Appendix F

CENRAP Technical Support Document

Draft Report

Technical Support Document for CENRAP Emissions and Air Quality Modeling to Support Regional Haze State Implementation Plans

Prepared for:
Central Regional Air Planning Association
10005 S. Pennsylvania, Suite C
Oklahoma City, OK 73159

Prepared by:
ENVIRON International Corporation
101 Rowland Way, Suite 220
Novato, CA 94945

and

University of California at Riverside
College of Engineering Center for
Environmental Research and Technology
Riverside, Ca 92517

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1.0 INTRODUCTION

This Technical Support Document (TSD) describes the Central Regional Air Planning Association (CENRAP) regional emissions and air quality modeling to support the central states Regional Haze Rule (RHR) State Implementation Plans (SIPs). The CENRAP 2002 annual emissions and air quality modeling was performed by the contractor team of ENVIRON International Corporation (ENVIRON) and the University of California at Riverside (UCR).

1.1 Background

The 1977 Clean Air Act Amendments (CAAA) added a new Section 169A for the protection of visibility in Federal Class I areas (specific national parks, wilderness areas and wildlife refuges). Section 169A(a)(1) of the CAAA established the national goal for visibility protection: "Congress hereby declares as a national goal the prevention of any future, and the remedying of any existing, impairment of visibility in mandatory class I Federal areas which impairment results from manmade air pollution." The CAAA require States to submit SIPs containing emission limits, schedules of compliance and to "promulgate regulations to assure reasonable progress toward meeting the national goal" (Section 169A(a)(4)). In response to these mandates EPA promulgated the Regional Haze Rule (RHR) on July 1, 1999 that requires States to "establish goals (expressed in deciviews) that provide for reasonable progress towards achieving natural visibility conditions" at Class I areas. The States' RHR SIPs are due December 17, 2007 and an important component of the SIP will be the 2018 Reasonable Progress Goals (RPGs) toward achieving natural conditions in 2064. Regional air quality models are used to project visibility to 2018 to determine the level of visibility improvement that is expected to be achieved in 2018. This information, along with other sources, can be used by the states to assist in setting their 2018 RPGs.

CENRAP is one of five Regional Planning Organizations (RPOs) that have responsibility for coordinating development of SIPs and Tribal Implementation Plans (TIPs) in selected areas of the U.S. to address the requirements of the RHR. CENRAP is a regional partnership of states, tribes, federal agencies, stakeholders and citizen groups established to initiate and coordinate activities associated with the management of regional haze and other air quality issues within the CENRAP states. The CENRAP region includes states and tribal lands located within the boundaries of Arkansas, Iowa, Kansas, Louisiana, Minnesota, Missouri, Nebraska, Oklahoma and Texas.

The CENRAP Emissions and Air Quality Modeling Team is composed of staff from ENVIRON and UCR, with assistance and coordination from the CENRAP states, tribes, federal agencies and stakeholders. The ENVIRON/UCR Team performs the emissions and air quality modeling simulations for states and tribes within the CENRAP region, providing analytical results used in developing implementation plans under the RHR. Figure 1-1 shows the states included in each of the five RPOs in the U.S., including CENRAP. Table 1-1 lists the Class I areas within the CENRAP states.

CENRAP is performing emissions and air quality modeling to project visibility to 2018. The modeling results will be used to determine the level of visibility improvement expected in 2018 under various emission scenarios. States will use these results to assist in determining their 2018 RPGs toward achieving natural conditions in 2064.

Figure 1-1. Regional Planning Organizations engaged in Regional Haze Modeling.

Table 1-1. Federal Mandated Class I Areas in the CENRAP States.

Class I Area	Acreage	Federal Land Manager	Public Law
Arkansas			
Caney Creek Wilderness Area	14,460	USDA-FS	93-622
Upper Buffalo Wilderness Area	12,018	USDA-FS	93-622
Louisiana			
Breton Wilderness Area	5,000+	USDI-FWS	93-632
Minnesota			
Boundary Waters Canoe Area Wilderness	810,088	USDA-FS	99-577
Voyageurs National Park	114,964	USDI-NP	99-261
Missouri			
Hercules-Glade Wilderness Area	12,314	USDA-FS	94-557
Mingo Wilderness Area	8,000	USDI-FWS	95-557
Oklahoma			
Wichita Mountains Wilderness	8,900	USDI-FWS	91-504
Texas			
Big Bend National Park	708,118	USDI-NP	74-157
Guadalupe Mountains National Park	76,292	USDI-NP	89-667

1.2 CENRAP Organizational Structure and Work Groups

The governing body of CENRAP is the Policy Oversight Group (POG) that is made up of voting members representing states and tribes within the CENRAP region and non-voting members representing local agencies, the EPA and other federal agencies. The work of CENRAP is accomplished through five standing workgroups:

- Monitoring;
- Emissions Inventory;
- Modeling;
- Communications; and
- Implementation and Control Strategies.

Participation in workgroups is open to all interested parties and the POG may form additional ad hoc workgroups to address specific issues (e.g., a Data Analysis workgroup was formed).

The RHR requires the states, and the tribes that may elect to, submit the first SIPs and TIPs that address progress toward natural conditions at federally mandated Class I areas by December 17, 2007. 40 CFR 51.308 (Section 308) discusses the following four core requirements to be included in SIPs/TIPs and Best Available Retrofit Technology (BART) requirements:

1. Reasonable progress goals;
2. Calculations of baseline and natural visibility conditions;
3. A Long-term strategy for regional haze;
4. A Monitoring strategy and other implementation plan requirements; and
5. BART requirements for regional haze visibility impairment.

One of CENRAP's goals is to provide support to states and tribes to meet each of these requirements of the RHR and to develop scientifically supportable, economical and effective control strategies that the states and tribes may adopt to reduce anthropogenic effects on visibility impairment at Class I areas. One component of CENRAP's support to states and tribes as part of compliance with the RHR is performing emissions and air quality modeling. These activities were implemented to:

- obtain a better understanding of the causes of visibility impairment and to identify potential mitigation measures for visibility impairment at Class I areas;
- to evaluate the effects of alternative control strategies for improving visibility; and
- to project future-year air quality and visibility conditions.

In October 2004, CENRAP selected the team of ENVIRON and UCR to perform their Emissions and Air Quality Modeling.

The CENRAP Emissions and Air Quality Modeling Team performs regional haze analyses by operating regional scale, three-dimensional air quality models that simulate the emissions, chemical transformations, and transport of gaseous and particulate matter (PM) species and consequently the effects on visibility in Class I Areas in the central U.S. A key element of this work includes the integration of emissions inventories and emissions models with regional transport models. The general services provided by the CENRAP Emissions and Air Quality Modeling Team include, but are not limited to:

- Emissions processing and modeling;
- Air quality and visibility modeling simulations;
- Analysis, display, and reporting of modeling results; and
- Storage/quality assurance of the modeling input and output files.

The CENRAP 2002 annual Emissions and Air Quality Modeling Team performs work for the CENRAP Modeling Workgroup through direction from the CENRAP Technical Director and CENRAP Executive Director.

1.3 Overview of 2002 Annual Emissions and Air Quality Modeling Approach

The CENRAP 2002 annual emissions and air quality modeling was initiated on October 16, 2004 and involved the preparation of numerous databases, model simulations, presentations and reports. Much of the modeling analyses have been posted to the CENRAP modeling website at: http://pah.cert.ucr.edu/aqm/cenrap/index.shtml. There were numerous versions and iterations of the modeling and interim results. The results presented in this TSD focus on the final modeling results and key findings in their development. The reader is referred to the modeling website for interim products.

