



#### **Revised Draft**

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

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# 1.0 INTRODUCTION

This Modeling Protocol describes the meteorological, emissions and air quality modeling to be conducted by the contractor team of ENVIRON International Corporation and Alpine Geophysics, LLC, as part of the Columbia River Gorge National Scenic Area Air Quality Study (Gorge Study). The meteorological, emissions and air quality modeling and analyses are 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) requested 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 that significantly contribute 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.

#### 1.1.1 Columbia River Gorge Air Quality Study Components

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

<u>Measurement Program</u>: 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.

<u>Haze Gradient Study</u>: 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., 2006a).

<u>Causes of Haze</u>: The Causes of Haze in the Gorge (CaHaGo) analysis is a follow-up to the Columbia River Gorge Haze Gradient Study. While the Haze Gradient Study used primarily nephelometer and surface meteorological data to understand spatial and temporal patterns in haze in the Gorge, CoHaGo made use of additional aerosol chemical composition to enhance understanding of haze in the Gorge. A CaHaGo draft report is now available (Green et al., 2006b).

<u>Modeling Analysis</u>: The modeling of visibility impairment in the Gorge is the subject of this Modeling Protocol.

# 1.2 Overview of Gorge Modeling Approach

To meet the goals of the Gorge Study, the Technical Team, drawing upon the experience of visibility modeling experts across the country, proposed chemical transport modeling as one of the study components. The plan called for using the state-of-the-science air quality models, such as the Comprehensive Air Quality Model with extensions (CAMx; ENVIRON, 2005) and EPA's Models-3 Community Multiscale Air Quality (CMAQ; Byun and Ching, 1999) model. These modeling platforms would be provided emission inputs from the EPA's Models-3 Sparse Matrix Operating Kernel Emissions (SMOKE; Coats, 1995; Houyoux and Vukovich, 1999) system, and meteorological inputs from the Pennsylvania State University / National Center for Atmospheric Research (PSU/NCAR), Fifth Generation Mesoscale Model (MM5; Dudhia, 1993; Grell et al., 1994).

The first element of the Gorge Study modeling component is the selection and prioritization of episodes to be examined. Based on visibility measurements during the 2003-2005 enhanced monitoring periods, several episodic periods will be selected and prioritized.

The approach for the Gorge Study modeling described in this Modeling Protocol is to leverage the considerable regional visibility modeling work already 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 federally protected 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 as well.

The WRAP Regional Modeling Center (RMC) has applied the MM5 meteorological model on a 36 km continental U.S. and a 12 km western U.S. grid for the 2002 calendar year. The SMOKE emissions model has been used to generate hourly gridded speciated emissions needed for photochemical grid modeling for both the 2002 base year, and the 2018 future year that includes all emission control regulations that are currently promulgated and "on-the-books." WRAP is currently using both the CMAQ and CAMx photochemical grid models to estimate base and future year PM components from which visibility impairment is calculated.





## 1.2.1 Modeling Analyses Supported by Gorge Study Funding

Following the WRAP modeling methodology, the Gorge Study modeling component was to employ both CAMx and CMAQ to simulate as many as four season-representative high PM/extinction episodes with a wide array of sensitivity tests and Probing Tool applications for both the base year and the 2018 future year. Modeling was to be conducted on a series of telescoping nested grids with resolution ranging from 36 km (the WRAP continental grid) to 12, 4, and 1.33 km focusing on the Gorge area. The final modeling project budget was established by the SWCAA in late Spring of 2006. This limited budget, coupled with unanticipated work associated with MM5 performance assessments and complications with incorporating state-specific emissions data into the WRAP inventory, has required a reduction in the original scope. Below we summarize the modeling analyses to be conducted under current funding.

The Gorge Study modeling component will utilize the MM5 meteorological, SMOKE emissions, and CAMx air quality models. The modeling domain will include the WRAP 36 km continental U.S. grid, with a set of smaller nested 12 and 4 km grids focusing on the primary area of study. Modeling inputs will be developed for two multi-day episodes in 2004. The Gorge Study modeling will expend significant effort developing refined 2004 emissions and episode-specific meteorological modeling inputs for the 12 km OR/WA/ID grid, and the 4 km Oregon/Washington grid, and will rely on the WRAP emissions set up for the regional 36 km grid. The WRAP 2002 emission inventory will be adjusted to 2004, and 2004 episode-specific emissions for Oregon and Washington will be used to replace the WRAP estimates for those states. Base case air quality model performance will be evaluated for the specific episodes to be simulated using operational and diagnostic techniques.

A 2018 future year episode will also be simulated to obtain a visibility forecast trend line for the Gorge monitoring sites. The WRAP 2018 emission projections will be used for this estimate for all grids, but will include additional emission reductions that will be applied to two specific large PM sources: the Boardman power plant near the eastern end of the Gorge, and the Camas pulp mill at the western end of the Gorge. The CAMx Particulate Source Apportionment Technology (PSAT) probing tool will be used to assess source category and region-specific attribution to sulfate, nitrate, organics, and primary particulates at several monitoring sites within the Gorge. PSAT will be applied for both 2004 base and 2018 future years. Finally, a group of five "what-if" scenarios will be simulated to provide estimated visibility improvements with the removal (or significant reduction) of emissions from specific sources.

# 1.3 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 by 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 <sup>1</sup>	Desert Research Institute
Frank Van Haren <sup>2</sup>	Washington Department of Ecology
Clint Bowman <sup>2</sup>	Washington Department of Ecology
Sally Otterson <sup>2</sup>	Washington Department of Ecology
Christiana Figueroa-	Washington Department of Ecology
Kaminsky <sup>2</sup>	

- 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 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 U.S. (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 Study modeling team (ENVIRON and Alpine Geophysics) 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 considered the following models for use in modeling particulate matter (PM) and regional haze:

- ➤ <u>MM5</u>: The Pennsylvania State University / National Center for Atmospheric Research (PSU/NCAR) Fifth Generation Mesoscale Model (MM5) is a nonhydrostatic, prognostic meteorological model routinely used for urban- and regional-scale photochemical, fine particulate, and regional haze regulatory modeling studies.
- ➤ <u>SMOKE</u>: The EPA Models-3 Sparse Matrix Operator Kernel Emissions (SMOKE) system is an emissions processor that generates hourly, gridded, speciated emissions from mobile, nonroad, area, point, fire and biogenic source categories for input to photochemical grid models.
- ➤ <u>CMAQ</u>: The EPA 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.
- ➤ <u>CAMx</u>: The Comprehensive Air Quality Model with Extensions (CAMx) 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

#### 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. In recent years, the MM5 modeling system has been widely adopted to support air quality modeling applications, and has been successfully applied in such 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).

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' airquality models (e.g., CMAQ and CAMx).

Distinct planetary boundary layer (PBL) parameterizations are available for air-quality applications, which represent sub-grid-scale vertical 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 scheme 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 several available North American





and Global large-scale analyses 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). There are two FDDA options in MM5: "analysis" nudging to 3-D and 2-D (surface-level) large scale analyses prepared by the NOAA National Center for Environmental Prediction (NCEP) and others worldwide; and "observational" nudging to specific arbitrarily-located measurement sites. Analysis nudging controls the entire 3-D grid system on a regular time interval (e.g., 3, 6, or 12-hourly), depending upon the source of the analyses. These analyses are prepared on global or continental scales with resolution ranging from 40-km to 2.5 degrees (latitude/longitude). Hence, the analyses are usually improved with local data when translated to the MM5 grids to improve their representation of winds, temperature, and humidity on the smaller-scale MM5 grids. Observational nudging is usually employed on smaller, high-resolution grids when a sufficiently high density of observations is available. Observation nudging is usually only applied at the surface layer at hourly intervals, within a user-specified radius of influence from each measurement site, so it usually does not impact the entire grid.

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. 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 MM5 was selected as the preferred meteorological model 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 consists 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;
- ➤ For the 12, and 4 km runs use two way nesting with no feedback (also called interactive one way nesting);
- > Initialization and boundary conditions from Eta analysis fields;
  - o Eta 3D and surface analysis data (ds609.2);





- o 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;
- ➤ No 2D surface FDDA analysis nudging; and
- ➤ No surface observational nudging.

Additional MM5 runs with changes to the various options will be carried out if the initial configuration does not perform adequately. The most sensitive components include the PBL model, land-surface model, cumulus parameterization, and FDDA options. These will be systematically altered to assess the impact of each to derive a meteorological simulation that adequately replicates observed conditions.

# 2.2.3 MM5 Input Requirements

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>: Multiple-resolution topographic information derived from the NCAR Geophysical Data Center global datasets is available for prescribing terrain elevations throughout the 36, 12, and 4 km grid domain.
- ➤ <u>Vegetation Type and Land Use:</u> Multiple-resolution vegetation type and land use information is available from NCAR for prescribing soil type, vegetative cover, and land use distributions throughout the 36, 12, and 4 km grid domain.
- Atmospheric Data: Initial and boundary conditions may be developed from operationally analyzed fields derived from the National Centers for Environmental Predictions (NCEP) EDAS (Eta Data Assimilation System at 40 km resolution) analyses following the procedures outlined by Stauffer and Seaman (1990). These 3-hr synoptic-scale analyses include horizontal winds, temperature, and humidity at standard pressure levels, plus sea-level pressure and ground/sea surface temperature. These coarse analyses are augmented for the MM5 grid structure by blending in surface and upper-air observational data in an objective analysis technique (a pre-processing step).
- ➤ Multi-Scale FDDA: The standard 3-D "multi-scale" analysis FDDA strategy to be used on the 36 and 12 km grids will employ objectively analyzed three-dimensional fields produced every 3-hr from the same NCEP EDAS analyses as used for initial and boundary conditions. Observational data will be used to improve the large-scale EDAS analyses, and to provide a source for observational nudging if that is needed to improve the simulation.





# 2.3 SMOKE Emissions Modeling System

#### 2.3.1 SMOKE Overview

The SMOKE 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, <a href="http://www.epa.gov/ttn/chief/software.html#pcbeis">http://www.epa.gov/ttn/chief/software.html#pcbeis</a>). 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 (<a href="http://www.epa.gov/asmdnerl/models3">http://www.epa.gov/asmdnerl/models3</a>). 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 (<a href="https://www.cmascenter.org">www.cmascenter.org</a>). 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 2-2 summarizes the version of the SMOKE system to be used and the sources of data to be employed in constructing the required modeling inventories.

## 2.3.3 SMOKE Input Requirements

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
- Wildfire, prescribed burns and agricultural burning emissions, day specific
- 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.

# 2.4 CMAQ Modeling System

For more than a decade, EPA has been developing 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 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 in September 2005.

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 provided 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 (two fine, and one coarse). Transfer of mass between the aerosol and gas phases is assumed to be in equilibrium and all secondary aerosols (sulfate, nitrate, SOA) are 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<sub>2</sub> 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), with the latest being the Secondary Organic Aerosol Model (SORGAM – last updated in August 2003), 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.





