaction rate (IRR) and (c) chemical process analysis (CPA). Several versions of process analysis (PA) have been implemented in air quality models (AQMs) including both trajectory models (Tonnesen, 1990, 1995) and grid models (Jang et al., 1995, Tonnesen and Dennis, 2000; Arnold et al., 1998; and Wang, 1997).

The fundamental approach in all versions of PA is similar: The AQM is modified to calculate the integral over time of the individual sink and source processes and each chemical reaction. These integrated sink/source process rates (IPR) and integrated reaction rates (IRR) can then be stored to a file and analyzed using a post-processor, or some processing can be performed internally in the model and a more limited set of process diagnostic information is output directly by the AQM. Chemical process analysis (CPA) is an improvement on the IRR method whereby some of the processing of IRR information is internalized within the AQM to output chemically meaningful parameters directly (e.g., budget terms for O_3, NOx and odd oxygen).

Process analysis measures for aerosol chemistry have not been analyzed as much as for ozone chemistry. Although the ozone chemistry process analysis is directly related to secondary sulfate and nitrate formation, there is additional process analysis information available in the aerosol modules that are not extracted in either CMAQ or CAMx. In particular, information on sulfate formation and oxidants from the aqueous-phase module and on the sulfate/nitrate equilibrium from the aerosol thermodynamics module would be a useful addition to the current process analysis output.

Because application of all three of these probing tools--source apportionment, DDM, and Process Analysis—are computational intensive and require a fair amount of analysis time to reap the benefits of using the methods, they are not part of the current Gorge Study core modeling effort. However, each method has potential for use in addressing key episodic periods or geographical locations in the Gorge Study domain where performance in the 2004 simulation may present a problem or where particular attention needs to be focused on emissions controls.

In such focused applications, one or more of these probing tools may indeed serve a purpose and will be considered where appropriate.

7.6 Gorge Study 2004 Episodic Model Evaluation Procedures

EPA guidance (EPA, 2001, pg. 227) suggests that the performance evaluation focus on two aspects:

- How well is the model able to replicate observed concentrations of components of $PM_{2.5}$, and total observed mass of $PM_{2.5}$? and
- How accurately does the model characterize the sensitivity of changes in component concentrations to changes in emissions?

Recognizing that the former is much easier to accomplish than the latter, EPA goes on to declare that testing of a model's reliability in estimating the actual effects of emissions changes is the more important. Over the past 20 years, a substantial body of information and analytical techniques has been developed to address the first aspect. Unfortunately, even today there are little rigorous methods available for quantifying the accuracy and precision of a model's predictions of ozone, PM or visibility changes as the result of emissions changes. In this section we explain how the Gorge Study model testing will address the first aspect of the performance evaluation, i.e., how does the model compare against observed data. In section 7.10 we consider the second performance consideration.

7.6.1 Assessment of Ground-Level Gas-Phase and Aerosol Species

Given that visibility in the model is expressed in terms of extinction and deciview built off of individual components of fine particulate matter, the model should be evaluated separately for each of the key fine particulate matter components that make up the extinction coefficient. Current EPA guidance suggests that the model should also be evaluated for ammonium as well as several key gas-phase species that are important for fine particulate modeling. For *particulate species* this includes SO_4 and/or S, NH_4, NO_3, mass associated with SO_4, mass associated with NO_3, elemental carbon (EC), organic carbon (OC), IP, mass of individual constituents of IP, and coarse matter (CM). The *gaseous species* include ozone (O_3), HNO_3, NO_2, PAN, NH_3, NOy, SO_2, CO, and H_2O_2.

Key measurements made as part of the Gorge Study monitoring include nephelometer (bsp) and athelometer measurements that measure light scattering and absorption would also be part of the core evaluation effort.

As part of the CMAQ/CAMx operational evaluation, model outputs will be compared statistically and graphically to observational data obtained from the IMPROVE, CASTNet, EPA-FRM, EPA-STN, special Gorge Study and other monitoring networks. These monitoring data will be obtained from AIRS, VIEWS, and other appropriate organizations. These comparisons will likely include:

- Hourly to daily averages for SO_2, SO_4, NO_3, EC, OC, $PM_{2.5}$, and PM_{10}, taking care to exclude periods of sampling interference in the observational data. We will look for systematic biases between the model results and observations, and if biases are found, identify possible sources of error in the model inputs.

- Hourly, high resolution PM species and gaseous species, concentrations and light scattering and absorption at sites where available (e.g., Gorge Study data).

- At sites with contrasting aerosol mass loadings, analysis of the temporal behavior of the major scattering and absorbing aerosol constituents along with the visibility trends, to establish correlations (e.g., Haze Gradient Sites).

The optional CMAQ/CAMx diagnostic model evaluations may entail several components, many of which can be identified presently. Of course, the actual diagnostic analyses to be performed and the scope of such analyses can only be determined once the initial operational model evaluation is underway. These potential diagnostics analyses will need to be carefully defined and rank-ordered in terms of their priority to ensure that they can be accommodated within available resources and schedule. Among the diagnostic model evaluation analyses that could be considered are:

- Evaluate seasonal trends in observations of organic and inorganic aerosol precursors and their effects on PM composition and visibility, and evaluate the ability of the model to capture these seasonal trends.
- Evaluate how well the model simulates various physicochemical processes by: (a) examining observed and modeled correlations between various species pairs, and (b) comparing model-predicted ratios of various species (individual or families) with observations to evaluate gas/particle partitioning (e.g., nitrate/total nitrate, SO_4/SO_x).
- Investigate the performance of the model at selected observational sites characterized by different chemical regimes that may be encountered either spatially or during different seasons to help identify any inadequacies in the model and to provide a better understanding of conditions under which model inferences may be weak.
- Create scatter plots of modeled vs. observed data and hourly and 24-hour averages by site and subregion to help identify any site-specific biases.
- Create time series plots of predicted and observed concentrations as appropriate.
- Evaluate for total sulfur ($SO_2 + SO_4$), nitrate ($HNO_3 + NO_3$) and ammonia ($NH_3 + NH_4$).
- Compare observed versus modeled mass fractions of PM constituents at various sites that are characterized by their proximity or remoteness relative to sources, or by specific meteorological conditions (e.g., frontal passage, stagnation, precipitation); these will enable identification of trends in the model of over- or under-prediction of specific PM constituents under these conditions.
- Calculate the measured and predicted relative abundance of key PM components and compare with EPA guideline recommendations and emergent alternative science recommendations (e.g., removing the soil component from the calculations, use of alternative extinction equations [i.e., Boylan, 2004]).
- Pay particular close attention to the model performance at the Gorge sites for SO_4, NO_3, EC, OC, IP and CM on the key episode days.