1.3.1 Modeling Protocol

A Modeling Protocol was prepared at the outset of the study to serve as a road map for performing the CENRAP emissions and air quality modeling and to communicate the modeling plans to the CENRAP participants. The Modeling Protocol was prepared following EPA guidance for preparation at the time it was prepared (EPA, 1991; 1999, 2001) and took into account CENRAP's long-term plan (CENRAP, 2003) and the modeling needs of the RHR SIPs. The first version (Version 1.0) of the Modeling Protocol was dated November 19, 2004. Based on comments received from CENRAP, the Modeling Protocol was updated to the current Version 2.0 (Morris et al., 2004a) that was dated December 8, 2004. This Modeling Protocol can be found on the CENRAP modeling Website at:

http://pah.cert.ucr.edu/aqm/cenrap/docs/CENRAP_Draft2.0_Modeling_Protocol_120804.pdf

1.3.2 Quality Assurance Project Plan (QAPP)

A Quality Assurance Project Plan (QAPP) was prepared for the CENRAP emissions and air quality modeling study that described the quality management functions performed by the modeling team. The QAPP was prepared and was based on the national consensus standards for quality assurance (ANSI/ASQC, 1994), followed EPA's guidelines for quality assurance project plans for modeling (EPA, 2002) and for QAPPs (EPA, 2001) and took into account the recommendations from the North American Research Strategy for Tropospheric Ozone (NARSTO) Quality Handbook for modeling projects (NARSTO, 1998). The EPA and NARSTO guidance documents were developed specifically for modeling projects, which have different quality assurance concerns than environmental monitoring data collection projects. The work performed in this project involves modeling at the basic research level and for regulatory/planning applications. In order to use model outputs for these purposes, it must be established that each model is scientifically sound, robust, and defensible. This is accomplished by following a project planning process that incorporates the following elements as described in the EPA modeling guidance document:

- A systematic planning process including identification of assessments and related performance criteria;
- Peer reviewed theory and equations;
- A carefully designed life-cycle development process that minimizes errors;
- Documentation of any changes from original plans;
- Clear documentation of assumptions, theory, and parameterization that is detailed enough so others can understand the model output;
- Input data and parameters that are accurate and appropriate for the analysis; and
- Output data that can be used to help inform decision makers.

The CENRAP QAPP can be found at:

http://pah.cert.ucr.edu/aqm/cenrap/docs/CENRAP_QAPP_Nov_24_2004.pdf).

A key component of the CENRAP emissions and air quality modeling QAPP was the graphical display of model inputs and outputs and multiple peer-review of each step of the modeling process. This was accomplished through use of the CENRAP modeling website where modelers posted displays of work products (e.g., emissions plots, model outputs, etc.) for review by the CENRAP modeling team, modeling workgroup and others. This website can be found at: http://pah.cert.ucr.edu/aqm/cenrap/index.shtml.

1.3.3 Model Selection

The selection of the meteorological, emissions and air quality models for the CENRAP regional haze modeling was based on a review of previous regional haze modeling studies performed in the CENRAP region (e.g., Pitchford et al., 2004; Pun, Chen and Seigneur, 2004; Tonnesen and Morris 2004) as well as elsewhere in the United States (e.g., Morris et al, 2004a; Tonnesen et al., 2003; Baker, 2004). The CENRAP emissions and air quality Modeling Protocol (Morris et al., 2004a) provides details on the justification for model selection and the formulation of the different models. Based on previous work (e.g., CENRAP, WRAP, VISTAS, MRPO, BRAVO and EPA), CENRAP selected the following models for use in modeling PM and regional haze in the central states:

- **MM5:** The Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Meteorological Model (MM5 Version 3.6 MPP) is a non-hydrostatic, prognostic meteorological model routinely used for urban- and regional-scale photochemical, fine particulate, and regional haze regulatory modeling studies (Anthes and Warner, 1978; Chen and Dudhia, 2001; Stauffer and Seaman, 1990, 1991; Xiu and Pleim, 2000).

- **SMOKE**: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is an emissions modeling system that generates hourly gridded speciated emission inputs of mobile, non-road, area, point, fire and biogenic emission sources for photochemical grid models. (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 tool for converting an existing base emissions inventory data into the hourly, gridded, speciated, and formatted emission files required by an air quality model.

- **CMAQ:** EPA's Models-3/Community Multiscale Air Quality (CMAQ) modeling system is a 'One-Atmosphere' photochemical grid model capable of addressing ozone, PM, visibility and acid deposition at a regional scale for extended periods of time (Dennis, et al., 1996; Byun et al., 1998a; Byun and Ching, 1999, Pleim et al., 2003).

- **CAMx:** ENVIRON's Comprehensive Air Quality Model with Extensions (CAMx) modeling system is also a state-of-science 'One-Atmosphere' photochemical grid model capable of addressing ozone, PM, visibility and acid deposition at a regional scale for extended periods of time. (ENVIRON, 2006).

1.3.3.1 MM5 Meteorological Model Configuration for CENRAP Annual Modeling

Application of the MM5 for the 2002 annual modeling on a 36 km grid for the continental US was performed by the Iowa Department of Natural Resources (IDNR; Johnson, 2007). Details of the 2002 36 km MM5 model application and evaluation procedures carried out by IDNR may be found in Johnson, 2007. Application of the MM5 model on a 12 km grid covering the Central States for portions of 2002 was performed by EPA Region VII and the Texas Commission on Environmental Quality (TCEQ).

The MM5 (Version 3.63) configuration used in the generation of the meteorological modeling datasets consists of the following (see Table 1-2 for more details):

- 36 km grid with 34 vertical layers;
- 12 km nested grid for episodic modeling;
- For 12 km runs use two way nesting (without feedback) within the 36 km grid;
- Initialization and boundary conditions from Eta analysis fields;
  - Eta 3D and surface analysis data (ds609.2);
  - Not using NCEP global tropospheric SST data (ds083.0) ;
  - Observational enhancement (LITTLE_R)
    - NCEP ADP surface obs (ds464.0)
    - NCEP ADP upper-air obs (ds353.4)
- Pleim-Xiu (P-X) land-surface model (LSM);
- Pleim-Chang Asymmetric Convective Mixing (ACM) PBL model;
- Kain-Fritsch 2 cumulus parameterization;
- Mixed phase (Reisner 1) cloud microphysics;
- Rapid Radiative Transfer Model (RRTM) radiation;
- No Shallow Convection (ISHALLO=0);
- Standard 3D FDDA analysis nudging outside of PBL; and
- Surface nudging of the winds only.

1.3.3.2 SMOKE Emissions Model Configuration for CENRAP Annual Modeling

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

As an emissions processing system, SMOKE has far fewer 'science configuration' options compared with the MM5 and CMAQ models. Table 1-3 summarizes the version of the SMOKE system that was used and the sources of data that were employed in constructing the required modeling inventories.

1.3.3.3 CMAQ Air Quality Model Configuration for CENRAP Annual Modeling

CENRAP used CMAQ Version 4.5 with the "SOAmods enhancement", described below, and used the model configuration as shown in Table 1-4. The model was set up and exercised on the same 36 km grid that was used by WRAP and VISTAS, the 36 km RPO national grid. CENRAP performed 12 km CMAQ sensitivity tests and found little change in model performance with a large penalty in computation time. Consequently, at the February 7, 2006 CENRAP Modeling

Workgroup Meeting a decision was made to proceed with the CENRAP emissions and air quality modeling using just the 36 km national RPO grid (Morris et al., 2006a).