# 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 (referred to as "Probing Tools"), including Process Analysis (IRR, IPR, and CPA), Decoupled Direct Method (DDM), and the Ozone and Particulate Source Apportionment Technology (OSAT/PSAT). CAMx has been widely used in recent years by a variety regulatory agencies for 1-hr and 8-hr ozone and 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 multiple levels of fully interactive grid nesting (e.g., 36/12/4 km);
- ➤ CB4 or SAPRC99 gas-phase photochemical mechanisms;
- ➤ Two gas-phase chemical solvers, the CAMx Chemical Mechanism Compiler (CMC) Fast Solver or the highly accurate Implicit Explicit Hybrid (IEH) solver;
- ➤ Two separate treatments of PM using the same ISOROPIA and RADM chemistry algorithms as CMAQ:
  - o A two mode option comparable to the approach in CMAQ;
  - o A multi-section "full-science" approach using the Multi-component Aerosol Dynamics Model (MADM; Pilinis et al., 2000) that treats the effects of condensation/evaporation, coagulation and nucleation upon the particle size distribution.
- ➤ Secondary organic aerosol thermodynamics represented using the semi-volatile scheme of Strader and co-workers (1999);
- ➤ Multiple numerical algorithms for horizontal transport including the Piecewise Parabolic Method (PPM) and Bott advection solvers;
- ➤ Subgrid-scale Plume-in-Grid (PiG) algorithm to treat the near-source plume dynamics and chemistry from point sources;
- ➤ Ability to interface with a variety of meteorological models including the MM5, RAMS, and WRF prognostic hydrostatic meteorological models and the CALMET diagnostic meteorological model (others also compatible);
- ➤ The Ozone and Particulate Source Apportionment Technology (OSAT/PSAT) that identifies the source contributions due to user-defined geographic regions and categories (e.g., mobile, point, biogenic, etc.);
- ➤ The Decoupled Direct Method (DDM) sensitivity method that provides first-order sensitivity coefficients for emissions, initial and boundary conditions.

CAMx provides two key options to users interested in simulating PM. For CPU-efficient PM modeling applications, CAMx may be run using a two mode size representation (fine and coarse) similar to the treatment in CMAQ. Alternatively, more rigorous aerosol simulations (perhaps for





shorter episodes) may be addressed using the version that treats N-size sections (N is typically 10) and the rigorous, but computationally-extensive MADM multi-section chemistry module.

Given its similar performance in the northwest compared to CMAQ in WRAP applications, its ability to run 2-way interactive nested grids together within a single run of the model, and its ability to track non-linear source category and region impacts through its innovative PSAT probing tool, the CAMx model was chosen for use in the Gorge Study.

## 2.5.2 CAMx Configuration for Gorge Modeling

Table 2-3 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 a subset of the 36, 12, and 4 km grids used in MM5. All grids will be run together in two-way interactive mode, which allows for both up- and down-scale transfer of information among the grids. The base configuration of CAMx will use 19 vertical layers up to 100 mb (~15 km AGL) that exactly match those used by CMAQ and CAMx in WRAP. While CAMx includes a PiG treatment for ozone and PM, it is designed primarily to represent point source plume dispersion and chemistry within coarse grids, and would probably not provide much benefit on the high resolution grids planned for this study (it adds considerable computer resources). The effect of the PiG option may be tested in sensitivity simulations. The PPM advection solver will be used along with the spatially varying (Smagorinsky) horizontal diffusion Vertical diffusion in CAMx will be modeled by K-theory, using diffusivity approach. coefficients derived from MM5 PBL output variables via the MM5CAMx interface processor. Alternative vertical diffusivity coefficients will be tested in sensitivity tests. In its base configuration, CAMx will be exercised with the CB4 gas-phase, RADM aqueous-phase, ISORROPIA inorganic aerosol chemistry, and the SOAP secondary organic aerosol schemes.

#### 2.5.3 CAMx Input Requirements

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

- ➤ Three-dimensional hourly meteorological fields generated by MM5 and prepared using the MMCAMx interface processor;
- ➤ Two-dimensional low-level (surface layer) emissions and elevated point source emissions generated by the SMOKE emissions processor.
- ➤ IC/BC inputs (seasonal average, diurnally-varying) used by WRAP and processed by the CMAQ-to-CAMx IC/BC processor;
- ➤ Photolysis rates look up table;
- ➤ Albedo/Haze/Ozone Column input file prepared from several available global satellite-derived datasets;
- ➤ Land use and topography, as prepared for MM5.

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





#### 2.6 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.

#### 2.6.1 MM5

MM5 has 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. The MM5 Pleim-Xiu LSM/PBL option used by WRAP and the other RPOs frequently predicts very low PBL heights, and can generate "holes" in the spatial distribution of PBL heights that don't appear physically realistic and may affect air quality modeling. Furthermore, the use of FDDA and the type of nudging performed can lead to significant differences in the generated meteorological fields.

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 and consistent cool bias in the Pacific Northwest has been raised as a major concern (Kemball-Cook et al., 2005). Concerns have also been raised concerning the MM5 performance over the western third of the continent in general, especially pertaining to temperature and humidity (Johnson, 2004).

#### 2.6.2 **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.

#### 2.6.3 CAMx

Like all air quality models, a major limitation of CAMx 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; since CAMx and CMAQ share many common chemistry algorithms, performance issues are common to both models. Preliminary modeling by the RPOs (e.g., WRAP, VISTAS and CENRAP) found both CAMx and CMAQ nitrate performance suspect with winter overestimations and summer underestimations (Pun, Chen and Seigneur, 2004; Tonnesen and Morris, 2004). While not as poor as CMAQ, the VISTAS and





CENRAP modeling also found CAMx performance for Organic Carbon (OC) to be less than ideal; much of the OC performance problems are due to deficiencies in the SOA module that fails to account for several known processes important to SOA (e.g., polymerization). 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.



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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, and 4 km	
36 km grid	165 x 129 cells	
12 km grid	145 x 130	
4 km grid	184 x 157	
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 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	
3D Data Assimilation	Analysis Nudging on 36 and 12	
2D Surface Data Assimilation	None	
Observation Nudging	None	
Integration Time Step	Variable	Grid scale dependent
Simulation Periods	Gorge episodes	
Platform	Linux Cluster	MPI multi-processing

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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 km	
36 km grid	148 x 112 cells	Use WRAP emissions
12 km grid	131 x 116 cells	Use WRAP emissions
4 km grid	146 x 137 cells	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
	Revised EPA Spatial Surrogates Used for coarse grids,	
Gridding	new surrogates for fine grids WRAP 2018 EI, modified to include specific controls	
Growth and Controls	at Boardman EGU and Camas Paper Mill	
Quality Assurance	QA Tools in SMOKE 2.0	
Simulation Periods	Gorge episodes	

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

Science Options	Configuration	Details
Model Code	CAMx (ver 4.30 or 4.40)	Available at: www.camx.com
Horizontal Grid Mesh	36, 12, and 4 km	36 km covering continental U.S
36 km grid	148 x 112 cells	
12 km grid	131 x 116 cells	
4 km grid	146 x 137 cells	
Vertical Grid Mesh	19 Layers	17 Layers sync'd w/ MM5
Grid Interaction	Two-way nesting	Grids run together, with feedback
Initial Conditions	~10 days full spin-up	36 km full 10 days
Boundary Conditions	<b>GEOS-CHEM</b> 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 (PiG)	To be tested in sensitivity runs
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	
Integration Time Step	Wind speed dependent	

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#### 3.0 EPISODE SELECTION

This chapter discusses 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 nor a nonattainment area so there is no requirement for a formal emissions control plan 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<sub>2.5</sub> 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<sub>2.5</sub> attainment and regional haze modeling, adapting them to the specific requirements of the Gorge study.

#### 3.1 Overview of EPA Guidance

EPA's current draft guidance on PM<sub>2.5</sub>/Regional Haze modeling (EPA, 2001) identifies specific goals to consider when selecting one or more episodes for use in demonstrating PM<sub>2.5</sub> attainment or reasonable progress in attaining the regional haze NAAQS. Since there is much in common with the goals for selecting episodes for annual and episodic PM<sub>2.5</sub> attainment demonstrations as well as regional haze, EPA's guidance addresses all three in a common document. More recently, EPA has published an updated summary of PM<sub>2.5</sub> 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<sub>2.5</sub>/regional haze NAAQS implementation process that is expected during 2006. These concepts are appropriate for application to the Gorge visibility modeling, except that Gorge modeling will have to account for more fine scale features than may be needed for PM<sub>2.5</sub> attainment and regional haze modeling.

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 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, this recommendation can be interpreted such 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 Haze Gradient 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, which include IMPROVE Protocol measurements, additional ozone, NOx, SO<sub>2</sub>, sulfate, nitrate, nephelometer and meteorological monitoring was performed over the period March 1, 2003 to February 28, 2005 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.

Two major components of the intensive monitoring program were developed as funding became available. The first major component was the Haze Gradient Study, which was comprised of a series of nine nephelometers located throughout the Gorge Scenic Area (Figure 3-2). These locations also included surface meteorological monitoring instruments with the exception of the Memaloose location. 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 inter-comparison of the bsp measurements across monitors at different RH so that gradients of visibility impairment in the Gorge can be analyzed. 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.

Results from the Haze Gradient Study were used to identify episodes that would be evaluated in greater detail. 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.







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].





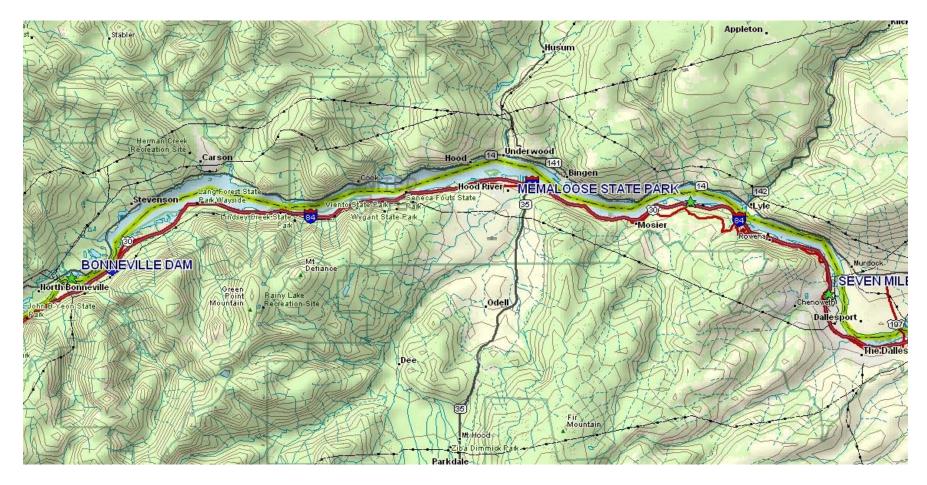


Figure 3-2b. Locations of Bonneville, Memaloose State Park, and Seven Mile Hill monitoring sites [Source: Green et al., 2006].