The suite of statistical metrics and graphical tools identified in the previous section for the core operational evaluation efforts would likely also be used to diagnose performance problems with the CMAQ/CAMx simulations should they exist and to highlight differences between model runs. Experience in ozone/PM modeling is the best basis upon which to identify obviously flawed simulation results. Efforts to improve the CMAQ/CAMx model's base case performance will be made, where necessary, warranted (i.e., to reduce the discrepancies between model estimates and observations), and consistent with the project resources and schedule; however, these model performance improvements efforts must be based on sound scientific principles. "Curve-fitting" exercises will be avoided.

7.7 Performance Goals and Benchmarks

Establishment of performance goals and benchmarks for modeling is a necessary but difficult activity. Here, performance goals refer to targets that we believe a good performing model should achieve, where as performance benchmarks are based on historical model performance measures for the best performing simulations. Performance goals are necessary in order to provide consistency in model applications and expectations across the country and to 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 (e.g., Houston, San Joaquin Valley, Los Angeles) 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 from breeding built-in compensating errors (Reynolds et al., 1996) as modelers strive to get good statistics as opposed to searching for the explanations for poor performance and then rectifying them. A NARSTO review of more than two-dozen urban-scale ozone SIP applications found this tendency to be all too prevalent in the regulatory modeling of the 1990s. (Roth et al, 1997).

Nearly 15 years ago, research sponsored by the California Air Resources Board (Tesche et al., 1990) led to the agency's adoption of three performance goals for 1-hour ozone modeling in the state:

> Unpaired (in time and space) peak prediction accuracy (≤ ± 20%);
> Mean normalized bias in hourly averaged concentrations (≤ ± 15%); and
> Mean normalized gross error in hourly concentrations (≤ 35%).

These performance goals for 1-hr ozone concentrations were adapted from previous surveys of several dozen urban-scale photochemical grid modeling studies (principally in California) focusing on ozone episodes of 1 to at most 3 days in duration. A surprising number of these studies did not include biogenic VOC emissions in the inventory under the then prevailing belief that biogenics were a negligibly small source category compared to automobile emissions. Most of the studies (Tesche, 1985, 1988; Tesche et al., 1985; 1990) comprising the data base from which the California ozone performance goals were derived entailed hourly ozone concentrations well above background levels (~40-50 ppb). As a result, it was common practice to use a "cutoff values" ranging between 40 ppb to 60 ppb to eliminate prediction-observations pairs that would cause these bias and error residual statistics to become extraordinarily large when measured concentrations were low. Accordingly, normalized statistics such as bias and error proved to be suitable in most applications since the observed concentrations were generally high. These three California ozone model performance goals were adopted by EPA (1991) as part of the nationwide photochemical modeling guidelines and have been heavily used since.

However, when these evaluation metrics and goals were later adapted to PM and PM species, difficulties arose because performance statistics that divide by low concentration observations become much less useful. Indeed, some PM species may approach zero (e.g., NO_3). In time, this has led to the introduction of the fractional and normalized mean bias and error metrics in addition to the mean normalized metrics and related performance expectations based on these alternative measures.

While the 1-hr metrics and goals still have value in interpreting ozone and some gas-phase species performance, it has been necessary to develop new performance metrics and goals for fine particulates. EPA's PM guidance document (EPA, 2001) guidance document identifies particulate matter components of interest to include: SO_4 and/or S, NH_4, NO_3, mass associated with SO_4, mass associated with NO_3, EC, OC, IP, and mass of individual constituents of inorganic primary particulate matter (i.e., IP). Gaseous pollutants of interest include ozone, HNO_3, NO_2, PAN, NH_3, NO_y, SO_2, CO, and H_2O_2. In addition, EPA guidance identifies several potentially useful statistical measures including: (a) accuracy of spatially averaged concentrations near a monitor, (b) fractional bias in means and standard deviations of predictions and observations, (c) normalized bias, (d) normalized gross error, (e) unpaired comparisons between predicted and observed peak concentrations. (Interested readers are referred to the EPA guidance document on the details of these metrics including mathematical formulae and implementation methods.)

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 for mean normalized gross error of $\leq$ 30% for southern California (SCAQMD, 1997; 2003) and $\leq$ 50% for Phoenix (ENVIRON, 1998) have been used. As correctly pointed out by Seigneur and co-workers (2003), the current ability of regional PM models to predicting regional PM and visibility is an area of research with improvements needed for characterizing meteorology and emissions as well as PM models themselves. To this list we would add the need for improvements in model evaluation methodologies as well.

When EPA's draft guidance was developed five years ago, an interim set of fine particulate modeling performance goals were suggested for aggregated mean normalized gross error and mean normalized bias as follows:

Pollutant	Gross Error	Normalized Bias
$PM_{2.5}$	~30-50%	~±10%
Sulfate	~30-50%	~±20-30%
Nitrate	~20-70%	~±15-50%
EC	~15-60%	NA
OC	~40-50%	~±38%

Because regional-scale fine particulate and regional haze modeling is an evolving science, and considerable practical application and performance testing has transpired in the intervening years since these goals were postulated, we consider them general guidelines. Results of the WRAP, VISTAS, and MRPO model evaluation together with recommendations from science workshops (e.g., EPA's PM Model Performance Evaluation Workshop in February 2004) and recently published scientific studies (e.g., Boylan, 2004) will be used to provide support to these recommendations.

7.8 Diagnostic and Sensitivity Testing

Rarely does a modeling team find that the first simulation satisfactorily meets all (or even most) model performance expectations. Indeed, our experience has been that initial simulations that 'look very good', usually do so as the result of compensating errors. The norm is to engage in a logical, documented process of model performance improvement wherein a variety of diagnostic probing tools and sensitivity testing methods are used to identify, analyze, and then attempt to remove the causes of inadequate model performance. This is invariably the most technically challenging and time consuming phase of a modeling study. We anticipate that the 2004 episode CMAQ/CAMx model base case simulations will present some performance challenges that may necessitate focused diagnostic and sensitivity testing in order for them to be resolved. Hopefully, these diagnostic and/or sensitivity tests can be adequately carried out within the resources and schedule of the current work effort. Below we identify the types of diagnostic and sensitivity testing methods that might be employed in diagnosing inadequate model performance and devising appropriate methods for improving the model response.

7.8.1 Traditional Sensitivity Testing

Model sensitivity experiments are useful in three distinct phases or 'levels' of an air quality modeling study and all will be used as appropriate in the Gorge Study modeling with CMAQ and CAMx. These levels are:

- **Level I**. Model algorithm evaluation and configuration testing;
- **Level II**. Model performance testing, uncertainty analysis and compensatory error diagnosis, and
- **Level III.** Investigation of model output response (e.g., ozone, aerosol, deposition) to changes in precursors as part of emissions control scenario analyses.