Initial CMAQ 2002 simulations performed by VISTAS found that the model greatly underestimates organic mass carbon (OMC) concentrations, especially in the summer. A review of the CMAQ formulation found that it failed to treat Secondary Organic Aerosol (SOA) formation from sesquiterpenes and isoprene and also failed to account for the fact that SOA can become polymerized so that it is no longer volatile and stays in the particle form. Thus, VISTAS updated the CMAQ SOA module to include these missing processes and found much improved OMC model performance (Morris et al., 2006c). CENRAP tested the CMAQ Version 4.5 with SOAmods enhancement and found it performed much better for OMC than the standard versions of CMAQ Version 4.5. Therefore, CMAQ Version 4.5, with the enhanced SOAmods (Morris et al., 2006c), was adopted for the CENRAP modeling. CMAQ Version 4.5 is available from the CMAS center (www.cmascenter.org).

1.3.3.4 CAMx Air Quality Model Configuration for CENRAP Annual Modeling

CAMx Version 4.40 was applied using similar options as used by CMAQ. CAMx was used initially in side-by-side comparisons with CMAQ. Comparative model performance results and other factors for CAMx V4 and CMAQ V4.4 with SOAmods were presented at the February 7, 2006 CENRAP modeling workgroup meetings that found (Morris et al., 2006b):

- No one model was consistently performing better than the other over all species and averaging times.
- Both models performed well for sulfate.
- CMAQ's winter nitrate over-prediction tendency not as large as CAMx's.
- CAMx performed slightly better than CMAQ for elemental carbon (EC).
- CMAQ performed much better than CAMx for organic mass carbon (OMC).
- Both models over-predicted Soil and under-predicted coarse mass (CM).
- CMAQ ran faster than CAMx due to MPI multi-processing capability.
- CAMx required much less disk space than CMAQ.

Based on these factors, CMAQ was selected as the lead air quality model for the CENRAP regional haze modeling with CAMx the secondary corroborative model. However, CAMx also contained a PM Source Apportionment Technology (PSAT) capability that was used widely in the CENRAP modeling. Table 1-4 lists the main CAMx configuration used for the CENRAP annual modeling that was selected, in part, to be consistent with the CMAQ model configuration (Table 1-4). One exception to this was that the CAMx PSAT simulations used the Bott advection solver rather than the PPM advection solver. The PPM advection solver is typically used in the standard CAMx and CMAQ runs. Bott, however, is more computationally efficient and the high computational requirements of the CAMx PSAT runs dictated this choice.

Table 1-2. MM5 Meteorological Model Configuration for CENRAP 2002 Annual Modeling (Johnson, 2007).

Science Options	Configuration	Details/Comments
Model Code	MM5 version 3.63	Grell et al., 1994
Horizontal Grid Mesh	36 km	
36 km grid	165 x 129 dot points	RPO MM5 Grid
Vertical Grid Mesh	34 layers	Vertically varying; sigma pressure coordinate system
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
Planetary Boundary Layer	ACM PBL	
Radiation	RRTM	
Vegetation Data	USGS	24 Category Scheme
Land Surface Model	Pleim-Xiu Land Surface Model (LSM)	
Shallow Convection	None	
Sea Surface Temperature	Eta Skin	Spatially varying
Thermal Roughness	Garratt	
Snow Cover Effects	None	
4D Data Assimilation	Analysis Nudging on 36 and 12	
Surface Nudging	Wind Field Only	
Integration Time Step	90 seconds	
Simulation Periods	Annual 2002 for 36 km	12 km episodic only
Platform	Linux Cluster	Done at IDNR[1]

[1] Twelve km episodic modeling completed by EPA Region VII and the Texas Commission on Environmental Quality.

Table 1-3. SMOKE Emissions Model Configuration for CENRAP Annual Modeling.

Emissions Component	Configuration	Details/Comments
Emissions Model	SMOKE Version 2.3	Several versions of SMOKE used during course of the study
Horizontal Grid Mesh	36 km	
36 km grid	148 x 112 cells	RPO National Grid
Area Source Emissions	CENRAP Domain: CENRAP State 2002 EI	Updated '02 developed by CENRAP states (Pechan, 2005d,e)
	Other States: '02 NEI augmented with other 2002	Generated from EPA NEI02 v.1 and RPO interaction (Pechan, 2005c)
On-Road Mobile Sources	CENRAP Domain: CENRAP VMT data	Updated '02 developed by CENRAP states (Reid et al., 2004a)
	Other States: EPA '02 NEI augmented with other 2002	Generated from EPA NEI02 v.1 and RPO interaction (Pechan, 2005c)
Point Sources	CENRAP Domain: CENRAP State 2002 EI	Updated '02 developed by CENRAP states and stakeholders (Pechan, 2005a,b)
	Other States: EPA '02 NEI augmented with other 2002	Generated from EPA NEI02 v.1 and RPO interaction (Pechan, 2005c)
Off-Road Mobile Sources	CENRAP Domain: CENRAP State 2002 EI	Updated '02 developed by CENRAP states (Pechan, 2005d,e)
	Other States: EPA '02 NEI augmented with other 2002	Generated from EPA NEI02 v.1 and RPO interaction (Pechan, 2005c)
Biogenic Sources	SMOKE BEIS-3	BELD3 vegetative database
Mexican Sources	1999 Emissions for 2002 and 2018	http://www.epa.gov/ttn/chief/net/mexico.html; (ERG, 2006)
Canadian Sources	2000 Emissions for 2002 and 2020 Emissions for 2018	http://www.epa.gov/ttn/chief/net/canada.html
Temporal Adjustments	Seasonal, day, hour	Based on latest collected information and CEM-based profiles
Chemical Speciation	Revised CBM-IV Chemical Speciation	Updated January 2004
Gridding	Revised EPA Spatial Surrogates Used	Gridding of surrogates from http://www.epa.gov/ttn/chief/emch/spatial/
Growth and Controls	CENRAP developed	Pechan (2005a,b)
Quality Assurance	QA Tools in SMOKE 2.0	Follow QAPP (Morris and Tonnesen, 2004) and QA refinements (Morris and Tonnesen, 2006)
Simulation Periods	Annual 2002 for 36 km	Episodic periods at 12 km

Table 1-4. CMAQ Air Quality Model Configuration for CENRAP Annual Modeling.

Science Options	Configuration	Details/Comments
Model Code	CMAQ Version 4.5 w/ SOAmods	Secondary Organic Aerosol enhancements as described by Morris et al., (2006c)
Horizontal Grid Mesh	36 km annual	36 km covering continental U.S; some episodic 12 km sensitivity runs were also performed
36 km grid	148 x 112 cells	RPO National Grid
Vertical Grid Mesh	19 Layers	First 17 layers sync'd w/ MM5
Grid Interaction	One-way nesting	
Initial Conditions	~15 days full spin-up	Separately run 4 quarters of 2002
Boundary Conditions	2002 GEOS-CHEM day-specific	2002 GEOS-CHEM day specific 3-hour average data
Emissions		
Baseline Emissions Processing	See SMOKE model configuration	MM5 Meteorology input to SMOKE, CMAQ
Sub-grid-scale Plumes	No Plume-in-Grid (PinG)	
Chemistry		
Gas Phase Chemistry	CBM-IV	
Aerosol Chemistry	AE3/ISORROPIA	
Secondary Organic Aerosols	Secondary Organic Aerosol Model (SORGAM) w/ SOAmods update	Schell et al., (2001); Morris et al., (2006c)
Cloud Chemistry	RADM-type aqueous chemistry	Includes subgrid cloud processes
N2O5 Reaction Probability	0.01 – 0.001	
Meteorological Processor	MCIP Version 2.3	Includes dry deposition and snow cover updates
Horizontal Transport		
Numerical Scheme	PPM advection solver	
Eddy Diffusivity Scheme	K-theory with Kh grid size dependence	Multiscale Smagorinsky (1963) approach
Vertical Transport		
Eddy Diffusivity Scheme	K-theory	
Diffusivity Lower Limit	Kzmin = 0.1 to 1.0	Land use dependent Kzmin
Deposition Scheme	M3dry	Directly linked to Pleim-Xiu Land Surface Model parameters
Numerics		
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) solver	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme	
Simulation Periods	Annual 2002 for 36 km	Episodic periods at 12 km
Integration Time Step	Calculated Internally	15 minute coupling time step

Table 1-5. CAMx Air Quality Model Configuration for CENRAP Annual Modeling.