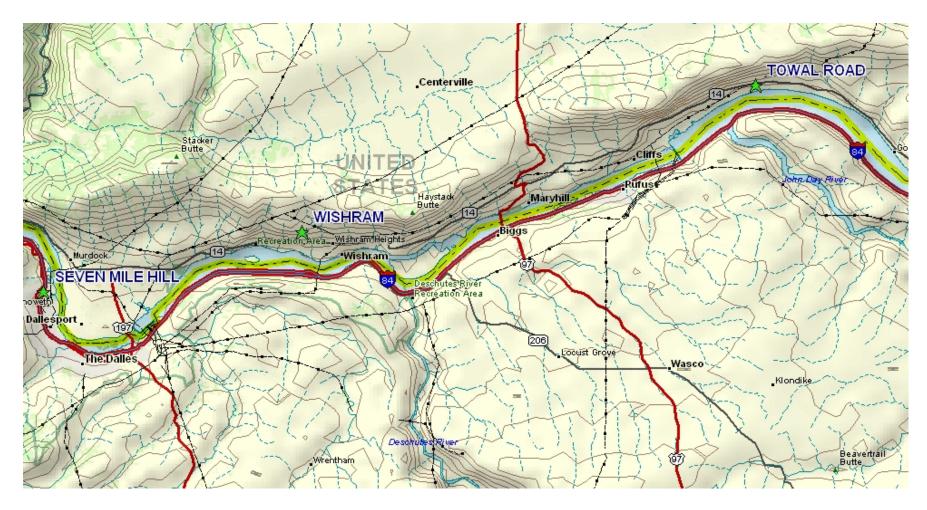


Figure 3-2c. Location of eastern monitoring sites (Seven Mile Hill, Wishram, and Towal Road) [Source: Green et al., 2006].







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

3-1. Monitors and equipment in close	e proximity to Columb	oia River Gorge Scenic
LONGVIEW	dry neph	Radiance M903
Olympic School	data logger	ESC 8816
1324 30th Ave, Longview, WA	00	
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"	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"	55	
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"	55	
elev 765 ft msl		
MCLOUGHLIN MIDDLE SCHOOL	dry neph	Radiance M903
5802 MacArthur, Blvd	data logger	ESC 8800
Vancouver, WA	33	
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"		S
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		
0.07 E IE II III 01		







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

PORTLAND - MILWAUKEE	ozopo analyzor	Dasibi 1003-AH
10955 SE 25th St, Milwaukie, Oregon	ozone analyzer	Dasibi 1003-AH
lat 45 26" 35.44"		
long -122 38' 16.95"		
elev 95 ft msl		
PORTLAND - SE LAFAYETTE	ozono onalyzor	Dasibi 1003-AH
5824 SE Lafayette, Portland, OR	ozone analyzer	Radiance M903
lat 45 - 29" - 47.83"	dry neph	Met One
long -122 36' - 10.52"	met gear PM2.5 FRM	R&P 2025
elev 246 ft msl		Odessa 3260
elev 240 it msi	data logger PM10	Odessa 3200
	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
	data loggol	040004 0200
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	Aaraaham/201
	Precip Collector Weigh rain guage	Aerochem/301 Belfort
VISTA HOUSE		DEHOLL
~ MP 25 on I-84, Oregon	camera	
lat 45 32' 20.18"		
long -122 14' 48.66"		
elev 800 ft msl		
CICA OOO II IIISI		







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

DOWNEY/U.F.DAM		D. II. Mana
BONNEVILLE DAM	dry neph	Radiance M903
~ MP 40 on I-84, OR/WA	met gear	
	chart recorder	L & N
( ; , , ) 00/04 1 ; , 04/05	data logger	ESC 8800
(winter/summer 03/04 and winter 04/05	140 140000 (5 17)	
study)	IAS IMPROVE like	IAS
(winter/summer 03/04 and winter 04/05	DDUM	110.5
study)	DRUM sampler	UC Davis
:	00040	Aerovironment model
installed 10/6/04	SODAR	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	dry nepri	Nadiance M903
lat 45 41' 51.96"	data laggar	ESC9900
	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 "	<b>,</b>	
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
(winter 00/04 or 104/05 to 10	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	radiance wood
elev 496 ft msl	chart recorder	Yokogawa 4 channel
lat 45 - 45' 13.867"	data logger	ESC 8800
	desktop	
long -120 - 37' 37.380"	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
	•	R&P 8400S Pulse
	sulfates	Generator
		R&P 8400S Pulse
		Analyzer
()Aliah rana wintar	u ituata a	R&P 8400N Pulse
(Wishram - winter	nitrates	Generator R&P 8400N Pulse
Mt Zion - Summer)		Analyzer
Wit Zion Gammon)		Teledyne - Adv. Air
	zero air gas generator	Pollution
	SO2	Thermo 43C
Robbins/Bradford Island 11/1/03 to	002	
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 conditionar	Coloman
MOBILE TRAILER 8X12	air conditioner Trailer	Coleman Wells Cargo 8X12
MOBILE TRAILER 6X12	OC/EC	Sunset Labs Mod 3
	OC/EC laptop	Suriset Labs Wod 3
	computer	Compaq Presario 2100
	•	R&P 8400S Pulse
	sulfates	Generator
		R&P 8400S Pulse
		Analyzer
(Bonneville Dam)	nitrates	R&P 8400N Pulse Generator
	าแเฉเธอ	R&P 8400N Pulse
Robbins/Bradford Is. OR Winter 03/04		Analyzer
Cascade Is. WA Summer 04 & Winter		Teledyne - Adv. Air
04/05	zero air gas generator	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 PI, 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

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 periods 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 discuss 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 concentrations 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<sup>-1</sup> on November 10 at the Wishram and Towal Road sites in the eastern end of the Gorge, and with elevated bsp in excess of 100 Mm<sup>-1</sup> at five other sites in the Gorge (Figure 3-3). Between November 7 and November 13, bsp was observed at over 100 Mm<sup>-1</sup> at more than one site in the Gorge. The elevated bsp was 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 started fairly clean on November 3, with all sites in the 30-50 Mm<sup>-1</sup> range, built to a peak in excess of 200 Mm<sup>-1</sup> at some sites on November 10, then dropped to relatively clean values (~20 Mm<sup>-1</sup>) 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 and February 24-27 (Figure 3-4). During both of these periods the highest values occurred in the east end of the Gorge at the Towal Road and 7 mile sites. During both elevated periods light scattering exceeded 80 Mm<sup>-1</sup>. 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<sup>-1</sup> occurred at several sites during the February 11-15, 2004 period, with values in excess of 100 Mm<sup>-1</sup> occurring at the Towal Road and Memaloose sites on the eastern end of the Gorge on February 14 (Figure 3-5). The scattering at Bonneville Dam tracked 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 was not as high during the summer periods with values exceeding 30 MM<sup>-1</sup> on July 24 and July 27-29 (Figure 3-6). Because NO3 was low during this summer period, light scattering was due to SO4 and OC. During the July 27-29 period, bsp was in mainly in the 40-60 Mm<sup>-1</sup> 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:

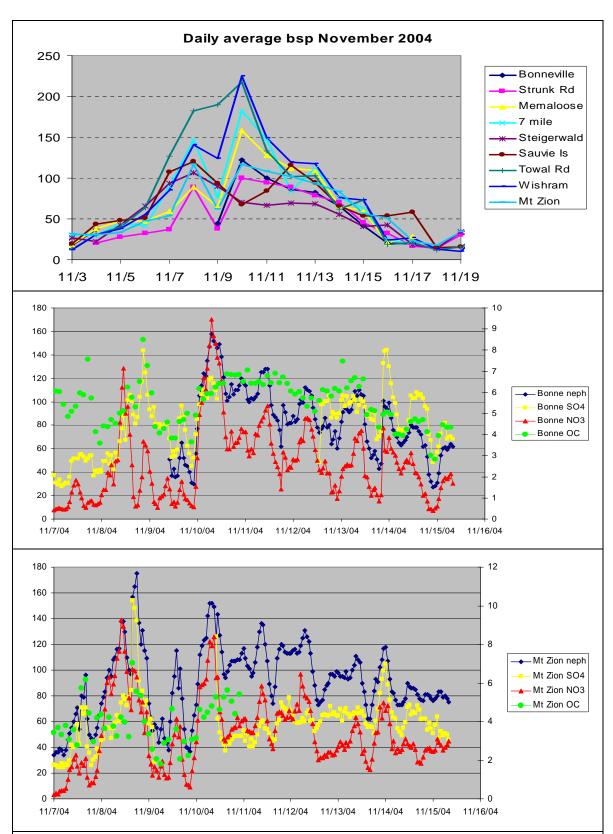
- July 24, 2004
- July 27, 2004
- July 28, 2004
- July 29, 2004

### 3.3.5 August 10-22, 2004

Most Gorge sites experienced elevated scattering in the 30-50 Mm<sup>-1</sup> range during August 11-16, with a secondary peak over August 18-19, 2004 (Figure 3-7). The continuous SO4 measurements at Bonneville Dam tracked the light scattering well. The IMPROVE monitors collected 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



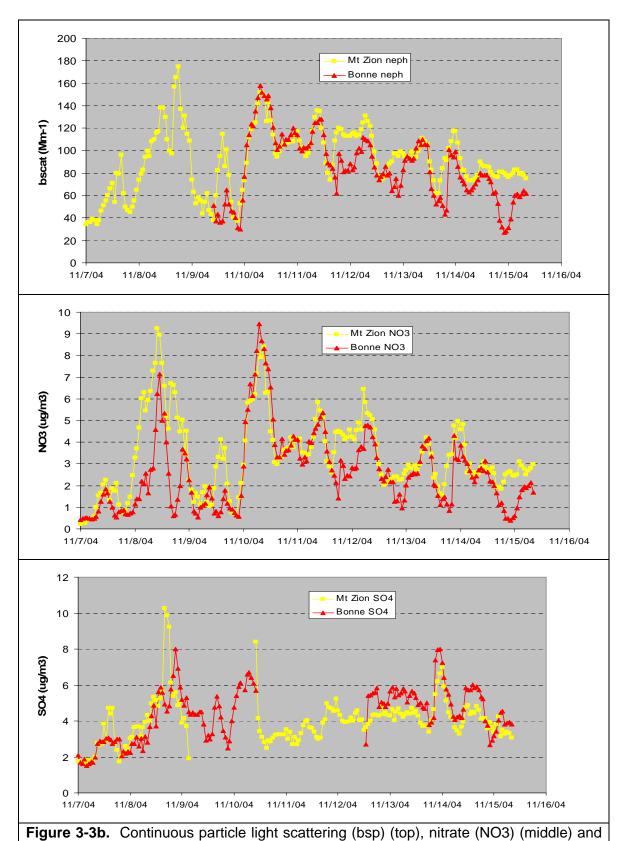


**Figure 3-3a.** Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (middle) and Mt. Zion (bottom) sites for November 2004.