Most of the Level I sensitivity tests with CMAQ and CAMx have already been completed by the model developers and the RPOs. However, given the open community nature of the CMAQ and CAMx models, and the frequent science updates to the model and supporting databases, it is possible that some additional configuration sensitivity testing will be necessary.

Potential Level II sensitivity analyses might be helpful in accomplishing the following tasks:

- To reveal internal inconsistencies in the model;
- To provide a basis for compensatory error analysis;
- To reveal the parameters (or inputs) that dominate (or do not dominate) the model's operation;
- To reveal propagation of errors through the model; and
- To provide guidance for model refinement and data collection programs.

At this time, it is not possible to identify one or more Level II sensitivity runs that might be needed to establish a reliable 2004 CMAQ or CAMx base case. The merits of performing Level II sensitivity testing will depend upon whether performance problems are encountered in the operational evaluation. Also, the number of tests possible, should performance difficulties arise, will be limited by the additional resources and schedule. Thus, at this juncture, one cannot be overly prescriptive on the number and emphasis of sensitivity runs that may ultimately be desirable. However, from past experience with CMAQ, CAMx and other models, it is possible to identify examples of sensitivity runs could be useful in model performance improvement exercises with the 2004 CMAQ/CAMx simulation. These include:

- Modified biogenic emissions estimates;
- Modified on-road motor vehicle emissions;
- Modified air quality model vertical grid structure;
- Modified boundary conditions;
- Modified fire emissions;
- Modified EGU emissions;
- Modified ammonia emission estimates.
- Modified aerosol/N_2O_5/HNO_3 chemistry; and
- Modified NH_3 and HNO_3 deposition velocities.

If necessary, Process Analysis extraction outputs can be included in these Level II diagnostic sensitivity simulations in order to provide insight into why the model responds in a particular way to each input modification. Again, the number, complexity, and importance of these types of traditional sensitivity simulations can only be determined once the initial CMAQ/CAMx 2004 simulation(s) are executed.

Level III sensitivity analyses have two main purposes. First, they facilitate the emissions control scenario identification and evaluation processes. Today, four complimentary sensitivity “tools” can be used in regional photochemical models depending upon the platform being used. These methods include: (a) traditional or ‘brute force’ testing, (b) the direct decoupled method (DDM), (c) Ozone Source Apportionment Technology (OSAT) and PM Source Apportionment Technology (PSAT), and (d) Process Analysis (PA). Each method has its strong points and they will be employed where needed and as resources are available. The second purpose of Level III sensitivity analyses is to help quantify the estimated reliability of the air quality model in simulating the atmosphere’s response to significant emissions changes. This important model evaluation need is addressed in further detail in section 7.9 below.

Based on experience in other regional studies, examples of Level III monthly or annual sensitivity runs for Gorge modeling might include:

- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to SO_2 emissions;
- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to elevated point source NO_x emissions;
- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to ground level NO_x emissions; and
- Sulfate, nitrate, ammonium and other aerosol sensitivities to ammonia.

Of course, traditional ‘brute force’ sensitivity experiments are just one way of quantifying these or other Level III sensitivities. Other methods that can be applies include DDM, OSAT, or PSAT simulations.

The need to perform sensitivity experimentation (Levels I, II, or III) will depend on the outcome of the Gorge operational performance evaluations. If such a need arises, the ability to actually carry out selected sensitivity and/or diagnostic experiments will hinge on the availability of additional resources and sufficient time to carry out the analyses. Clearly, selection of the specific analysis method will depend upon the nature of the technical question(s) being addressed at the time.

7.8.2 Diagnostic Tests

A rich variety of diagnostic probing tools are available for investigating model performance issues and devising appropriate means for improving the model and/or its inputs. Previously, in section 7.4.4 we introduced the suite of 'probing tools' available for use in the CMAQ and CAMx modeling systems. Where the need exists (i.e., if performance problems are encountered) and assuming the Gorge Study elects to fund the use of the probing tool applications, these techniques could be employed as appropriate to assist in the model performance improvement efforts associated with the CMAQ/CAMx base case development. .

7.9 Corroborative and Weight of Evidence Modeling Analyses

This section identifies additional modeling analyses that might be worth pursuing under additional funding to add strength to the core model evaluation efforts already planned as part of the Gorge Study operational evaluation.

7.9.1 Corroborative Models

Noteworthy in EPA's new ozone, PM, and regional haze guidance documents is the encouragement of the use of alternative modeling methods to corroborate the performance findings and control strategy response of the primary air quality simulation model. This endorsement of the use of corroborative methodologies stem from the common understanding that no single photochemical modeling system can be expected to provide exact predictions of the observed ozone and PM species concentrations in a region with complex topography and sources as the Gorge. Although the photochemical/PM models identified in EPA's PM/regional haze guidance document possess many up-to-date science and computational features, there still can be important differences in modeled gas-phase and aerosol predictions when alternative models are exercised with identical inputs.

Mindful of EPA's endorsement of corroborative modeling methods and the rigorous use of 'weight of evidence' investigations, we recommend that the most recent version of CMAQ and CAMx be carried through the study, including the 2018 future-year modeling. Among other things, this will permit us to more explicitly identify the expected range of model uncertainty and to corroborate the general effectiveness of the CMAQ and CAMx visibility improvements. Other corroborative modeling methods such as the CMAQ-AIM and CMAQ-MADRID should also be considered. However, as these models are derivatives of CMAQ they would not provide as robust independent corroboration as CAMx.

7.9.2 Weight of Evidence Analyses

EPA's guidance recommends three general types of 'weight of evidence' analyses in support of the attainment demonstration: (a) use of air quality model output, (b) examination of air quality and emissions trends, and (c) the use of corroborative modeling such as observation-based (OBM) or observation-driven (OBD) models. The exact details of the 'weight of evidence' analyses must wait until the Gorge Study evolves further. It is premature to prescribe which, if any of the WOE analyses would be performed since the model's level of performance with the 2004 episodes is obviously not known at this time and the time and remaining project resources available to support WOE analyses is unknown as well. Nonetheless, we outline below our thoughts regarding what would likely be considered should the operational CMAQ/CAMx model evaluation need to be bolstered with WOE analyses.

Use of Emissions and Air Quality Trends. A limited scope emissions and trend analysis could be employed to support the 'weight of evidence' determinations. However, traditionally, these types of analyses are performed by the lead agency's own staff. With this expectation, we would coordinate our efforts with the Gorge Study Technical Team to develop a trends analysis supporting the future year applications of CMAQ/CAMx.