Science Options	Configuration	Details
Model Code	CAMx Version 4.40	Available at: www.camx.com
Horizontal Grid Mesh	36 km annual	36 km covering continental U.S
36 km grid	148 x 112 cells	
Vertical Grid Mesh	19 Layers	17 Layers sync'd w/ MM5
Grid Interaction	Two-way nesting	
Initial Conditions	~15 days full spin-up	Separately run 4 quarters of 2002
Boundary Conditions	2002 GEOS-CHEM day-specific	2002 GEOS-CHEM day specific 3-hour average data
Emissions		
Baseline Emissions Processing	See SMOKE model configuration	MM5 Meteorology input to SMOKE, CAMx
Sub-grid-scale Plumes	No Plume-in-Grid (PinG)	Consistent with CMAQ
Chemistry		
Gas Phase Chemistry	CBM-IV	with Isoprene updates
Aerosol Chemistry	ISORROPIA equilibrium	Dynamic and hybrid also available but not used
Secondary Organic Aerosols	SOAP	
Cloud Chemistry	RADM-type aqueous chemistry	Alternative is CMU multi-section aqueous chemistry
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 = 0.1 to 1.0	Land use dependent Kzmin
Planetary Boundary Layer	No Patch	
Deposition Scheme	Wesely	
Numerics		
Gas Phase Chemistry Solver	CMC Fast Solver	
Horizontal Advection Scheme	Piecewise Parabolic Method (PPM) scheme. PSAT w/ Bott scheme.	
Simulation Periods	Annual 2002 at 36 km	
Integration Time Step	Wind speed dependent	

1.3.4 Modeling Domains

The CENRAP emissions and air quality modeling was conducted on the 36 km national RPO domain as depicted in Figure 1-2. This domain consists of a 148 by 112 array of 36 km by 36 km grid cells and covers the continental United States. Sensitivity simulations were also performed for episodes on a 12 km modeling domain covering the central states, however the results were very similar to the 36 km results so CENRAP elected to proceed with the 2002 annual modeling using the 36 km domain for computational efficiency (Morris et al., 2006a).

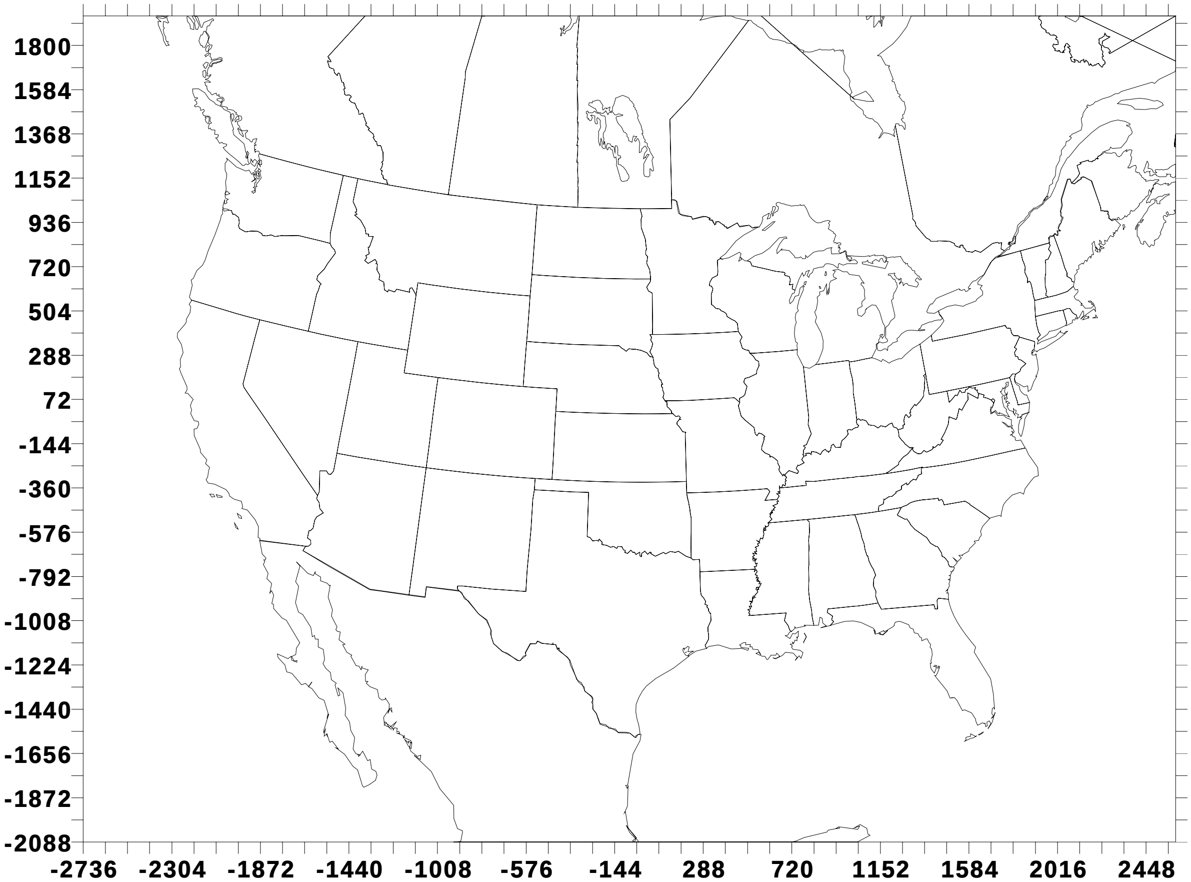

Figure 1-2. National Inter-RPO 36 km modeling domain used for the CENRAP 2002 annual SMOKE, CMAQ and CAMx modeling.

1.3.5 Vertical Structure of Modeling Domain

The MM5 meteorological model was exercised using 34 vertical layers from the surface to a pressure level of 100 mb (approximately 15 km above ground level). Both the CMAQ and CAMx air quality models can employ layer collapsing in which vertical layers in the MM5 are combined in the air quality model, which improves computational efficiency. The sensitivity of the CMAQ model estimates to the number of vertical layers was evaluated by the Western Regional Air Partnership (WRAP) and Visibility Improvements State and Tribal Association of the Southeast (VISTAS) (Tonnesen et al., 2005; 2006; Morris et al., 2004a). CMAQ model simulations were performed with no layer collapsing (i.e., the same 34 layers as used by MM5) and with various levels of layer collapsing. These studies found that using 19 vertical layers up to 100 mb (i.e., same model top as MM5) and matching the eight lowest MM5 vertical layers near the surface produced nearly identical results as with no layer collapsing. They also found that very aggressive layer collapsing (e.g., 34 to 12 layers) produced results with substantial differences compared to no layer collapsing. Therefore, based on the WRAP/VISTAS sensitivity analysis, CENRAP adopted the 19 vertical layer configuration up to the 100 mb model top. Figure 1-3 displays the definition of the 34 MM5 vertical layers and how they were collapsed to 19 vertical layers in the air quality modeling performed by CENRAP.