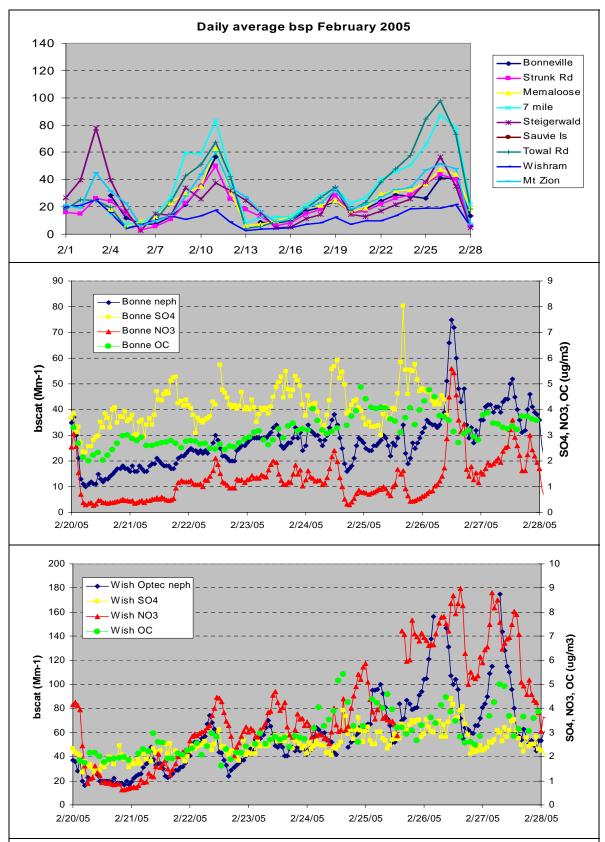


sulfate (SO4) (bottom) at the Bonneville Dam and Mt. Zion sites during November 2004.







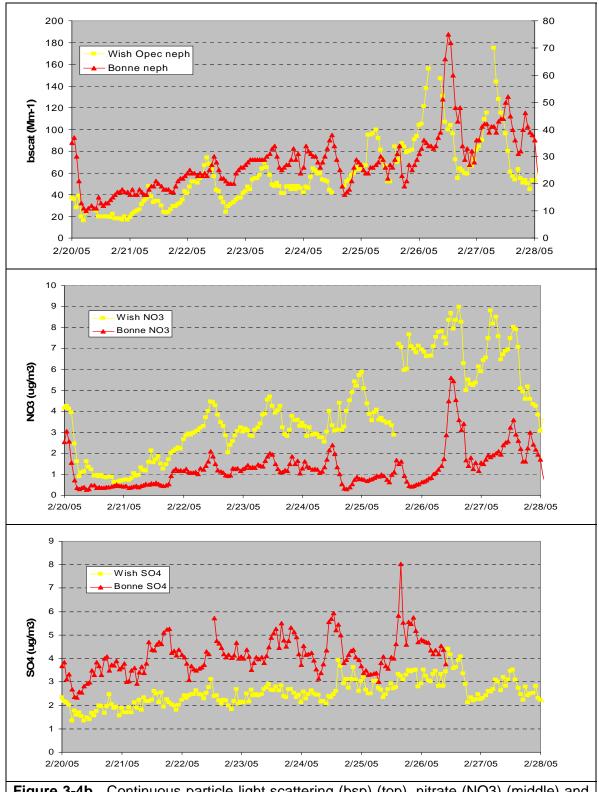


**Figure 3-4a.** Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (middle) and Wishram (bottom) sites for February 2005.







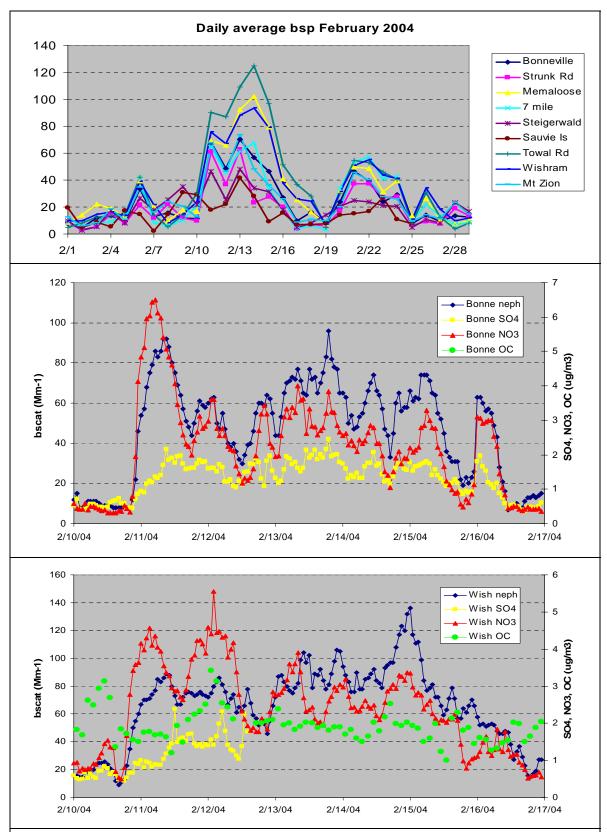


**Figure 3-4b.** Continuous particle light scattering (bsp) (top), nitrate (NO3) (middle) and sulfate (SO4) (bottom) at the Bonneville Dam and Wishram sites during February 2005.







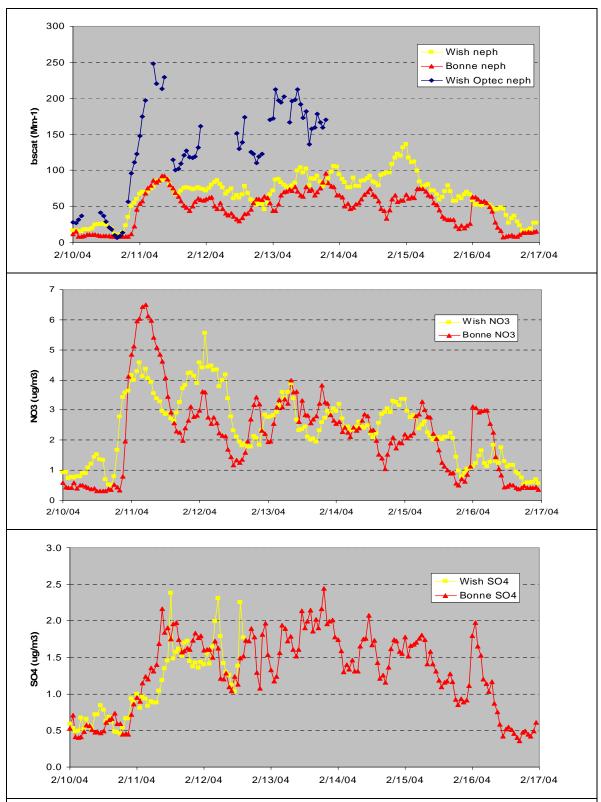


**Figure 3-5a.** Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (middle) and Wishram (bottom) sites for February 2004.



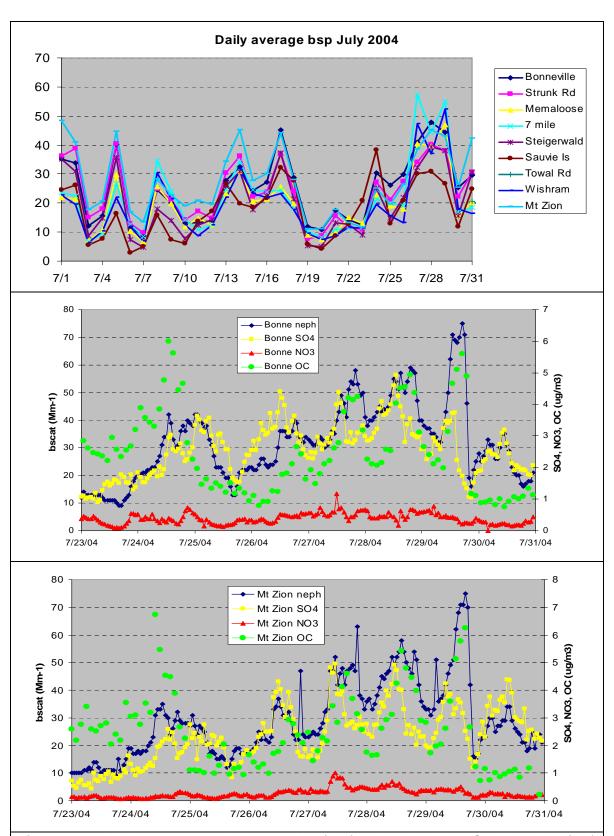






**Figure 3-5b.** Continuous particle light scattering (bsp) (top), nitrate (NO3) (middle) and sulfate (SO4) (bottom) at the Bonneville Dam and Wishram sites during February 2004.



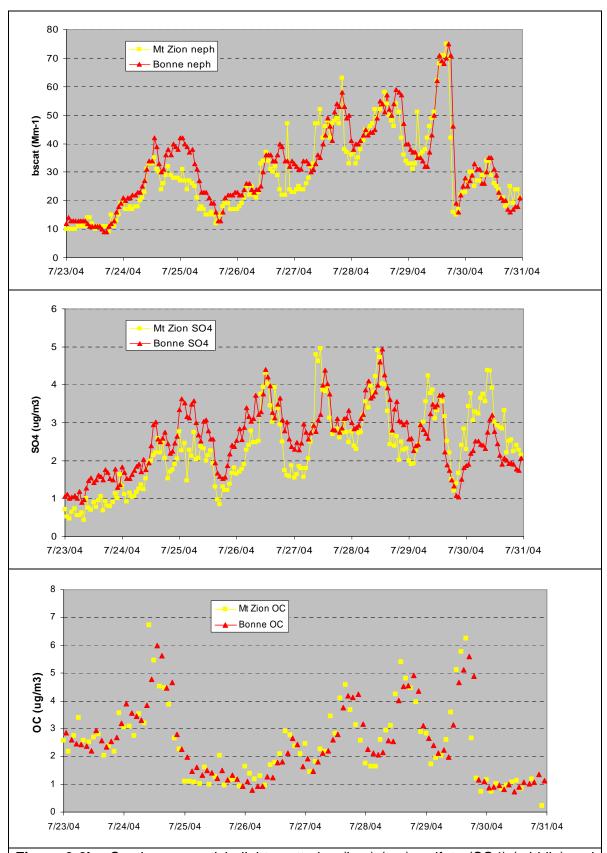


**Figure 3-6a.** Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (middle) and Mt. Zion (bottom) sites for July 2004.







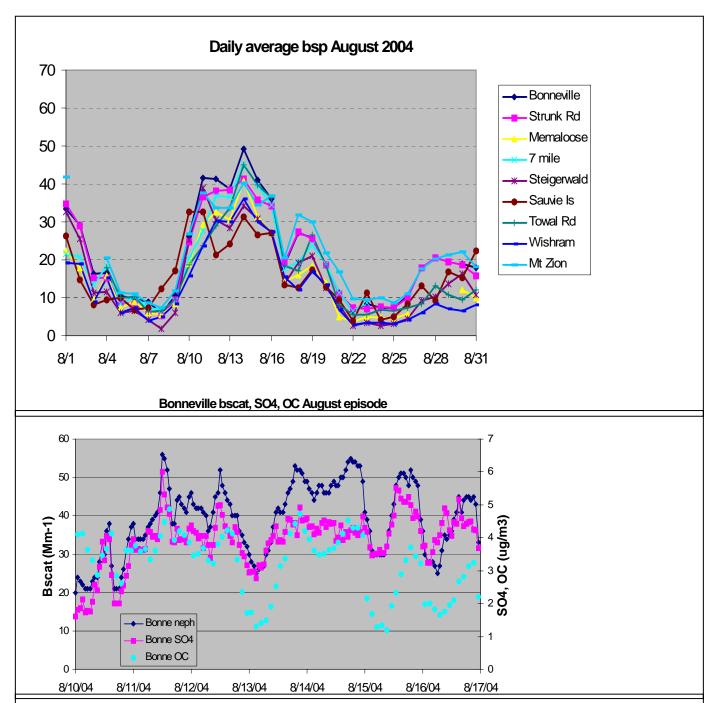


**Figure 3-6b.** Continuous particle light scattering (bsp) (top), sulfate (SO4) (middle) and Organic Carbon (OC) (bottom) at the Bonneville Dam and Mt. Zion sites during July 2004.