Use of Corroborative Observational Modeling. While regulatory modeling studies for ozone attainment demonstrations have traditionally relied upon photochemical models to evaluate ozone control strategies, there has recently been growing emphasis on the use of data-driven models to corroborate the findings of air quality models. As noted, EPA's guidance now encourages the use of such observation-based or observation-driven models (OBMs/ODMs). We will consider the merits of using these techniques as supportive weight of evidence. While the OBD/OBM models cannot predict future year air quality levels, they do provide useful corroborative information on the extent to which specific subregions may be VOC-limited or NOx-limited, for example, or where controls on ammonia or SO2 emissions might be most influential in reducing $PM_{2.5}$. Information of this type, together with results of DDM and traditional 'brute-force' sensitivity simulations, can be extremely helpful in postulating emissions control scenarios since it helps focus on which pollutant(s) to control. The Co Ha Go component of the Gorge Study should provide useful information to address this.

7.10 Assessing Model Reliability in Estimating the Effects of Emissions Changes

EPA identifies three methods (EPA, 2001, pg. 228) potentially useful in quantifying a model's reliability in predicting air quality response to changes in model inputs, e.g., emissions. These include:

- Examination of conditions for which substantial changes in (accurately estimated) emissions occur;
- Retrospective modeling, that is, modeling before and after historical significant changes in emissions to assess whether the observed air pollution changes are adequately simulated; and

- Use of predicted and observed ratios of 'chemical indicator species'.

We note that in some urban-scale analyses, the use of weekday/weekend information has been helpful in assessing the model's response to emissions changes. However, we suspect that this approach would not prove feasible to address visibility issues in the Gorge.

Recent analytical and numerical modeling studies have demonstrated how the use of ambient data and indicator species ratios can be used to corroborate the future year control strategy estimates of Eulerian air quality models. Blanchard et al., (1999), for example used data from environmental (i.e., smog) chambers and photochemical models to devise a method for evaluating the 1-hr ozone predictions of models due to changes in precursor NOx and VOC emissions. Reynolds et al., (2003) followed up this analysis, augmented with process analysis, to assess the reliability of SAQM photochemical model estimate of 8-hr ozone to precursor emissions cutbacks. With respect to secondary aerosol PM, the recent CMAQ evaluation by Arnold et al. (2003) clearly demonstrated how the use of indicator species analysis could be use to develop insight into the expected reliability and adequacy of a photochemical/PM model for simulating the effects of emissions control scenarios. These researchers used three indicator ratios (or diagnostic 'probes') to quantify the model's response to input changes:

- The ozone response surface probe [O_3/NO_x];
- The chemical aging probe [NO_z/NO_y]; and
- The ozone production efficiency probe [O_3/NO_z].

By closely examining the model's response to key input changes, properly focused in time and spatial location, Arnold et al., (2003) were able to conclude that the photochemical processing in CMAQ was substantially similar to that in the atmosphere

Thus, the extension of these techniques to address CMAQ and CAMx predictions for secondary aerosols will doubtless be quite challenging, but the use of indicator species (e.g., ammonia or HNO_3 limitation for nitrate particle formation) and species ratios appears to offer, at this time, the only real opportunity to quantify the expected reliability of the air quality model to correctly simulate the effects of emissions changes. In the CMAQ and CAMx model evaluation, we will remain alert to opportunities to extend the indicator species ratio analyses to the problem of fine particulate and visibility.

8.0 MODELING SCENARIOS

Currently, the Gorge Study modeling intends to run a current and future-year base case simulation to estimate how visibility is expected to change in the Gorge due to anticipated changes in emissions. There may also be a desire to perform a set of “what if” scenarios. Although not currently funded, a set of potential scenarios is also presented in this section.

8.1 Base Modeling Scenarios

As the core modeling effort for the Gorge Study we will simulate a 2004 Base Case and 2018 On-the-Books (OTB) Base Case using both the CMAQ and CAMx models and analyze the changes in PM species and visibility that the two models estimate. These changes will be calculated using the absolute modeling results as well as using the models in a relative sense to project changes in PM species and resultant visibility through the use of Relative Projection Factor (RRFs) as is done for the regional haze rule (RHR). Changes in other pollutants will be analyzed also.

8.2 Potential Alternative Analysis

There are several potential alternative types of analysis that can be conducted using the Gorge Study modeling system that would help elucidate the causes of visibility impairment and other air quality related concerns in the Gorge (e.g., fog acidity and acid deposition).

8.2.1 Emission Sensitivity Tests

There are numerous emission sensitivity tests that could be conducted. Below is one such set that could be investigated:

- Boardman Electrical Generating Unit (EGU)
    - Apply BART level of controls
    - Eliminate Emissions
- Three Mile Canyon Farm
    - Control emissions by some level
    - Eliminate emissions
    - Combination controls with Boardman EGU
- Eliminate emissions from Mt. St. Helens
- Eliminate emissions from counties within the Gorge
    - In combination
    - One at a time or in groups
- Eliminate barge traffic emissions
- Eliminate railroad emissions
- Eliminate on-road mobile sources
- Eliminate non-road mobile sources

8.2.2 Use of Probing Tools

As discussed in Chapter 7, CMAQ and CAMx have a set of “Probing Tools” that can extract more information on model sensitivity and source-receptor relationships from the model. Of particular note is the PM Source Apportionment Technology (PSAT) that performs PM source apportionment for source groups. A source group consists of a combination of a geographic source region and source category. For example, PSAT could be set up to obtain all of the emissions listed in Section 8.2.1 above in one run.

Potential Source Categories that could be analyzed separately by PSAT include:

- Boardman EGU
- Three Mile Canyon Farm
- On-Road Mobile Sources
- Barges
- Locomotives
- Other Non-Road Sources
- Mt. St. Helens
- Other (non-Boardman) EGUs
- Non-EGU Point Sources
- Biogenic Sources
- Open Ocean Vessels
- Other Anthropogenic Sources

Geographic source regions could look like:

- Portland
- Western Gorge Counties
- Central Gorge Counties
- Eastern Gorge Counties
- Columbia Plateau Counties
- Counties North of Gorge
- Counties South of Gorge
- Seattle
- Spokane
- Remainder Washington
- Remainder Oregon
- Idaho
- Canada
- Remainder US

Although not currently funded, the application of PSAT could provide valuable information to the Gorge Technical Team.

9.0 DOCUMENTATION

This section describes the documentation and schedule for the Gorge Study air quality modeling

9.1 Planned Documentation

Documentation associated with the emissions and air quality modeling performed during the Gorge Study modeling will include all relevant input data bases and scripts associated with the pre- and post-processing associated with model input development, model application, sensitivity and diagnostic analyses, and performance evaluations. PowerPoint presentations, technical memorandums, interim and final reports that describe the methodologies and results of the model performance evaluation, model intercomparison, and visibility assessment will be provided. Table 9-1 below lists the current schedule of deliverables under the Gorge Study modeling and analysis study.