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

Figure 1-3. MM5 34 vertical layer definitions and scheme for collapsing the 34 layers down to 19 layers for the CENRAP CMAQ and CAMx 2002 annual modeling.

1.3.6 2002 Calendar Year Selection

The calendar year 2002 was selected for CENRAP regional haze annual modeling as described in the CENRAP Modeling Protocol (Morris et al., 2004a). EPA's applicable guidance on $PM_{2.5}$/Regional Haze modeling at that time (EPA, 2001) identified specific goals to consider when selecting modeling periods for use in demonstrating reasonable progress in attaining the regional haze goals. However, since there is much in common with the goals for selecting episodes for annual and episodic $PM_{2.5}$ attainment demonstrations as well as regional haze, EPA's current guidance addresses all three in a common document. (EPA, 2007) At the time of the modeling period selection EPA had also published an updated summary of $PM_{2.5}$ and Regional Haze Modeling Guidance (Timin, 2002) that served, in some respects, as an interim placeholder until the final guidance was issued as part of the $PM_{2.5}$/regional haze NAAQS implementation process that was ultimately published in April 2007 (EPA, 2007). The interim EPA modeling guidance for episode selection (EPA, 2001; Timin, 2002) was consistent with the final EPA regional haze modeling guidance (EPA, 2007).

EPA recommends that the selection of a modeling period derive from three principal criteria:

- A variety of meteorological conditions should be covered that includes the types of meteorological conditions that produce the worst 20 percent and best 20 percent visibility days at Class I areas in the CENRAP States during the 2000-2004 baseline period;

- To the extent possible, the modeling data base should include days for which enhanced data bases (i.e. beyond routine aerometric and emissions monitoring) are available; and

- Sufficient days should be available such that relative response 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 percent worst and 20 percent best visibility days determined for each Class I area 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. 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.

Due to limited available resources CENRAP was restricted to modeling a single calendar year. The RHR uses the five-year baseline of 2000-2004 period as the starting point for projecting future-year visibility. Thus, the modeling year should be selected from this five-year baseline period. The 2002 calendar year, which lies in the middle of the 2000-2004 Baseline, was selected for the following reasons:

- Based on available information, 2002 appears to be a fairly typical year in terms of meteorology for the 5-year Baseline period of 2000-2004;

- 2003 and 2004 appeared to be colder and wetter than typical in the eastern US;
- The enhanced IMPROVE and IMPROVE Protocol and Supersites PM monitoring data were fully operational by 2002. Much less IMPROVE monitoring data was available during 2000-2001, especially in the CENRAP region;
- IMPROVE data for 2003 and 2004 were not yet available at the time that the CENRAP modeling was initiated; and
- 2002 was being used by the other RPOs.

1.3.7 Initial Concentrations and Boundary Conditions

The CMAQ and CAMx models were operated separately for each of four quarters of the 2002 year using a ~15 day spin up period (i.e., the models were started approximately 15 days before the first day of interest in each quarter in order to limit the influence of the assumed initial concentrations, e.g., start June 15 for quarter 3 whose first day of interest is July 1). Sensitivity simulations demonstrated that with ~15 initialization days, the influence of initial concentrations (ICs) was minimal using the 36 km Inter-RPO continental U.S. modeling domain. Consequently, clean ICs were specified in the CMAQ and CAMx modeling using a ~15 day spin up period.

Boundary Conditions (BCs) (i.e., the assumed concentrations along the later edges of the 36 km modeling domain, see Figure 1-2) were based on a 2002 simulation by the GEOS-CHEM global circulation/chemistry model. GEOS-CHEM is a three-dimensional global chemistry model driven by assimilated meteorological observations from the Goddard Earth Observing System (GEOS) of the NASA Global Modeling and Assimilation Office. It is applied by research groups around the world to a wide range of atmospheric composition problems, including future climates and planetary atmospheres using general circulation model meteorology to drive the model. Central management and support of the model is provided by the Atmospheric Chemistry Modeling Group at Harvard University.

A joint RPO study was performed, coordinated by VISTAS, in which Harvard University applied the GEOS-CHEM global model for the 2002 calendar year (Jacob, Park and Logan, 2005). The University of Houston (UH) was retained to process the 2002 GEOS-CHEM output into BCs for the CMAQ model (Byun, 2004). The GEOS-CHEM simulations for the RPOs used GEOS meteorological observations for the year 2002. These were obtained from the Global Modeling and Assimilation Office(GMAO) as a 6-hourly archive (3-hour for surface quantities such as mixing depths). The data through August 2002 were from the GEOS-3 assimilation, with horizontal resolution of 1^ox1^o and 55 vertical layers. The data after August 2002 were from the updated GEOS-4 assimilation, with horizontal resolution of 1^ox1.25^o and 48 vertical layers (note 1^o latitude is equal to approximately 110 km). The GEOS-CHEM output was processed by mapping the GEOS-CHEM chemical compounds to the species in the CBM-IV chemical mechanism used by CMAQ/CAMx and mapping the GEOS-CHEM vertical layers to the 19 layer vertical layer structure used by CMAQ/CAMx in the CENRAP modeling (Byun, 2004). The results were day-specific three-hourly BC inputs for the CMAQ model. The CMAQ2CAMx processor was then used to transform the CMAQ day-specific 3-hourly BCs to the format used by CAMx.

There were several quality assurance (QA) checks of the BCs generated from the 2002 GEOS-CHEM output. The first QA/QC check was a range check to assure reasonable values. The BCs were compared against the GEOS-CHEM outputs to assure the mapping and interpolation was performed correctly. The code used to map the GEOS-CHEM output to the CMAQ BC format was obtained from UH, reviewed and the BC generation duplicated for several time periods during 2002.

1.3.8 Emissions Input Preparation

The CENRAP SMOKE emissions modeling was based on an updated 2002 emissions data for the U.S. (Pechan, 2005c,e; Reid et al., 2004a,b), 1999 emissions data for Mexico (ERG, 2006), and 2000 emissions data for Canada. These data were used to generate a final base 2002 Base G Typical (Typ02G) annual emissions database. Numerous iterations of the emissions modeling were conducted using interim databases before arriving at the final Base G emission inventories (e.g., Morris et al., 2005). The 2018 Base G base case emissions (Base18G) for most source categories in the U.S. were based on projections of the 2002 inventory assuming growth and control (Pechan, 2005d). 2018 EGU emissions were based on the run 2.1.9 of the Integrated Planning Model (IPM) updated by the CENRAP states. Canadian emissions for the Base18G scenario were based on a 2020 inventory, whereas the Mexican 1999 inventory was held constant for 2018.

The Typ02G and Base18G emission inventories represent significant improvements to the preliminary emissions modeling performed by CENRAP (Morris et al., 2005). While the preliminary 2002 modeling served its purpose to develop the infrastructure for modeling large emissions data sets and producing annual emissions simulations, much of the input data (both as inventories and ancillary data) were placeholders for actual 2002 data that were being prepared through calendar year 2005. As these actual 2002 data sets became available, they were integrated into the SMOKE modeling and QA system that was developed during the preliminary modeling, to produce a high-quality emissions data set for use in the final CMAQ and CAMx modeling. The addition of entirely new inventory categories, like marine shipping, added complexity to the modeling. By the end of the emissions data collection phase, there were 23 separate emissions processing streams covering a variety of sources categories necessary to general model-ready emission inputs for the 2002 calendar year.

Details on the emissions modeling are provided in Chapter 2 with additional information contained in Appendix B.