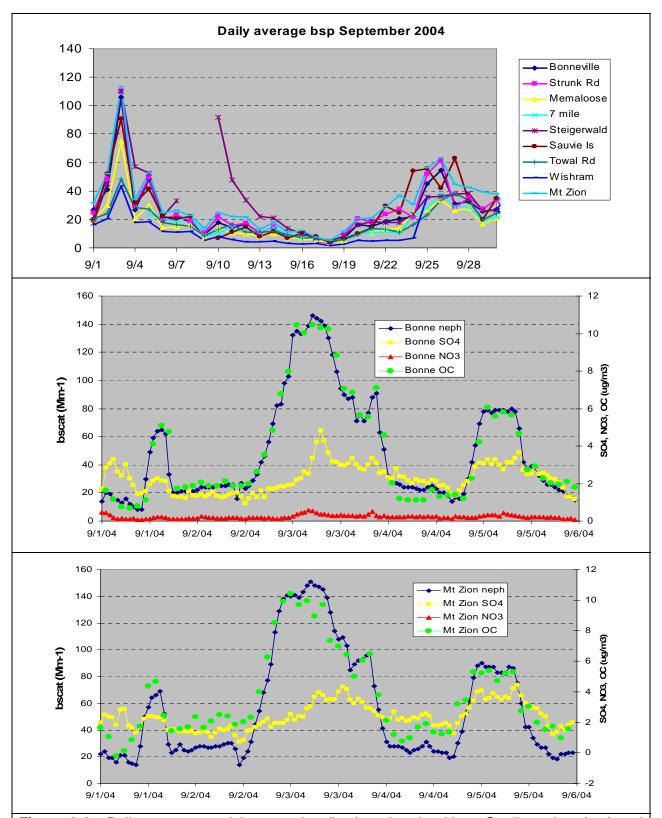


**Figure 3-7.** Daily average particle scattering (bsp) at the nine Haze Gradient sites (top) and continuous bsp, sulfate (SO4), nitrate (NO3) and Organic Carbon (OC) measurements at the Bonneville Dam (bottom) sites for August 2004.









**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.





### 3.3.6 September 1-6 and 24-28, 2004

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

### 3.3.7 Episode Selection and Prioritization

Resources for the Gorge Study modeling component have limited the number of episodes to be addressed to two. Although visibility impairment appears to be greater in the Gorge in the winter than summer, it is important that both seasons be analyzed. Most visitors enjoy the scenic vistas along the Gorge during the summer season.

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
Light Up Gorge	Light up gorge, increasing with	Peak in transition months April and
	distance into gorge	October, more common in winter
		than summer
<ol><li>Moderate Up Gorge</li></ol>	Moderate up gorge, increasing	Late summer- early fall Peak in
	with distance into gorge, large	August, most common cluster
	diurnal variation in speed	August to October
<ol><li>Strong Up Gorge</li></ol>	Strong up gorge, increasing with	Peak in July, most common cluster
	distance into gorge	May-July
4. Light Down Gorge	Light down gorge, except diurnally	Mainly Autumn and Spring (most
	changing direction at eastern	common cluster November),
	sites, up gorge Sauvie Island	uncommon summer
5. Winter Down Gorge	Down gorge, light in eastern end,	Predominantly winter – most
	increasing through gorge, light	common cluster December-
	down at Sauvie Island	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
	1	2	3	4	5	IMPROVE
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 Gorge Study modeling component will address 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 visibility 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 CAMx air quality modeling domain will be contained within in the MM5 domain. The selection of the MM5 domain is described by Johnson (2004). To achieve finer spatial resolution in the Gorge Region we will also use nested higher resolution grids with 12 and 4 km grid spacing.

Both MM5 and 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. It is diffiled domain definition.				
Parameter	Value			
Projection	Lambert-Conformal			
Alpha	33 degrees			
Beta	45 degrees			
x center	97 degrees			
y center	40 degrees			

Table 4-1. RPO unified domain definition.

The MM5 36 km grid includes 164 cells in the east-west dimension and by 128 cells in the north-south dimension. The CAMx 36 km grid will include 148 cells in the east-west dimension and 112 cells in the north-south dimension. Because the MM5 model is provided boundary conditions from the NOAA/NCEP Eta model, there is a possibility of boundary artifacts within MM5 that occur as the Eta-derived boundary conditions 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 CAMx 36 km domain. This is designed to eliminate any potential boundary artifacts from entering into the air quality model. 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, 12, and 4 km grids for both MM5 and CAMx. In Table 4-2 "Dot" refers to the MM5 grid mesh defined at the vertices of the grid cells, while "cross" refers to the MM5 grid mesh defined by the grid cell centers. Thus, the dimension of the dot mesh is equal to the cross mesh plus one. Note that SMOKE and CAMx are defined by grid cells only. Finally, we note that the grid definition for the SMOKE emissions model and CAMx model are identical.





Table 4-2	Grid definitions	for MM5	SMOKE and CAMx.
I abic 4-2.	GIIU UGIII IIIIOI 13	IUI IVIIVIJ.	SIVIONE ALIU CAIVIX.

	Columns	Rows	Xorigin	Yorigin
Model	Dot (cross)	Dot (cross)	(m)	(m)
MM5 36 km	165 (164)	129 (128)	-2952000	-2304000
MM5 12 km	145 (144)	130 (129)	-2700000	108000
MM5 4 km	184 (183)	157 (156)	-2196000	612000
SMOKE/CAMx 36 km	148	112	-2736000	-2088000
SMOKE/CAMx 12 km	131	116	-2640000	168000
SMOKE/CAMx 4 km	146	137	-2164000	644000

### 4.2 Vertical Modeling Domain

The CAMx vertical structure is defined by the vertical grid used in the MM5 modeling. The MM5 model employs a terrain following coordinate system defined by pressure, using 34 layers that extend from the surface to a pressure altitude of 100 mb. Table 4-3 lists the layer definitions for both MM5 and CAMx. A layer aggregation or "collapsing" scheme will be used for CAMx to reduce the computational cost of the air quality simulations. 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 CAMx. In the Gorge Study modeling we will collapse from 34 layers in MM5 output into 19 layers for the CAMx air quality simulations. The first 8 layers of CAMx, up to approximately 450 m AGL, will match the MM5 vertical layer structure exactly. The CAMx model top will be the same as used by MM5, 100mb (approximately 15 km AGL). 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 air quality model simulations were compared to ambient monitoring data (Morris et al., 2004a).

### 4.3 Higher Resolution Modeling Domains

A 12 km higher resolution modeling domain will be nested within the continental US Inter-RPO 36 km domain to 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. Figure 4-1 displays the proposed MM5 36/12/4 km nested grid modeling domains. The SMOKE emissions and 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. The SMOKE/CAMx modeling domains are shown in Figure 4-2. The same vertical grid will be employed for all grids.

#### 4.4 Input Data Availability

The CAMx modeling system requires emissions, meteorological, initial and boundary conditions (IC/BC) and ozone column data for defining the inputs.





**Table 4-3.** Vertical layer definition for MM5 simulations (left most columns), and approach for

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

### 4.4.1 Emissions Data

The base year emissions inventory for the Gorge episodic modeling will be developed by the ODEQ and SWCAA for the states of Oregon and Washington, respectively, based on the 2002 NEI and projected out to 2004. The inventory for the remainder of the domain will be based on the 2002 WRAP emissions, also projected out to 2004. Figure 4-3 lists the counties for which the SWCAA and ODEQ are collecting refined emission estimates for the Gorge study.







**Figure 4-1a.** MM5 36 km (D01), 12 km (D02), and 4 km (D03) nested-grid modeling domains. D04 will not be used in the Gorge visibility modeling study.





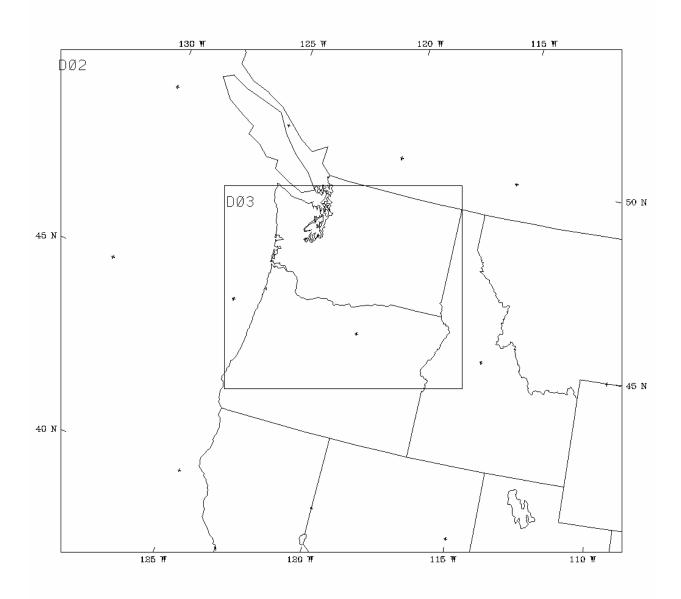
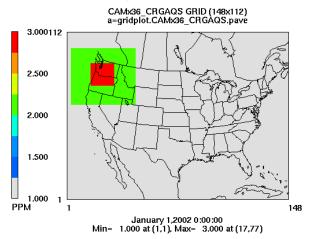


Figure 4-1b. MM5 12 km (D02) and 4 km (D03) nested-grid modeling domains.

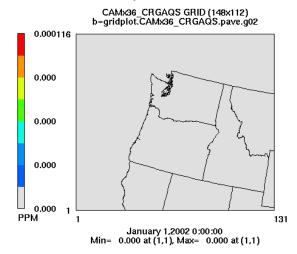




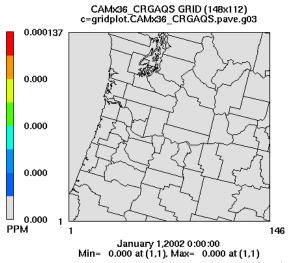
## Layer 1 ALLGRIDSa



### Layer 1 GRID02b



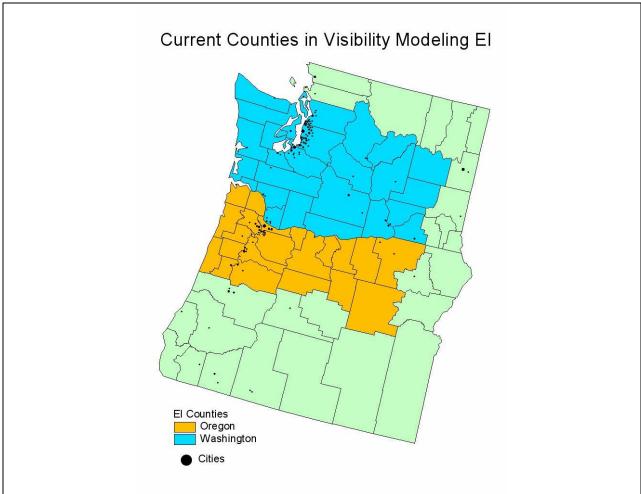
# Layer 1 GRID03c



**Figure 4-2.** SMOKE/CAMx modeling domains for the 36 km (top), 12 km (middle), and 4 km grids.







**Figure 4-3.** Counties where ODEQ and SWCAA are assembling emissions for Gorge Study modeling (Spokane is also included).