Table 9-1. Current list of deliverables and schedule under the Gorge Study air quality modeling study.

Deliverable	Deliverable Due Date
Task 1. Study Design and Modeling Protocol	
Draft Modeling Protocol	February 2006
Final Modeling Protocol	Within 1 week of comments
Task 2. MM5 Meteorological Modeling	
MM5 Evaluation PPT Presentation	June 2006
MM5 Processed Data for CMAQ and CAMx	June 2006
Task 3. SMOKE Emissions Modeling	
Emissions Summary Presentation (PPT)	August 2006
Model-ready 2004 emission inputs	August 2006
Model-ready 2018 emission inputs	October 2006
Task 4. CMAQ and CAMx Air Quality Modeling	
Presentation on 2004 Base Case Modeling and Model Performance Evaluation	November 2006
Presentation on 2018 Modeling Results	December
Task 5. Reporting	
Monthly progress reports and invoices	3rd week of following month
Draft Final Report	December 2006
Final Report	Two weeks after comments

In addition to a draft final and final report, a hard drive with the modeling databases will be provided to one of the project sponsors.

REFERENCES

Adelman, Z. 2004. Quality Assurance Protocol: WRAP RMC Emissions Modeling with SMOKE, Prepared for WRAP Modeling Forum, January.

Anthes, R.A. 1977. "A Cumulus Parameterization Scheme Utilizing a One-Dimensional Cloud Model", *Mon. Wea. Rev.*, Vol. 105, pp. 270-286.

Anthes, R.A. and T.T. Warner. 1978. "The Development of Mesoscale Models Suitable for Air Pollution and Other Mesometeorological Studies", *Mon. Wea. Rev.*, Vol. 106, pp, 1045-1078.

Arnold, J.R.; R.L. Dennis, and G.S. Tonnesen. 1998. Advanced techniques for evaluating Eulerian air quality models: background and methodology. In: Preprints of the 10th Joint Conference on the Applications of Air Pollution Meteorology with the Air & Waste Management Association, January 11-16, 1998, Phoenix, Arizona. American Meteorological Society, Boston, Massachusetts, paper no. 1.1, pp. 1-5.

Arnold, J.R., R.L. Dennis, and G.S. Tonnesen. 2003. "Diagnostic Evaluation of Numerical Air Quality Models with Specialized Ambient Observations: Testing the Community Multiscale Air Quality Modeling System (CMAQ) at Selected SOS 95 Ground Sites", *Atmos. Environ.*, Vol. 37, pp. 1185-1198.

ARS. 2002a. *Analysis of IMPROVE and SEARCH Speciated* $PM_{2.5}$ *Data.* Air Resource Specialists, Inc. Report to VISTAS, August 28, 2002. http://www.vistas-sesarm.org.

ARS. 2002b. *Analysis of Alternative Methods.* Air Resource Specialists, Inc. Report to VISTAS, August 28, 2002. http://www.vistas-sesarm.org.

ARS. 2002c. *Review of Selected Factors Responsible for High and Low Extinction.* Air Resource Specialists, Inc. Report to VISTAS, October 14, 2002. http://www.vistas-sesarm.org.

Baker, K. 2004. Presentations on latest MRPO modeling results at November 11, 2004 MRPO meeting in Chicago, Illinois. Available at: http://www.ladco.org/tech/photo/photochemical.html.

Barchet, W.R., and R.L. Dennis. 1990. "ANAPAP Model Evaluation, Volume 1: Protocol", prepared for the U.S. Environmental Protection Agency, prepared by Battelle Pacific Northwest Laboratories, Richland, WA.

Boylan, J. W., 2004. "Calculating Statistics: Concentration Related Performance Goals", paper presented at the EPA PM Model Performance Workshop, Chapel Hill, NC. 11 February.

Byun, D.W., and J.K.S. Ching. 1999. "Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System", EPA/600/R-99/030.

Carter, W.P.L. 1999. Documentation of the SAPRC-99 Chemical Mechanism for VOC Reactivity Assessment, Draft report to the California Air Resources Board, Contracts 92-329 and 95-308, 9/13/99.

CENRAP. 2003. CENRAP Long Range Plan. Central States Regional Air Planning Association, Oklahoma City, Oklahoma. October 29.

Chang, J.S., R.A. Brost, I.S.A. Isakson, S. Madronic, P. Middleton, W.R. Stockwell and C.J. Walcek. 1987. A three-dimensional Eulerian acid deposition model: Physical concepts and formulation. *J. Geophys. Res.*, 92, 14681-14700.

Chang, J. S., et al. 1997. "The SARMAP Air Quality Model", prepared for the California Air Resources Board, prepared by the State University of New York, Albany, New York.

Coe D. and S. Reid. 2003. "Research and Development of Ammonia Emission Inventories for the Central States regional Air Planning Association". Final Report. Sonoma Technology, Inc. (STI). October 30.

Coella, P., and P. L., Woodward. 1984. "The Piecewise Parabolic Method (PPM) for Gas-Dynamical Simulations", *J. Comp. Physics*, Vol. 54, pp. 174-201.

Dennis, R. L., et al. 1990. "Evaluation of Regional Acid Deposition Models", State-of-Science/Technology Report No. 5, National Acid Precipitation Assessment Program, Washington, D.C.

Dentener, F. J., and P. J. Crutzen. 1993. Reaction of N_2O_5 on tropospheric aerosols: Impact on global distributions of NO_x, O_3, and OH, *J. Geophys. Res.*, *98*, 7149-7163.

Donahue, N.M., M.K. Dubey, R. Mohrschladt, K.L. Demerjian, and J.G. Anderson. 1997. High-pressure flow study of the reactions $OH+NO_x \rightarrow HONO_x$: Errors in the falloff region. *J. Geophys. Res.* **102**, 6159-6168.

Dudhia, J. 1993. "A Non-hydrostatic Version of the Penn State/NCAR Mesoscale Model: Validation Tests and Simulation of an Atlantic Cyclone and Cold Front", *Mon. Wea. Rev.*, Vol. 121. pp. 1493-1513.

Edgerton, E. S., *Sources of PM2.5 Carbon in the Southeast US*, presentation at the MARAMA Science Meeting, Baltimore, MD, January 22, 2003. http://www.marama.org.

ENVIRON, Alpine Geophysics, UC Riverside and UC Davis. 2003a. "VISTAS Emissions and Air Quality Modeling – Phase I Task 4a/b Report: Review of Model Sensitivity Simulations and Recommendations of Initial CMAQ Model Configurations and Sensitivity Tests." Revised Draft July 25.

ENVIRON, Alpine Geophysics , UC Riverside and UC Davis. 2003b. "VISTAS Emissions and Air Quality Modeling – Phase I Task 3 Report: Review and Assessment of Available Ambient

Air Quality Data to Support Modeling and Modeling Performance Evaluation for the Three VISTAS Phase I Episodes." Revised Draft July 22.