1.3.9 Meteorological Input Preparation

The 2002 36 km MM5 meteorological modeling was conducted by the Iowa Department of Natural Resources (IDNR) who also performed a preliminary model performance evaluation (Johnson, 2007). CENRAP performed an additional MM5 evaluation of the CENRAP 2002 36 km MM5 simulation that included a comparative evaluation against the final VISTAS 2002 36 km MM5 and an interim WRAP 2002 36 km simulation (Kemball-Cook et al., 2004). Kemball-Cook and co-workers (2004) found the following in the comparative evaluation of the CENRAP, WRAP and VISTAS 2002 36 km MM5 simulations, (details are provided in Appendix A):

Surface Meteorological Performance within the CENRAP Region

- The three MM5 simulations (CENRAP, VISTAS and WRAP) obtained comparable model performance for winds and humidity that were within model performance benchmarks.
- The WRAP MM5 simulation obtained better temperature model performance than the other two simulations due to the use of surface temperature data assimilation.
    - In the final WRAP MM5 simulation the use of surface temperature assimilation was dropped because it introduced instability in the vertical structure of the atmosphere.
- For all three runs, the Northern CENRAP domain had a cold bias in winter and a warm bias in summer.

Surface Meteorological Performance outside the CENRAP Region

- All three runs had similar surface wind model performance in the western U.S. that was outside the model performance benchmarks
- For temperature, the WRAP MM5 simulation had the best performance overall due to the surface temperature data assimilation that was dropped in the final WRAP run.
- The three runs had comparable humidity performance, although WRAP exhibited a larger wet bias in the summer and the southwestern U.S.

Upper-Air Meteorological Performance

- The VISTAS and CENRAP MM5 simulations were better able to reproduce the deep convective summer boundary layers compared to the WRAP MM5 simulations, which exhibited a smoother decrease in temperature with increase in altitude.
- CENRAP and VISTAS MM5 simulations better simulated the surface temperature inversions than WRAP.
- WRAP was better able to simulate the surface temperature.
- All three models exhibited similar vertical wind profiles.

Precipitation Performance

- In winter, all three MM5 simulations exhibited similar, fairly good, performance in reproducing the spatial distribution and magnitudes of the monthly average observed precipitation.
- In summer, all runs had a wet bias, particularly in the desert southwest where the interim WRAP run had the largest wet bias.

In conclusion, the VISTAS simulation appeared to perform best, the CENRAP MM5 model performance was generally between the VISTAS and WRAP performance, with performance more similar to VISTAS than WRAP. Although the interim WRAP MM5 simulation performed best for surface temperature due to the surface temperature data assimilation, the surface temperature assimilation degraded the MM5 upper-air performance including the ability to assimilate surface inversions and was ultimately dropped from the final WRAP MM5 simulations (Kemball-Cook et al., 2005).

The IDNR 12 km[2] MM5 simulations were also evaluated and compared with the performance of the 36 km MM5 simulation (Johnson et al., 2007). The IDNR 36 km and 12 km MM5 model performance was similar (Johnson, 2007), which supported the findings of the CMAQ and CAMx 36 and 12 km sensitivity simulations that there was little benefit of using a 12 km grid for simulating regional haze at rural Class I areas (Morris et al., 2006a). However, as noted by Tonnesen and co-workers (2005; 2006) and EPA modeling guidance (1991; 1999; 2001; 2007) this finding does not necessarily hold for 8-hour ozone and $PM_{2.5}$ modeling that is characterized by sharper concentration gradients and frequently occurs in the urban environment as compared to the more rural nature of regional haze.

1.3.10 Photolysis Rates Model Inputs

Several chemical reactions in the atmosphere are initiated by the photodissociation of various trace gases. To accurately represent the complex chemical transformations in the atmosphere, accurate estimates of these photodissociation rates must be made. The Models-3/CMAQ system includes the JPROC processor, which calculates a table of clear-sky photolysis rates (or J-values) for a specific date. JPROC uses default values for total aerosol loading and provides the option to use default ozone column data or to use measured total ozone column data. These data come from the Total Ozone Mapping Spectrometer (TOMS) satellite data. TOMS data that is available at 24-hour averages was obtained from http://toms.gsfc.nasa.gov/eptoms/ep.html. Day-specific TOMS data was used in the CMAQ radiation model (JPROC) to calculate photolysis rates. The TOMS data were missing or erroneous for several periods in 2002: August 2-12; June 10; and November 18-19. Thus, the TOMS data for August 1, 2002 was used for August 2-7 and TOMS data for August 13 was used for August 8-12. Similarly, TOMS data for June 9 was used for June 10 and data for August 17 was used for August 18-19. Note that the total column of ozone in the atmosphere is dominated by stratospheric ozone which has very little day-to-day variability so the use of TOMS data within a week or two of an actual day introduces minimal uncertainties in the modeling analysis.

JPROC produces a "look-up" table that provides photolysis rates as a function of latitude, altitude, and time (in terms of the number of hours of deviation from local noon, or hour angle). In the current CMAQ implementation, the J-values are calculated for six latitudinal bands (10º, 20º, 30º, 40º, 50º, and 60º N), seven altitudes (0 km, 1 km, 2 km, 3 km, 4 km, 5 km, and 10 km), and hourly values up to ∀8 hours of deviation from local noon. During model calculations, photolysis rates for each model grid cell are estimated by first interpolating the clear-sky photolysis rates from the look-up table using the grid cell latitude, altitude, and hour angle, followed by applying a cloud correction (attenuation) factor based on the cloud inputs from MM5.

The photolysis rates input file was prepared as separate look-up tables for each simulation day. Photolysis files are ASCII files that were visually checked for selected days to verify that photolysis are within the expected ranges.

[2] The IDNR twelve 12 km annual simulation domain was not sufficient for CENRAP's needs, thus Bret Anderson with EPA Region 7 in cooperation with Texas completed an episodic 12km simulation on a larger domain.

The Tropospheric Ultraviolet and Visible (TUV) Radiation Model (http://cprm.acd.ucar.edu/Models/TUV/) is used to generate the photolysis rates input file for CAMx. TOMS ozone data and land use data were used to develop the CAMx Albedo/Haze/Ozone input file for 2002. As for CMAQ, the missing TOMS data period in the fall of 2002 was filled-in using observed TOMS data on either side of the missing period using the same procedures as described above for CMAQ. Default land use specific albedo values were used and a constant haze value used, corresponding to rural conditions over North America.

1.3.11 Air Quality Input Preparation

Air quality data used with the CMAQ and CAMx modeling systems include: (1) Initial Concentrations (ICs) that are the assumed initial three-dimensional concentrations throughout the modeling domain.; (2) the Boundary Conditions (BCs) that are the concentrations assumed along the lateral edges of the RPO national 36 km modeling domain; and (3) air quality observations that are used in the model performance evaluation (MPE). The MPE is discussed in Section 3 and Appendix C of this TSD.

As noted in Section 1.3.7, CMAQ default clean Initial Concentrations (ICs) were used along with an approximately 15 day spin up (initialization) period to eliminate any significant influence of the ICs on the modeled concentrations for the days of interest. The same ICs were used with CAMx as well. Both CMAQ and CAMx were run for each quarter of the year. Each quarter's model run was initialized 15 days prior to the first day of interest (e.g., for quarter 3, Jul-Aug-Sep, the model was initialized on June 15, 2002 with the first modeling day of interest July 1, 2002). The CMAQ Boundary Conditions (BCs) for the Inter-RPO 36 km continental U.S. grid (Figure 1-2) were based on day-specific 3-hour averages from the output of the GEOS-CHEM global simulation model of 2002 (Jacob, Park and Logan, 2005). The 2002 GEOS-CHEM output was mapped to the species and vertical layer structure of CMAQ and interpolated to the lateral boundaries of the 36 km grid shown in Figure 1-2 (Byun, 2004).