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 spatial, 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 surrogate factors developed by the Study Team. Spatial surrogates will be developed from population and landuse distributions provided by EPA (as used in the WRAP modeling). National/continental surrogate fields have been prepared by EPA on a 4-km Lambert Conformal projection grid covering the entire North American continent. These data will be processed to each of the Gorge Study modeling grids for emissions processing. Information and data fields are available from <a href="http://www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html">http://www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html</a>.





For the 36 km grid, we will use the WRAP seasonal 2002 anthropogenic emissions projected to 2004. For biogenic sources, the SMOKE-BEIS-3 module will be run with the MM5 temperature fields to generate day-specific 36 km biogenic emissions for the Gorge modeling episodes. The BELD3 landuse/landcover dataset will be used in the BEIS3 module to define the vegetative cover types over the grid. For the 12/4 km grids, the WRAP 2002 emissions will also be projected to 2004 and used for counties outside the specific OR/WA counties for which local estimates will be provided. Biogenic emissions will be generated using SMOKE-BEIS-3 using grid-specific MM5 temperature fields and the BELD3 landcover data. The SMOKE-MOBILE6 module will be used for on-road mobile sources, coupled with OR/WA specific and/or WRAP activity data (roadway locations, VMT, speed distributions, vehicle fleet mix, etc.).

Volcanic emissions from Mt. St. Helens will be estimated for SO2 and primary PM (ash). A Mt. St. Helens eruption chronology posted at

 $\underline{www.vulcan.wr.usgs.gov/Volcanoes/MSH/Eruption04/Chronology/framework.html}.$ 

Volcanic emissions estimates will be based on three measurements that were performed on 3 November 2004, 10 November 2004, and 12 November 2004. This was a period of increasing geologic activity which resulted in escalating emissions from Mt. St. Helens. Based on conversations with USGS specialists, a simple linear interpolation could be used to estimate emissions for the days in the November episode. According to the USGS, there was no volcanic activity during August 2004; hence, emissions for this episode will be set to zero. The USGS does not estimate emissions of ash, which could be used as a surrogate for PM10. However, given that there was no ash plume activity reported in either November or August 2004, PM emissions will be considered nonexistent. Therefore, only the SO2 emission estimates will be used in this effort.

#### 4.4.2 Air Quality

Data from routine ambient monitoring networks as well as the intensive Gorge Study 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 Study intensive monitoring was described in Chapter 3. Figure 4-4 displays the locations for the routine ambient monitoring sites for all networks except for the Gorge Study network, which contains so many sites they would obscure the other networks.

### 4.4.3 Ozone Column Data

Additional data used in the air quality modeling include ozone column burdens obtained from the Total Ozone Mapping Spectrometer (TOMS). Global TOMS data are available for 24-hour averages and are obtained from <a href="http://toms.gsfc.nasa.gov/eptoms/ep.html">http://toms.gsfc.nasa.gov/eptoms/ep.html</a>. The TOMS data are used in the CAMx (TUV) radiation model to calculate photolysis rates.





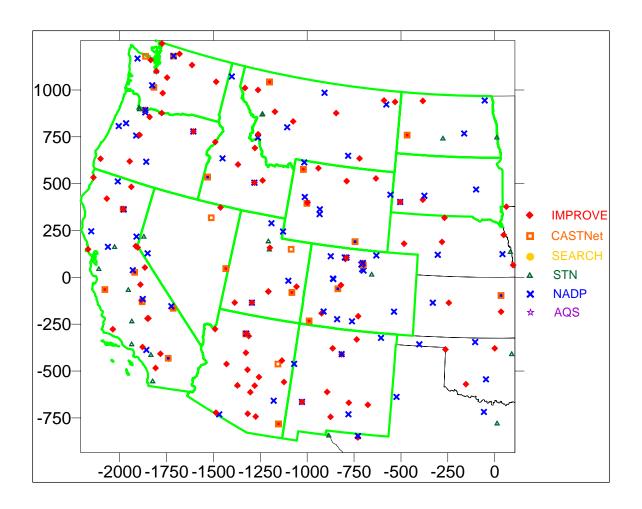
Table 4-4. Overview of routine ambient data monitoring networks.

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/IMPRO VE/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

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

#### 4.4.4 Meteorological Data

Meteorological data will be generated using the MM5 prognostic meteorological model as described in Chapter 2. The MM5CAMx interface program will be used to translate raw MM5 output fields to the CAMx input format requirements, as described in Section 5.

### 4.4.5 Initial and Boundary Conditions Data

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

The 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) 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.

#### 4.4.6 Landuse/Landcover Data

CAMx requires the specification of gridded landuse fields for each grid used in a simulation. The distribution of 11 landuse categories is needed to define dry deposition rates for gas and PM species. This file can be developed independently using landuse datasets developed for either the meteorological modeling or emission processing (i.e., surrogate data). In this project, the MM5CAMx interface program will be used to translate the MM5 landuse fields to the CAMx categories and input formats needed by CAMx.





#### 5.0 MODEL INPUT PREPARATION AND APPLICATION PROCEDURES

In this section we describe the procedures to be used to develop the CAMx model inputs for the Gorge Study visibility modeling episodes. The development of the CAMx meteorological and emissions inputs are discussed first followed by the science options to be used in 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 PSU/NCAR 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. The modeling results in the Gorge using the 4 km grid will be analyzed.

The SMOKE emissions processor requires specific gridded meteorological inputs from MM5, which are processed through the Models-3 Meteorological-Chemical Interface Processor (MCIP). CAMx requires that MM5 output fields be processed to specific meteorological input file formats, which are generated using the MM5CAMx interface processor.

## **5.1.1** MCIP Reformatting Methodology

MCIP version 3.0 will be used to convert the MM5 generated meteorological data to consistent Models-3 I/O API data structures for use in SMOKE. The key functions of MCIP include:

- 1. Reading in meteorological model output files;
- 2. Extracting meteorological data for the domain window;
- 3. Interpolating coarse meteorological model output for finer grids;
- 4. Collapsing meteorological profile data if coarser vertical resolution data is requested;
- 5. Computing or passing through surface and PBL parameters;
- 6. Diagnosing cloud parameters;
- 7. Computing species-specific dry deposition velocities;
- 8. Generating coordinate dependent meteorological data for the generalized coordinate air quality model simulation;
- 9. Outputting meteorological data in Models-3 I/O API format





The MCIP processor transforms the data into I/O API format while also using appropriate diagnostic algorithms to calculate 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 (1.5 m and 10 m, respectively). MCIP is 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. The PBL "pass through" option in MCIP will be used in the Gorge Study modeling. Details on the CAMx modeling domain definitions are provided in Chapter 4.

The Models-3 I/O API meteorological 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

## 5.1.2 MM5 Reformatting Methodology

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

CAMx requires meteorological input data for the parameters described in Table 5-2. All of these input data will be derived from the MM5 results. MM5CAMx performs several functions:

1. Extracts data from the MM5 grids to the corresponding CAMx grids; in this study, the extraction will include a simple one-to-one mapping from the MM5 Lambert Conformal grid to the CAMx Lambert Conformal grid, with appropriate windowing to remove the extra row/columns in the MM5 grids.





**Table 5-2**. CAMx meteorological input data requirements.

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

- 2. Performs mass-weighted vertical aggregation of data for CAMx layers that span multiple MM5 layers.
- 3. Diagnoses key variables that are not directly output by MM5 (e.g., vertical diffusion coefficients and some cloud information).

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

The data prepared by MM5CAMx will be directly input to CAMx. Vertical diffusivities (Kv) are an important input to the CAMx simulation since they determine the rate and depth of mixing in the planetary boundary layer (PBL) and above. In general, our experience has been that diffusivities from meteorological models require careful examination before they are used in air quality modeling. This may be because the air quality model results are much more sensitive to diffusivities than the meteorological model results. We will evaluate the CAMx diffusion inputs by comparing the Kv values from several diagnostic calculation approaches. Two sets of vertical turbulent diffusivity (Kv) files will be generated by MM5CAMx:

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

Sensitivity simulations will be undertaken with the various Kv fields.

#### 5.1.3 Treatment of Minimum K<sub>V</sub>

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<sup>2</sup>/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<sup>2</sup>/s, depending on the amount of urban land use present. We propose to do something similar for CAMx.

MM5CAMx will be operated initially with a  $0.1~\text{m}^2/\text{s}$  value for Kz\_min, however values of  $1.0~\text{m}^2/\text{s}$  will be generated as a sensitivity test. Additional pre-processing of the Kv fields is often





performed to adjust minimum Kv values based on landuse, similarly to the approach used for CMAQ. This will also be undertaken as a sensitivity test in these CAMx base case applications.

## 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 SMOKE set up developed for the WRAP study as the starting point for the Gorge emissions modeling. For the 36, 12, and 4 km grids, the 2002 WRAP anthropogenic emissions will be projected to 2004 and the biogenic and on-road mobile emissions will be updated.

The WRAP projected 2004 emissions will be replaced by local 2004 emissions data provided by SWCAA/ODEQ for several counties in Washington and Oregon (See Section 4, 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 SMOKE processor. Included in these runs will be the temporal, spatial, and speciation profiles and cross-reference data currently provided with SMOKE and augmented with any recommended and approved emission profile data provided by SWCAA, ODEQ, WAECY or others.

## **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 36, 12, and 4 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 on-road mobile source emissions that are generated using BEIS and MOBILE6 modules in SMOKE, respectively, precomputed 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.

Spatial surrogate (allocation factors) will be based on landuse and population fields provided by EPA (as described in Section 4). 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 the 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 parameters for the SMOKE runs are as follows:

Episodes: November 2004 and August 2004 Gorge Study 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

(Longitude: -97, Latitude: 40)

<u>Domain and Layer Structure</u>: 36/12/4 km grids as defined in Section 4 of this protocol

<u>CAMx Model Species</u>: The CAMx configuration will be set 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.

<u>Meteorology Data</u>: Daily (25-hour) MCIP files. These files need to match the grid projection and overlap with the emissions modeling region but can be larger in the horizontal dimensions than the modeling region shown in Section 4.

<u>Elevated Sources</u>: All point 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. To temporally allocate the remaining EGU point sources, the NOx, SO2, and heat input data will be 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. This will ensure that the annual emission values are maintained, but distributed using hourly to annual profiles.

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 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. Whereas the onnetwork 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 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 km predictions.

#### **5.2.7** Other Sources

If the SWCAA or ODEQ provide any emissions from wildfires, prescribed burns, or agricultural burns, they will be processed separately and merged with the final model-ready emissions. All other emission estimates for these sources, and windblown dust and sea salt, will be taken from the WRAP inventory. Volcanic emissions of SO2 from Mt. St. Helens will be estimated from USGS information and processed as a point source.

#### **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 CAMx Mechanism version 4 (CBM-IV, CB-IV or CB4). 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, modified to include planned controls on the Boardman EGU and Camas paper mill, for the Gorge grid structure and modeling episodes.