ENVIRON. 2002. "User's Guide Comprehensive Air Quality Model With Extensions (CAMx) Version 3.10." ENVIRON International Corporation, Novato, California (available at www.camx.com) April.

ENVIRON. 2003a. "Development of an Advanced Photochemical Model for Particulate Matter: PMCAMx." ENVIRON International Corporation, Novato, CA. Prepared for Coordinating Research Council, Inc. Project A-30 (available at www.crcao.com).

ENVIRON, 2003b. "VISTAS Emissions and Air Quality Modeling – Phase I Task 2 Report: Recommended Model Configurations and Evaluation Methodology for Phase I Modeling." Prepared by ENVIRON International Corporation, Alpine Geophysics, LLC and University of California at Riverside. Novato, California. (available at: http://pah.cert.ucr.edu/vistas/docs.shtml). August 4.

ENVIRON, 2003c. "VISTAS Emissions and Air Quality Modeling – Phase I Task 3 Report: Review and Assessment of Available Ambient Air Quality Modeling and Performance Evaluation for the Three VISTAS Phase I Episodes." Prepared by ENVIRON International Corporation, Alpine Geophysics, LLC and University of California at Riverside. Novato, California. (available at: http://pah.cert.ucr.edu/vistas/docs.shtml). July 22.

ENVIRON, 2003d. "VISTAS Emissions and Air Quality Modeling – Phase I Task 4a/b Report: Review of Model Sensitivity Simulations and Recommendations of Initial CMAQ Model Configurations and Sensitivity Tests." Prepared by ENVIRON International Corporation, Alpine Geophysics, LLC and University of California at Riverside. Novato, California. (available at: http://pah.cert.ucr.edu/vistas/docs.shtml). July 25.

EPA, 1991. "Guidance for Regulatory Application of the Urban Airshed Model (UAM), "Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, N.C.

EPA, 1999. "Draft Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-hr Ozone NAAQS". Draft (May 1999), U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, N.C

EPA. 2001. "Guidance for Demonstrating Attainment of Air Quality Goals for $PM_{2.5}$ and Regional Haze", Draft Report, U.S. Environmental Protection Agency, Research Triangle Park, NC.

EPA. 2003a. "Guidance for Tracking Progress Under the Regional Haze Rule", U.S. Environmental Protection Agency, Research Triangle Park, NC.

EPA. 2003b. "Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule", U.S. Environmental Protection Agency, Research Triangle Park, NC.

Fahey, K.M., and S.N. Pandis. 2001. Optimizing model performance: variable size reduction in cloud chemistry modeling. *Atmos. Environ*. Vol. 35, pp. 4471-4478.

FLAG. 2000. Federal Land Manager's Air Quality Related Values Workgroup (FLAG) Phase I Report. (http://www2.nature.nps.gov/ard/flagfiee/AL.doc).

Gery, M. W., G.Z. Whitten, J.P. Killus, and M.C. Dodge. 1989. A photochemical mechanism for urban and regional-scale computer modeling. *J. Geophys. Res.* 94, 12925-12956.

Gipson, G, and J. Young. 1999. Process Analysis, in *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System*, Chapter 16, U.S. EPA, Office of Research and Development, Washington, DC 20460.

Green M., N. Adhikari, J. Xiu and G. Nikolich. 2006. Columbia River Gorge Haze Gradient Study. Final Report. Desert Research Institute, Division of Air Sciences, Las Vegas, Nevada. (http://www.swcleanair.org/reports.html). January 27.

Grell, G. A., J. Dudhia, and D. R. Stauffer. 1994. "A Description of the Fifth Generation Penn State/NCAR Mesoscale Model (MM5). NCAR Tech. Note, NCAR TN-398-STR, 138 pp.

Hanna, S.R., A.G. Russell, J. Wilkinson, and J. Vukovich. 2002. Review of BEIS3 Formulation and Consequences Relative to Air Quality Standards: Estimation of Uncertainties in BEIS3 Emissions Outputs. EPRI Technical Report 1005159, EPRI, 3412 Hillview Ave., Palo Alto, CA 94304.

Hanna, S.R., A.G. Russell, J. Wilkinson, and J. Vukovich. 2003. Review of BEIS3 Formulation and Consequences Relative to Air Quality Standards: Estimation of Effects of Uncertainties in BEIS3 Emissions on Uncertainties in Ozone Predictions by Chemical Transport Models, EPRI, Palo Alto, CA: 2002 (report is currently under review by EPRI).

Hanna, S. R. 1994. "Mesoscale Meteorological Model Evaluation Techniques with Emphasis on Needs of Air Quality Models", in Mesoscale Modeling of the Atmosphere, R. A. Pielke and R. P. Pierce (Eds.), American Meteorological Society, Boston, MA.

Hermann, H. et al., 2000. manuscript submitted to *J. Geophys. Res.*

IPCC. 2001. "Climate Change 2001: The Scientific Basis -- Contribution of Working Group I to the Third Assessment Report of IPCC." Intergovernmental Panel on Climate Change. ISBN: 0521014956.

Jacob, D. J. 1999. Heterogeneous chemistry and tropospheric ozone. *Atmos. Environ.*, special issue, 1999 NARSTO Assessment.

Johnson, M. 2004. "Annual 2002 MM5 v363 Simulation Evaluation." Iowa Department of natural Resources, Air Quality Bureau. November. (Available at www.ladco.org/tech/photo/present/mm5v363_eval.pdf).

Khasibatla, P. et al. 1997. Impact of inert organic nitrate formation on ground-level ozone in a regional air quality model using the Carbon Bond Mechanism 4. *Geophys. Res. Letters*, **24**, 3205-3208.

Liu, G., C. Hogrefe, and S.T. Rao. 2003. “Evaluating the Performance of Regional-Scale Meteorological Models: Effects of Clouds Simulation on Temperature Prediction”, *Atmos. Environ.*, Vol. 36, pp. 1691-1705.

Malm, W.C.; Pitchford, M.L; Scruggs, M.; Sisler, J.F.; Ames, R.; Cepeland, S.; Gebhart, K.; Day, D.E. 2000. *Spatial and Seasonal Patterns and Temporal Variability of Haze and Its Constituents in the United States. Report III.* Cooperative Institute for Research in the Atmosphere, May.

Matthias-Maser, S. and R. Jaenicke. 1995. "The size distribution of primary biological aerosol particles with radii >0.2 mm in an urban-rural influenced region." *Atmos. Res.*, 39, 279-286.

McNally, D.E., and T.W. Tesche. 1994. "MAPS2.3 User's Guide", Alpine Geophysics, LLC, Golden, CO.