Table 1-6 summarizes the surface air quality monitoring networks and the number of sites available in the CENRAP region that were used in the model performance evaluation. Data from these monitoring networks were also used to evaluate the CMAQ and CAMx models outside of the CENRAP region.

Table 1-6. Ground-level ambient data monitoring networks and stations available in the CENRAP states for calendar year 2002 used in the model performance evaluation.

Monitoring Network	Chemical Species Measured	Sampling Frequency; Duration	Approximate Number of Monitors
IMPROVE	Speciated $PM_{2.5}$ and PM_{10}	1 in 3 days; 24 hr	11
CASTNET	Speciated $PM_{2.5}$, Ozone	Hourly, Weekly; 1 hr, 1 Week	3
NADP	WSO4, WNO3, WNH4	Weekly	23
EPA-STN	Speciated $PM_{2.5}$	Varies; Varies	12
AIRS/AQS	CO, NO, NO_2, NO_x, O_3	Hourly; Hourly	25

1.3.12 2002 Base Case Modeling and Model Performance Evaluation

The CMAQ and CAMx models were evaluated against ambient measurements of PM species, gas-phase species and wet deposition. Table 1-6 summarizes the networks used in the model evaluation, the species measured and the averaging times and frequency of the measurements. Numerous iterations of CMAQ and CAMx 2002 base case simulations and model performance evaluations were conducted during the course of the CENRAP modeling study, most of which have been posted on the CENRAP modeling website (http://pah.cert.ucr.edu/aqm/cenrap/cmaq.shtml) and presented in previous reports and presentations for CENRAP (e.g., Morris et al., 2005; 2006a,b). Details on the final 2002 Base F 36 km CMAQ base case modeling performance evaluation are provided in Chapter 3 and Appendix C (because of the similarity between 2002 Base F and 2002 Base G and resource constraints the model evaluation was not re-conducted for Base G). In general, the model performance of the CMAQ and CAMx models for sulfate (SO4) and elemental carbon (EC) was good. Model performance for nitrate (NO3) was variable, with a summer underestimation and winter overestimation bias. Performance for organic mass carbon (OMC) was also variable, with the inclusion of the SOAmods enhancement in CMAQ Version 4.5 greatly improving the CMAQ summer OMC model performance (Morris et al., 2006c). Model performance for Soil and coarse mass (CM) was generally poor. Part of the poor performance for Soil and CM is believed to be due to measurement-model incommensurability. The IMPROVE measured values are due, in part, to local fugitive dust sources that are not captured in the model's emission inputs and the 36 km grid resolution is not conducive to modeling localized events.

1.3.13 2018 Modeling and Visibility Projections

Emissions for the 2018 base case were generated following the procedures discussed in Section 1.3.8 and Chapter 2. 2018 emissions for Electrical Generating Units (EGUs) were based on simulations of the Integrated Planning Model (IPM) that took into the account the effects of the Clean Air Interstate Rule (CAIR) on emissions from EGUs in CAIR states using an IPM realization of a CAIR cap-and-trade program. Emissions for on-road and non-road mobile sources were based on activity growth and emissions factors from the EPA MOBILE6 and NONROAD models, respectively. Area sources and non-EGU point sources were grown to 2018 levels (Pechan, 2005d). The Canadian year 2000 emissions inventory was replaced by a Canadian 2020 emissions inventory for the 2018 CMAQ/CAMx simulations. The following sources were assumed to remain constant between the 2002 and 2018 base case simulations:

- Biogenic VOC and NOx emissions from the BEIS3 biogenic emissions model;
- Wind blown dust associated with non-agricultural sources (i.e., natural wind blown fugitive dust);
- Off-shore emissions associated with off-shore marine and oil and gas production activities;
- Emissions from wildfires;
- Emissions from Mexico; and
- Global transport (i.e., emissions due to BCs from the 2002 GEOS-CHEM global chemistry model.

The results from the 2002 and 2018 CMAQ and CAMx simulations were used to project 2018 PM levels from which 2018 visibility estimates were obtained. The 2002 and 2018 modeling results were used in a relative sense to scale the observed PM concentrations from the 2000-2004 Baseline and the IMPROVE monitoring network to obtain the 2018 PM projections. The 2018/2002 modeled scaling factors are called Relative Response Factors (RRFs) and are constructed as the ratio of modeling results for the 2018 model simulation to the 2002 model simulation. Two important regional haze metrics are the average visibility for the worst 20 percent and best 20 percent days from the 2000-2004 five-year Baseline. For the 2018 visibility projections, EPA guidance recommends developing Class I area and PM species specific RRFs using the average modeling results for the worst 20 percent days during the 2002 modeling period and the 2002 and 2018 emission scenarios. The results of the CENRAP 2018 visibility projections following EPA guidance procedures (EPA, 2007a) are provided in Chapter 4 and Appendix D. CENRAP has also developed alternative procedures for visibility projections that are discussed in Chapter 5 and Appendix D. For example, much of the coarse mass (CM) impacts at Class I area IMPROVE monitors is believed to be natural and primarily from local sources that are subgrid-scale to the modeled 36 km grid so are not represented in the modeling. So, one alternative visibility projection approach is to set the RRF for CM to 1.0. That is, the CM impacts in 2018 are assumed to be the same as in the observed 2000-2004 Baseline. Similarly, the Soil impacts at IMPROVE monitors are likely mainly due to local dust sources so another alternative approach is to set the RRFs for both CM and Soil to 1.0.

The 2018 visibility projections for the worst 20 percent days are compared against a 2018 point on the Uniform Rate of Progress (URP) glidepath or the “2018 URP point”. The 2018 URP point is obtained by constructing a linear visibility glidepath in deciviews from the observed 2000-2004 Baseline (EPA, 2003a) for the worst 20 percent days to the 2064 Natural Conditions (EPA, 2003b; Pitchford, 2006). Where the linear glidepath crosses the year 2018 is the 2018 URP point. States may use the modeled 2018 visibility to help define their 2018 RPG in their RHR SIPs. The 2018 URP point is used as a benchmark to help judge the 2018 modeled visibility projections and the state’s RPG. However, as noted in EPA’s RPG guidance “The glidepath is not a presumptive target, and States may establish a RPG that provides for greater, lesser, or equivalent visibility improvement as that described by the glidepath” (EPA, 2007b). Chapter 4 and Appendix D present the 2018 visibility projections for the CENRAP Class I areas and their comparisons with the 2018 URP point using EPA default visibility projection procedures (EPA, 2007a) and EPA default URP glidepaths (EPA, 2003a,b; 2007b).

Various techniques have been developed to display the 2018 visibility modeling results including “DotPlots” that display the 2018 visibility projections as a percentage of meeting the 2018 point on the URP glidepath. A value of 100% on the DotPlot indicates that the Class I area is predicted to meet the 2018 point on the URP glidepath. Over 100% means the 2018 visibility projection obtains more visibility improvements (reductions) than required to meet the 2018 point on the URP glidepath (i.e., projected value is below the glidepath). And less than 100% indicates that fewer visibility improvements are projected than are needed to meet the 2018 point URP on the glidepath (i.e., above the glidepath). Figure 1-4 displays a DotPlot that compares the 2018 visibility projections from the CENRAP 2018 Base G CMAQ simulation with the 2018 URP point using the EPA default RRFs and alternative RRFs that set the CM and Soil RRFs to unity (i.e., assume CM and Soil are natural so remain unchanged from the 2000-2004 Baseline). For these results, the 2018 visibility projections at the Hercules Glade (HEGL1) Class I area meets the 2018 point on the URP glidepath (100%), whereas the 2018 visibility projections at Caney

Creek (CACR), Mingo (MING) and Upper Buffalo (UPBU) achieve more visibility improvements than needed to meet the 2018 URP point so are below the 2018 URP glidepath. However, the 2018 visibility projections at Breton Island comes up slightly short (~5%) of meeting the 2018 point on the URP glidepath and Wichita Mountains (WIMO) comes up approximately 40% short of meeting the 2018 point on the URP glidepath. Class I areas at the northern (e.g., VOYA, BOWA and ISLE) and southern (e.g., BIBE and GUMO) boundaries of the U.S. also fall short of achieving the 2018 URP point. High contributions of international transport and/or natural sources (e.g., wind blown dust) affect the ability of these Class I areas to be on the URP glidepath. These issues are discussed in more detail in Chapters 4 and 5.