### **5.2.10** Products of the Emissions Inventory Development Process

In addition to the 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 into CB-IV compounds 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 CAMx Modeling Methodology**

This section describes 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 5-3 summarizes the proposed configuration for CAMx. The latest version of CAMx is currently version 4.31 and is proposed for use in the Gorge Study modeling. However, version 4.40 should be available in time for this application.

### **5.3.1 CAMx Science Components**

The CAMx base configuration will run the 36 km grid 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 entire 36/12/4 km grid structure will be run using two-way nesting. Day-specific 2004 emissions will be used with the 12/4 km grids, but the WRAP 2002 emissions will be used for the 36 km grid. The base configuration of CAMx 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 will 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 m²/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.





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

Model Option	CAMx
Model Version	Version 4.30 (2006)
Horizontal Resolution	36/12/4 km
No. Vertical Layers	19
Horizontal Advection	PPM
Horizontal Diffusion	Spatially Varying
Vertical Diffusion	K <sub>√</sub> (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
Inorganic Aerosol Chemistry	ISORROPIA
Dry Deposition	Wesley
Plume-in-Grid	Off (possibly used in sensitivity tests)
Initial Concentrations	CMAQ Default
Boundary Conditions	Monthly Average Diurnally Varying
	GEOS-CHEM
Emissions	WRAP 2002 augmented by
	SWCAA/ODEQ data for WA and OR

The CAMx chemical Mechanism 4 Course/Fine (CF) approach will be used for the Gorge Study modeling. Mechanism 4 employs an enhanced version of the CB-IV gas-phase chemical mechanism appropriate for regional ozone and PM modeling. Mechanism 4 CF includes the following PM chemistry algorithms: RADM aqueous-phase chemistry; SOAP secondary organic aerosol equilibrium; and ISORROPIA inorganic equilibrium. The CF approach assumes that all secondary PM is in the fine mode, and that the size modes are static.

## 5.3.2 Spin-Up Initialization

For the 2004 episodic CAMx modeling, initial conditions will be set according to CMAQ defaults. Then the model will be exercised for the two Gorge 2004 episodes using a 10 day initialization period on the 36 km grid only, and for the last two spin-up days on the 36/12 km grids.

### **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.





CAMx boundary conditions will utilize the monthly average diurnally-varying BCs described above. The CMAQ-to-CAMx BC processor will be used to process the CMAQ BCON files for input into CAMx.

### **5.3.4** Photolysis Rates

Several chemical reactions in the atmosphere are initiated by the photo-dissociation of various trace gases. To accurately represent the complex chemical transformations in the atmosphere, accurate estimates of these photolysis rates must be made. The CAMx system includes the TUV pre-processor, which calculates a table of clear-sky photolysis rates (or J-values) for a specific date. TUV applies user-defined values for total aerosol loading, satellite-derived column ozone data from TOMS instrumentation, and default surface UV albedo as a function of landuse. The TUV photolysis rates processor will be used to generate the photolysis rates input file for CAMx for the two 2004 Gorge episodes.

TUV produces a "look-up" table provides the photolysis rates as a function of solar zenith angle, altitude, surface UV albedo, ozone column, and haze turbidity. During model calculations, the input photolysis rates for each grid cell are estimated by first interpolating the clear-sky photolysis rates from the look-up table using the grid cell latitude/longitude, altitude, and other environmental parameters, and then applying a cloud correction factor. Photolysis files are ASCII files, and these will be visually checked for selected days to verify that photolysis are within the expected ranges.





#### 6.0 MODEL PERFORMANCE EVALUATION

### 6.1 Overview

This section describes a range of *potential* model testing methodologies that can be performed to adequately evaluate the performance of CAMx for the two 2004 modeling episodes. Since one cannot know at this juncture the specific performance problems that may arise in the 2004 CAMx base case simulations, we set forth in this chapter a broad range of methods and techniques that *may* be brought to bear in examining 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 and subject to available project resources. However, our base effort model performance evaluation is intended to provide a robust assessment of the operational ability of CAMx predict fine particulates and visibility at sites in and around the Columbia River Gorge National Scenic Area.

At a minimum, the evaluation of the CAMx modeling system for this project 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. Emphasis is placed upon assessing: (a) how accurately the model predicts observed concentrations; and (b) how accurately 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 for 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 available time and 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 will depend on how smoothly the integration of other data (e.g., emissions and meteorology) 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 need to be diverted to other activities, then work is dropped on the back end (usually placing limits on the model performance evaluation).

# 6.2 Context for the Gorge Study Model Evaluation

We begin the discussion of the Gorge Study modeling evaluation methodology by reviewing how the 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<sup>1</sup>. 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.

CAMx does not directly estimate visibility, instead it estimates 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:

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

where:

b<sub>ext</sub> is the estimated extinction coefficient (Mm<sup>-1</sup>);

[SO<sub>4</sub>] is the sulfate concentration assumed to be ammonium sulfate;

[NO<sub>3</sub>] 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 ( $< 2.5 \mu m$ ) concentration excluding primary sulfates and nitrates;

[CM] is the coarse particulate (> 2.5 µm and <10 µm) concentration;

b<sub>rayleigh</sub> is the light-scattering due to Rayleigh scattering (assumed to be 10 Mm<sup>-1</sup>);

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.

CAMx model testing will concentrate on an operational evaluation of those model predictions that are most necessary for estimating visibility (e.g., SO<sub>4</sub>, NO<sub>3</sub>, 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 predictions. This evaluation would focus on the Gorge and surrounding areas, and could also be 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 nephelometer 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.

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<sup>&</sup>lt;sup>1</sup> Members of the Gorge Study modeling team participated on the EPA fine particulate modeling work group over the two-year span of its activities.





## **6.3** Multi-Layered Model Testing Process

EPA's "Draft Guidance for Demonstrating Attainment of Air Quality Goals for PM<sub>2.5</sub> 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 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:

<u>Operational Evaluation</u>: 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";

<u>Diagnostic Evaluation:</u> Tests the ability of the model to predict visibility and extinction, PM chemical composition including PM precursors (e.g., SOx, NOx, and NH<sub>3</sub>) 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);

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

<u>Probabilistic Evaluation:</u> 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, efforts 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.

# 6.4 Development of Consistent Evaluation Data Sets

#### **6.4.1 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<sub>2</sub> 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., including: (a) Interagency Monitoring of Protected Visual Environments (IMPROVE), (b) Clean Air Status and Trends Network (CASTNET), (c) EPA PM<sub>2.5</sub> and PM<sub>10</sub> 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<sub>4</sub>, NO<sub>3</sub>, organic carbon (OC), elemental carbon (EC), soil (IP), CM, PM<sub>2.5</sub> and PM<sub>10</sub>. 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 6-1, supplemented with the routine AIRS/AQS data, as appropriate, for CAMx model performance testing.

**Table 6-1**. Ground-level ambient data monitoring networks and stations available in the United States.

States.			
Monitoring Network	Chemical Species Measured	Sampling Frequency; Duration	Approximate Number of Monitors
IMPROVE	Speciated PM <sub>2.5</sub> and PM <sub>10</sub>	1 in 3 days; 24 hr	11
CASTNET	Speciated PM <sub>2.5</sub> , 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 <sub>2.5</sub> )	1 in 3 days; 24 hr	(?)
EPA-STN	Speciated PM <sub>2.5</sub>	Varies; Varies	12
AIRS/AQS	CO, NO, NO <sub>2</sub> , NO <sub>x</sub> , O <sub>3</sub>	Hourly; Hourly	25
EPA-SPEC	Various as part of St. Louis Super Site	Various	1+
GORGE	PM, gaseous, bsp	Various	~20

Another important consideration is that different PM monitoring networks may use different protocols to "measure" different amounts of the same species, which may in turn differ 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. CAMx 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.





### **6.5** 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 Study evaluation of the CAMx modeling system. 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.

#### **6.5.1 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 6-2). 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<sub>2</sub>, SO<sub>2</sub>) we will 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 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 6-2 will be computed for sub-domains 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<sub>2</sub>, CO, SO<sub>2</sub>; 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 6-2 will be calculated for each gas phase species and each fine particulate species in the extinction equation as well as separately for SO<sub>4</sub>, NO<sub>3</sub>, ammonium (NH<sub>4</sub>), EC, OC, bsp, etc. on sub-domains 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 6-2.** 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).

model evaluation with ground-level data (see ENVIRON, 2003b,d for details).  Statistical Shorthand Mathematical				
Measure	Notation	Expression	Notes	
Accuracy of paired peak ( $A_p$ )	Paired_Peak	$rac{P-O_{peak}}{O_{peak}}$	P <sub>peak</sub> = paired (in both time and space) peak prediction	
Coefficient of determination ( <i>r</i> <sup>2</sup> )	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 $P_i$ , $\overline{i}$ =1,2,, $N$ ; $\overline{O}$ = arithmetic average of $O_i$ , $i$ =1,2,, $N$	
Normalized Mean Error ( <i>NME</i> )	Norm_Mean_Err	$rac{\displaystyle\sum_{i=1}^{N}ig P_{i}-O_{i}ig }{\displaystyle\sum_{i=1}^{N}O_{i}}$	Reported as %	
Root Mean Square Error ( <i>RMSE</i> )	Rt_Mean_Sqr_Err	$\left[\frac{1}{N}\sum_{i=1}^{N}(P_{i}-O_{i})^{2}\right]^{\frac{1}{2}}$	Reported as %	
Fractional Gross Error ( <i>F<sub>E</sub></i> )	Frac_Gross_Err	$\frac{2}{N} \sum_{i=1}^{N} \left  \frac{P_i - O_i}{P_i + O_i} \right $	Reported as %	
Mean Absolute Gross Error ( <i>MAGE</i> )	Mean_Abs_G_Err	$\frac{1}{N} \sum_{i=1}^{N} \left  P_i - O_i \right $		
Mean Normalized Gross Error ( <i>MNGE</i> )	Mean_Norm_G_Err	$\frac{1}{N} \sum_{i=1}^{N} \frac{\left  P_i - O_i \right }{O_i}$	Reported as %	





Statistical Measure	Shorthand Notation	Mathematical Expression	Notes
Mean Bias ( <i>MB</i> )	Mean_Bias	$\frac{1}{N} \sum_{i=1}^{N} \left( P_i - O_i \right)$	Reported as concentration (e.g., μg/m³)
Mean Normalized Bias ( <i>MNB</i> )	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, <b>MFB</b> )	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 ( <i>NMB</i> )	Norm_Mean_Bias	$rac{\displaystyle\sum_{i=1}^{N}(P_i-O_i)}{\displaystyle\sum_{i=1}^{N}O_i}$	Reported as %
Bias Factor ( <i>BF</i> )	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).

## **6.5.2** Graphical Representations

The CAMx operational air quality model evaluation will utilize numerous graphical displays to facilitate quantitative and qualitative comparisons between the predictions and measurements. Together with the statistical metrics listed in Table 6-2, 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 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.

# **6.5.3** Probing Tools and Allied Methods

The CAMx operational model evaluation will employ routine operational evaluation methods and standard statistical metrics (Table 6-2) and graphical displays to support the assessment of whether the model is shown to perform with sufficient accuracy and reliably for its intended purpose. Ideally, this operational evaluation will confirm that the modeling system is performing consistently 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 CAMx operational evaluation is completed. 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 CAMx model.