McNally, D. E. 1997. “Development of Methodology for Mapping MM5 Fields onto Arbitrary Eulerian Photochemical Air Quality Simulation Models (PAQSM)”, Alpine Geophysics, LLC, Arvada, CO.

Morris, R.E., B. Koo, S. Lau, T.W. Tesche, D. McNally, C. Loomis, G. Stella, G. Tonnesen and Z. Wang. 2004. “VISTAS Emissions and Air Quality Modeling – Phase I Task 4cd Report: Model Performance Evaluation and Model Sensitivity Tests for Three Phase I Episodes”, prepared for the VISTAS Technical Analysis Committee, prepared by ENVIRON International Corporation, Alpine Geophysics, LLC, and the University of California, Riverside (CE-CERT).

Morris, R.E., D. McNally, T. Tesche, G. Tonnesen, J. Boylan and P. Brewer. 2004. “Regional Haze Modeling over the VISTAS States: Preliminary Verification of Models-3/CMAQ for the 2002 Annual Period.” Presented at AWMA Visibility Conference, Asheville, North Carolina. October.

NARSTO (1999) NARSTO Quality Planning Handbook, Appendix A: Quality Integrated Work Plan Template for Monitoring and Measurement Research and Development Projects. www.cgenv.com/Narsto.

Pielke, R. A., and M. Uliasz. 1998. “Use of Meteorological Models as Input to Regional and Mesoscale Air Quality Models C Limitations and Strengths”, *Atmos. Environ*. Vol. 32, No. 8, pp. 1455-1466.

Pilinis, C. and J. H. Seinfeld. 1987. “Continued Development of a General Equilibrium Model for Inorganic Multicomponent Atmospheric Aerosols”, *Atmos. Environ*. Vol.21, pp.2453.

Pilinis, C., K.P. Capaldo, A. Nenes, and S.N. Pandis. 2000. "MADM - A new multicomponent aerosol dynamics model." *Aerosol Sci. Tech.*, Vol. 32(5), pp. 482-502. 2000.

Pitchford M.L., I. Tombach, M. Barna, K. Gebhart, M. Green, E. Knipping, N. Kumar, W. Malm, B. Pun, N. Schichtel and C. Seigneur. 2004. "Big Bend Aerosol and Visibility Study". Final Report. September.

Pleim, J.E. and J.S. Chang. 1992. A non-local closure model for vertical mixing in the convective boundary layer. *Atmos. Env*., **26A**, pp. 965-981.

Pun B., S-Y. Chen and C. Seigneur. 2004. "CENRAP Model Simulations and Performance Evaluations". Atmospheric and Environmental Research, Inc. (AER). August.

Russell, A.G., and R.L. Dennis. 2000. "NARSTO Critical Review of Photochemical Models and Modeling", *Atmos. Environ*., Vol. 34, No. 12-14, pp. 2283-2324.

Schere, K.L., and R.A. Wayland. 1989. "EPA Regional Oxidant Model (ROM2.0): Evaluation on 1980 NEROS Data Bases", EPA/600/3-80/057, Atmospheric Research and Exposure Assessment Laboratory, Research Triangle Park, NC.

Seaman, N.L. 1995. "Status of Meteorological Pre-Processors for Air Quality Modeling", *International Conf. On Particulate Matter*, Air and Waste Mgt. Assn., Pittsburgh, PA.

Seaman, N.L. 1995. "Status of Meteorological Pre-Processors for Air Quality Modeling", *International Conf. On Particulate Matter*, Air and Waste Mgt. Assn., Pittsburgh, PA.

Seaman, N.L. 1996. "Study of Meteorological Variables Needed in Air-Quality Modeling', Annual Progress Report prepared for the Coordinating Research Council (CRC), Interim Report, Project A-11, prepared by the Department of Meteorology, Penn State University, State College, PA.

Seaman, N.L. 2000. "Meteorological Modeling for Air Quality Assessments", *Atmos. Environ*., Vol. 34, No. 12-14, 2231-2260.

Seaman, N. L., and D. R. Stauffer. 1996. "SARMAP Meteorological Model Final Report", prepared for the San Joaquin Valleywide Air Pollution Study Agency, prepared by the Department of Meteorology, Pennsylvania State University, University Park, PA.

Seaman, N.L., and S.A. Michelson. 1998. "Mesoscale Meteorological Structure of a High-Ozone Episode During the 1995 NARSTO-Northeast Study", *J. Appl. Meteo*., (submitted).

Seaman, N.L., D.R. Stauffer, and T.W. Tesche. 1992. "The SARMAP Meteorological Model: A Four-Dimensional Data Assimilation Technique Used to Simulate Mesobeta-Scale Meteorology During a High-Ozone Episode in California", International Specialty Conference on Tropospheric Ozone Nonattainment and Design Value Issues, U.S. EPA/AWMA, 27-30 October, Boston, MA.

Seaman, N.L., D.R. Stauffer, and L.M. Lario. 1995. "A MultiScale Four-Dimensional Data

Assimilation System Applied to the San Joaquin Valley During SARMAP. Part I: Modeling Design and Basic Performance Characteristics", *J. Appl. Meteo.*, Vol. 34, pp. 1739-1761.

Seaman, N.L., D.R. Stauffer, and D.E. McNally. 1996a. "Application of the MM5-FDDA Meteorological Model to the Southern California SCAQS-1997 Domain: Preliminary Test Using the SCAQS August 1987 Case", Ninth Joint Conference on Applications of Air Pollution Meteorology, American Meteorological Society, 28 January-2 February, Atlanta, GA.

Seinfeld, J.H. and S.N. Pandis. 1998. Atmospheric Chemistry and Physics: From Air Pollution to Global Change. Wiley, New York.

Seigneur, C., et al. 2000. "Guidance for the Performance Evaluation of Three-Dimensional Air Quality Modeling Systems for Particulate Matter and Visibility", *J. Air & Wast Manage. Assoc.* Vol. 50, pp. 588-599.

Simoneit, B.R.T., J.N. Cardoso and N. Robinson. 1990. "An assessment of the origin and composition of higher molecular weight organic matter in aerosols over Amazonia." *Chemosphere*, 21, 1285-1301.

Solomon, P.S., T. Klamser-Williams, P. Egeghy, D. Crumpler and J. Rice. 2004. "STN/IMPROVE Comparison Study Preliminary Results". Presented at PM Model Performance Workshop. Chapel Hill, NC. February 10.

Stockwell, W.R., P. Middleton, J.S. Chang, and X. Tang. 1990. The second generation Regional Acid Deposition Model chemical mechanism for regional air quality modeling. *J. Geophys. Res.*, **95**, 16,343-16,367.

Stockwell, W.R., P. Middleton, J.S. Chang, and X. Tang, X. 1997. The second generation Regional Atmospheric Chemistry Mechanism regional air quality modeling. *J. Geophys. Res.*, **102**.