CAMx has 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 are: (a) ozone and particulate source apportionment technology (OSAT/PSAT), (b) process analysis (PA), and (c) the decoupled direct method (DDM) of sensitivity analysis.

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 that has been fully tested and evaluated; it works in a similar manner to OSAT, and tracks source region and category-specific contributions to sulfate, nitrate, organics, and primary PM.

**Decoupled Direct Method (DDM)**: Various forms of the Decoupled Direct Method (DDM) have been installed in 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, (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 in excellent agreement with brute force sensitivities

Process Analysis (PA): Photochemical air quality model simulations are usually evaluated primarily in terms of their ability to simulate observed criteria pollutant 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 ozone and PM formation and their sensitivity to emissions reductions (Arnold et al., 1998). Process analysis is a method for explaining model simulations by adding algorithms to the model 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 ozone, 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 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).

PA is implemented in CAMx, which supports three complementary aspects of the method: (a) the integrated process rate (IPR), (b) integrated reaction rate (IRR) and (c) chemical process analysis (CPA). The integrated sink/source process rates (IPR) and integrated reaction rates (IRR) are stored to a file and can be analyzed using a post-processor. 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<sub>3</sub>, 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 extracted by PA in CAMx.

Because application of all three of these probing tools – source apportionment, DDM, and PA — are computational intensive and require a fair amount of analysis time to reap the benefits of





using the methods, not all will be employed in the current Gorge Study core modeling effort. However, PSAT is considered to provide the most potential for use in addressing potential key issues in the Gorge Study modeling domain where particular attention needs to be focused on emission attribution. Thus, the use of PSAT has been explicitly funded as part of the Gorge Study modeling effort.

# 6.6 Gorge Study 2004 Episodic Model Evaluation Procedures

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

- The ability of the model to replicate observed concentrations of components of PM<sub>2.5</sub>, and total observed mass of PM<sub>2.5</sub>;
- The accuracy of the model in characterizing 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 6.10 we consider the second performance consideration.

## 6.6.1 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<sub>4</sub> and/or S, NH<sub>4</sub>, NO<sub>3</sub>, mass associated with SO<sub>4</sub>, mass associated with NO<sub>3</sub>, elemental carbon (EC), organic carbon (OC), IP, mass of individual constituents of IP, and coarse matter (CM). The *gaseous species* include ozone (O<sub>3</sub>), HNO<sub>3</sub>, NO<sub>2</sub>, PAN, NH<sub>3</sub>, NO<sub>y</sub>, SO<sub>2</sub>, CO, and H<sub>2</sub>O<sub>2</sub>. Key measurements made as part of the Gorge Study monitoring include nephelometer (bsp) and athelometer measurements that measure light scattering and absorption, respectively; these would also be part of the core evaluation effort.

As part of the 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<sub>2</sub>, SO<sub>4</sub>, NO<sub>3</sub>, EC, OC, PM<sub>2.5</sub>, and PM<sub>10</sub>, 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 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<sub>4</sub>/SO<sub>x</sub>).
- 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.
- $\triangleright$  Evaluate for total sulfur (SO<sub>2</sub> + SO<sub>4</sub>), nitrate (HNO<sub>3</sub> + NO<sub>3</sub>) and ammonia (NH<sub>3</sub> + NH<sub>4</sub>).
- ➤ 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<sub>4</sub>, NO<sub>3</sub>, 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 will likely also be used to diagnose performance problems with the





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 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.

## 6.7 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 achieve 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 ( $\leq \pm 20\%$ );
- Mean normalized bias in hourly averaged concentrations ( $\leq \pm 15\%$ ); and
- Mean normalized gross error in hourly concentrations ( $\leq 35\%$ ).

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<sub>3</sub>). 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) identifies particulate matter components of interest to include: SO<sub>4</sub> and/or S, NH<sub>4</sub>, NO<sub>3</sub>, mass associated with SO<sub>4</sub>, mass associated with NO<sub>3</sub>, EC, OC, IP, and mass of individual constituents of inorganic primary particulate matter (i.e., IP). Gaseous pollutants of interest include ozone, HNO<sub>3</sub>, NO<sub>2</sub>, PAN, NH<sub>3</sub>, NO<sub>y</sub>, SO<sub>2</sub>, CO, and H<sub>2</sub>O<sub>2</sub>. 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.

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 <sub>2.5</sub>	~30-50%	~±10%
Sulfate	~30-50%	~±20-30%
Nitrate	~20-70%	~±15-50%
EC	~15-60%	NA
ОС	~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.

# 6.8 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", occasionally 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 episodic CAMx 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.

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. 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 CAMx have already been completed by the model developers and the RPOs. However, given the open community nature of CAMx, 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 CAMx base case. The merits of performing Level II sensitivity testing will depend upon whether performance problems are encountered in the





operational evaluation. 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 CAMx and other models, it is possible to identify examples of sensitivity runs could be useful in model performance improvement exercises with the 2004 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;
- AAAAA Modified EGU emissions;
- Modified ammonia emission estimates.
- Modified aerosol/N<sub>2</sub>O<sub>5</sub>/HNO<sub>3</sub> chemistry; and
- Modified NH<sub>3</sub> and HNO<sub>3</sub> 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 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 (traditional or 'brute force' testing, DDM, and OSAT/PSAT, as described earlier). Only the PSAT approach is specifically funded for the Gorge Study modeling. 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 6.9 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<sub>2</sub> emissions;
- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to elevated point source NO<sub>x</sub> emissions;
- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to ground level NO<sub>x</sub> emissions; and
- Sulfate, nitrate, ammonium and other aerosol sensitivities to ammonia.

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.





# 6.9 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.

### **6.9.1** Corroborative Models

Noteworthy in EPA's new ozone, PM, and regional haze guidance documents are 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, the use of both CMAQ and CAMx could be carried through the study from base case development through 2018 future-year modeling if additional funding was made available. Among other things, this would permit more explicit identification of 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.

## 6.9.2 Weight of Evidence Analyses

EPA's guidance recommends three general types of "weight of evidence" (WOE) 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 WOE 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. Nonetheless, we outline below our thoughts regarding what would likely be considered should the operational CAMx model evaluation need to be bolstered with WOE analyses and additional funding is made available.

<u>Use of Emissions and Air Quality Trends.</u> A limited scope emissions and trend analysis could be employed to support the WOE 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 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 would 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 sub-regions may be VOC-limited or NOx-limited, for example, or where controls on ammonia or SO2 emissions might be most influential in reducing PM<sub>2.5</sub>. 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 CoHaGo component of the Gorge Study should provide useful information to address this.

# 6.10 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<sub>z</sub>/NO<sub>y</sub>]; and
- $\triangleright$  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 CAMx predictions for secondary aerosols would doubtless be quite challenging, but the use of indicator species (e.g., ammonia or HNO<sub>3</sub> 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 CAMx model evaluation, we will remain alert to opportunities to extend the indicator species ratio analyses to the problem of fine particulate and visibility.





## 7.0 MODELING SCENARIOS

The Gorge Study modeling will include 2004 base year and 2018 future-year simulations for both August and November episodes to forecast expected visibility changes in the Gorge due to anticipated changes in emissions. Additionally, the PSAT probing tool will be employed for both 2004 base and 2018 future year runs, and up to five "what if" scenarios will be undertaken for the 2018 future year.

# 7.1 Base Modeling Scenarios

The core modeling effort for the Gorge Study will include a 2004 Base Case and 2018 On-the-Books (OTB) Base Case (with additional planned controls for the Boardman EGU and the Camas paper mill) using the CAMx model. Changes in PM species concentrations and visibility will be analyzed. 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.

## 7.2 Alternative Analyses

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

## 7.2.1 Emission Sensitivity Tests

The modeling team has been funded to perform five "what-if" scenarios applied to the 2018 future year emissions inventory. The exact set of scenarios will be selected at a later time. The list below provides the potential types of scenarios that could be investigated:

- Boardman Electrical Generating Unit (EGU)
  - o Apply BART level of controls
  - o Eliminate Emissions
- Three Mile Canyon Farm
  - o Control emissions by some level
  - o Eliminate emissions
  - o 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





## **7.2.2** Use of PSAT Probing Tools

As discussed in Chapter 7, CAMx posseses a set of "Probing Tools" that can extract detailed information on model sensitivity and source-receptor relationships from the model. Of particular note is the PM Source Apportionment Technology (PSAT) that tracks source category and source region-specific contributions to sulfate, nitrate, organics, and primary PM over the entire modeling grid. Thus, source attribution for speciated and total PM (and visibility) can be determined at specific monitoring site locations. For example, PSAT could be set up to obtain 2004 and 2018 attributions for all of the emission sources listed in Section 7.2.1 in a single run.

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

### Low-level emissions:

- Biogenics
- Area (minus woodstoves)
- On-road mobile
- Non-road mobile
- River shipping
- Railroads
- Ammonia sources (dairies, CAFO, fertilizer)
- Woodstove residential heating

## Elevated (point) emissions:

- EGU
- Non-EGU
- Pulp Mills
- Lumber mills
- Wild Fires
- Other Fires

### The regions to consider are:

- In Gorge
- Portland/Vancouver metro (by county)
- Morrow County
- East of Gorge (minus Morrow)
- NW of Portland/Vancouver (downriver sources)
- Willamette Valley
- TriCities/Spokane

The PSAT probing tool will be used to evaluate source apportionment to sulfate, nitrates, primary PM, and/or organics for both the 2004 and 2018 years. Selection of specific source categories and regions to be tracked will be determined at a later time.





#### 8.0 DOCUMENTATION

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

### 8.1 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 memoranda, interim and final reports that describe the methodologies and results of the model performance evaluation, model intercomparison, and visibility assessment will be provided. Table 8-1 below lists the current schedule of deliverables under the Gorge Study modeling and analysis study.

**Table 8-1.** 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	September 2006
Task 2. MM5 Meteorological Modeling	
MM5 Evaluation PPT Presentation	May – August 2006
MM5 Processed for CAMx	August 2006
Task 3. SMOKE Emissions Modeling	
Emissions Summary Presentation (PPT)	August 2006
Model-ready 2004 emission inputs	September 2006
Task 4. CAMx Air Quality Modeling	
Presentation on 2004 Base Case Modeling and Model	September 2006
Performance Evaluation	
Presentation on 2018 Modeling Results	October 2006
Source Apportionment and Model Sensitivity (e.g., "What	October – November 2006
if") Simulations	
Presentation on Future Year, Source Apportionment,	November 2006
and "What if" Simulations	
Task 5. Reporting	
Monthly progress reports and invoices	3rd week of following month
Draft Final Report	November 2006
Final Report	January 2007

# 8.2 Technology Transfer

All final model inputs and major model outputs, job scripts, and models will be provided to SWCAA or it's designate on IDE hard drives for subsequent distribution. These drives can be hooked up to a drive kit that is Firewire and/or USB compatible for external connection (hot), or can be plugged into an internal PC hard disk slot. The ENVIRON/Alpine Team will be available to answer questions from the SWCAA staff and it's designates as needed. Current resource constraints will preclude any on-site, hands-on training for model use, analysis, or interpretation.





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