Strader, R., F.W. Lurmann and S.N. Pandis. 1999. "Evaluation of secondary organic aerosol formation in winter." *Atmos. Environ.* Vol. 33, pp. 4849-4864.

Strait, R., S. Roe and J. Vukovich. 2004. "2002 Base Case Modeling Inventory – Work Plan." E.H. Pechan and Associates, Inc. Durham, North Carolina. July 30.

Tang, Y. 2002, "A Case Study of Nesting Simulation for the Southern Oxidants Study 1999 at Nashville", *Atmos. Environ.*, Vol. 36, pp. 1691-1705.

Tesche, T. W., et al., 1990. "Improved Treatment of Procedures for Evaluating Photochemical Models", prepared for the California Air Resources Board, prepared by Alpine Geophysics, Crested Butte, CO. Contract No. A832-103.

Tesche, T.W., and D.E. McNally. 1993a. “Operational Evaluation of the CAL-RAMS Meteorological Model for LMOS Episode 1: 26-28 June 1991", prepared for the Lake Michigan Air Directors Consortium, prepared by Alpine Geophysics, LLC, Crested Butte, CO.

Tesche, T.W., and D.E. McNally. 1993b. "Operational Evaluation of the CAL-RAMS Meteorological Model for LMOS Episode 2: 17-19 July 1991", prepared for the Lake Michigan Air Directors Consortium, prepared by Alpine Geophysics, LLC, Crested Butte, CO.

Tesche, T.W., and D.E. McNally. 1993c. "Operational Evaluation of the CAL-RAMS Meteorological Model for LMOS Episode 3: 25-26 August 1991", prepared for the Lake Michigan Air Directors Consortium, prepared by Alpine Geophysics, LLC, Crested Butte, CO.

Tesche, T.W., and D.E. McNally. 1993d. "Operational Evaluation of the CAL-RAMS Meteorological Model for LMOS Episode 4: 20-21 June 1991", prepared for the Lake Michigan Air Directors Consortium, prepared by Alpine Geophysics, LLC, Crested Butte, CO.

Tesche, T. 1994. Evaluation Procedures for Regional Emissions, Meteorological, and Photochemical Models. Presented at the 86th Annual Meeting for the Air and Waste Management Association, 14-18 June, Denver, CO.

Tesche, T.W. and D.E. McNally. 1996a. “Superregional Ozone Modeling and Analysis Study C Phase I: Work Element 3: Assessment of the OTAG Data Sets -- Task 2 Technical Memorandum: Review of the OTAG Meteorological Inputs and Outputs”, prepared for the Midwest Ozone Group, prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W. and D.E. McNally. 1996b. “Superregional Ozone Modeling and Analysis Study C Phase II: Work Element 5 Technical Report: Comparative Evaluation of the MM5 and RAMS Models for the July 1991 OTAG Episode”, prepared for the Midwest Ozone Group, prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W., and D.E. McNally. 1997a. “Superregional Ozone Modeling and Analysis Study C Final Report: Assessment of the Reliability of the OTAG Modeling System”, prepared for the Midwest Ozone Group, prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W., and D.E. McNally. 1997b. “Methodology for Climatological Analysis of Multi-Year Aerometric Data to Support the Development of the Breton Conceptual Model and Field Program Design”, prepared for Walk Heydel Environmental, prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W., and D.E. McNally. 1997c. "The Use of the San Joaquin Valley Meteorological Model in Preparation of a Field Program in the South Coast Air Basin and Surrounding Regions of Southern California: Volume I: Final MM5 Evaluation for the 3-6 August 1990 SARMAP Episode", prepared for the California Air Resources Board, prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W. and D.E. McNally. 1999. "Comparative Evaluation of the MM5 and RAMS3c Prognostic Meteorological Models Over the Midwestern U.S. for Two 1999 LMOS Intensive Measurement Episodes", prepared for the Coordinating Research Council, Project A-25 draft Final Report, prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W., and D.E. McNally. 2001. "Evaluation of CAMx and Models-3/CMAQ Over the Lower Lake Michigan Region with Inputs from the RAMS3c and MM5 Models", prepared for the Coordinating Research Council, prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Tesche, T.W., and H.E. Jeffries. 2002. "Findings From BCCA-AG Science Studies", prepared for the Business Coalition for Clean Air- Appeals Group, (2002), prepared by Alpine Geophysics, LLC, Ft. Wright, KY.

Timin, B. 2002. "PM$^{-}_{2.5}$ and Regional Haze Modeling Guidance". Prepared by the U.S. EPA/OAQPS. April 24.

Timin, B. 2004. "PM$_{2.5}$ Model Performance Evaluation: Purpose and Goals". Presented at PM Model Evaluation Workshop, Chapel Hill, NC. February.

Tonnesen, G.S. 1999. Effects of uncertainty in the reaction of the hydroxyl radical with nitrogen dioxide on model simulated ozone control strategies. *Atmos. Environ.* **33***:*1587-1598.

Tonnesen, G.S. and R.L. Dennis. 2000. Analysis of radical propagation efficiency to assess ozone sensitivity to hydrocarbons and NO$_x$. Part 1: Local indicators of odd oxygen production sensitivity. *J. Geophys. Res.*, **105**, 9213–9225.

Tonnesen, G., R.E. Morris, J. Vimont, M. Uhl, K. Briggs and T. Moore. 2003. "The WRAP Regional Modeling Center – Application and Evaluation of Regional Visibility Models." Presented at AWMA Annual Meeting and Exhibition. June.

Tonnesen G. and R. Morris. 2004. "Evaluation of Existing Regional Haze Modeling Results for the CENRAP Region". UCR and ENVIRON. July.

Watson, J.G. and J.C. Chow. 1999. Reconciling Urban Fugitive Dust Emissions Inventory and Ambient Source Contribution Estimates: Summary of Current Knowledge and Needed Research. Document No. 61110.4D2, Desert Research Institute, Reno NV, September 3.

Western Regional Air Partnership (2003) Western Regional Air Partnership 2004 Work Plan, October.

Western Regional Air Partnership (2003a) Strategic Plan 2003-2008 of the Western Regional Air

Partnership, September.

Xiu, A. and J.E. Pleim (2000) Development of a land surface model. Part I: application in a mesoscale meteorology model. *J. App. Met.*, **40**, pp. 192-209.

Zaveri, R.A and L.K. Peters. 1999. A new lumped structure photochemical mechanism for large scale applications, *J. Geophys. Res*., 30,387-30,415

Zheng,, M.; Cass, G.R.; Schauer, J.J.; Edgerton, E.S. *Environ. Sci. Tech.* 2002, 36, 2361-2371.