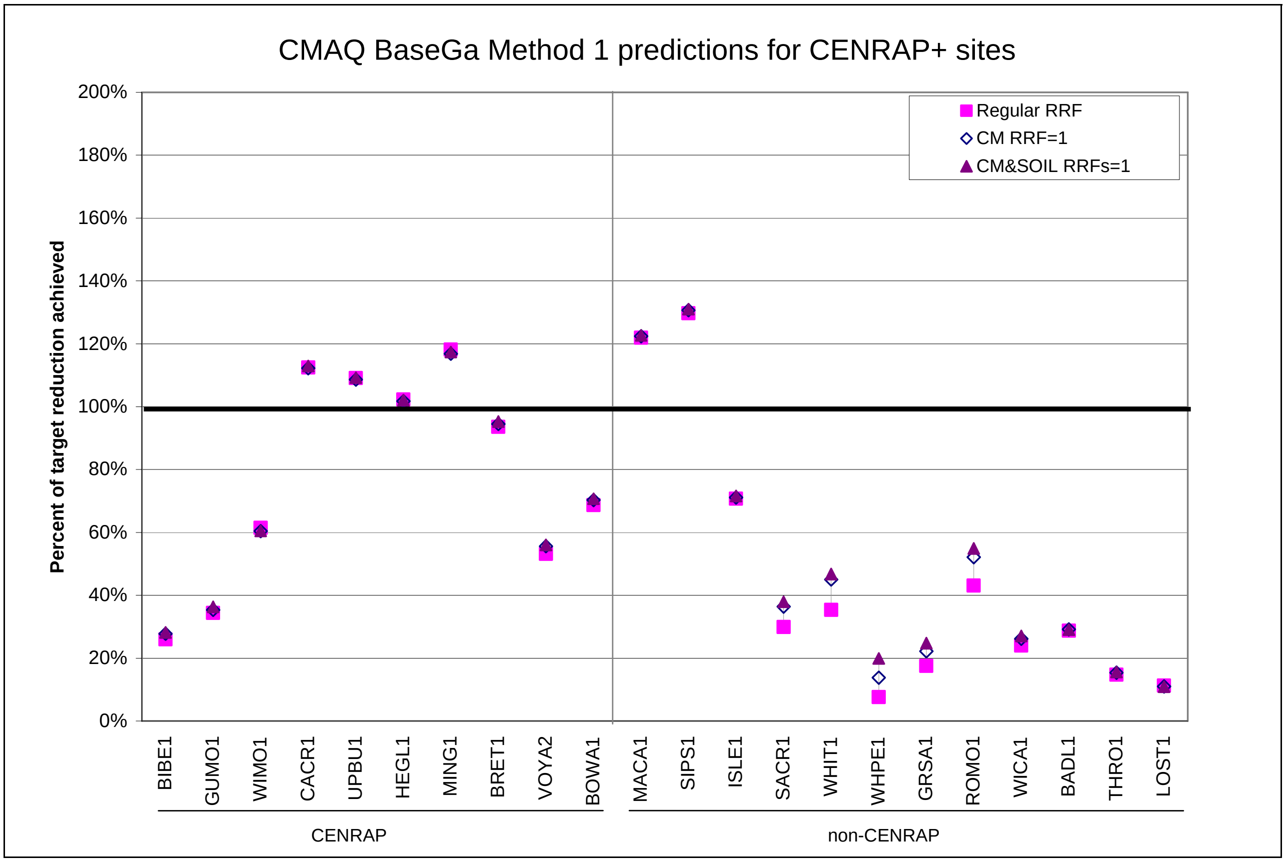

Figure 1-4. 2018 visibility projections expressed as a percent of meeting the 2018 URP point for the 2018 BaseG CMAQ base case simulation using the EPA default (EPA, 2007) Regular RRF and alternative projections procedures that set the RRFs for CM=1.0 and CM&SOIL=1.0.

1.3.14 Additional Supporting Analysis

CENRAP performed numerous supporting analyses of its modeling results including analyzing alternative glidepaths and 2018 projection Approaches and performing confirmatory analysis of the 2018 visibility projections. Details on the additional supporting analysis are contained discussed in Chapter 5, which include:

- The CENRAP 2018 visibility projections were compared with those generated by VISTAS and MRPO. There was close agreement between the CENRAP and VISTAS 2018 visibility projections at almost all common Class I areas. With the only exception being Breton Island where the CENRAP's projections were slightly more optimistic than VISTAS'. The MRPO 2018 visibility projections were less optimistic than CENRAP's at the four Arkansas-Missouri Class I area that may have been due to CENRAP's BART emission controls in CENRAP states not included in the 2018 MRPO inventory.
- Extinction based glidepaths were developed and the CENRAP 2018 visibility projections were shown to produce nearly identical estimates of achieving the 2018 URP point when using total extinction glidepaths as when the linear deciview glidepaths were used. With the extinction based glidepaths the analysis of 2018 URP could be made on a PM species-by-species basis where it was shown that 2018 extinctions due to SO4 and, to a lesser extent, NO3 and EC, achieve the URP, but the other species do not and in fact extinction due to Soil and CM is projected to get worse.
- 2018 visibility projections were made using EPA's new Modeled Attainment Test Software (MATS) program and the CENRAP Typ02G and Base18G modeling results. The CENRAP 2018 visibility projections exactly agreed with those generated by MATS with three exceptions: Breton Island, Boundary Waters and Mingo Class I areas, At these three Class I areas MATS did not produce any 2018 visibility projections due to insufficient data in the raw IMPROVE database to produce a valid observed 2000-2004 Baseline. CENRAP used filled data for these three Class I areas.
- PM Source Apportionment Technology (PSAT) modeling was conducted to estimate the contributions to visibility impairment at Class I areas by source region (e.g., states) and major source category. Source contributions were obtained for a 2002 and 2018 base case and the PSAT modeling results were implemented in a PSAT Visualization Tool that was provided to CENRAP states and others. Major findings from the PSAT source apportionment modeling include the following:
    - Sulfate from elevated point sources was the highest source category contribution to visibility impairment at CENRAP Class I areas for the worst 20 percent days.
    - International transport contributed significantly to visibility impairment at CENRAP Class I areas on the southern (BIBE and GUMO) and northern (BOWA and VOYA) borders of the U.S. and to a lesser extent at WIMO as well.
- Alternative visibility projections were made assuming that coarse mass (CM) alone and CM and Soil were natural in origin that confirmed the original 2018 visibility projections.
- Visibility projections were made using an alternative model (CAMx) that verified the projections made by CMAQ.
- The effects of International Transport were examined several ways and found that the inability of the 2018 visibility projections to achieve the 2018 URP point at the northern and southern border Class I areas was due to high contributions due to International Transport.

- Visibility trends for the worst 20 percent days, best 20 percent days and all monitored days were analyzed at CENRAP Class I areas using the period of record IMPROVE observations. At most Class I areas there was insufficient years of data to produce a discernable trend. In addition, there was significant year-to-year variability in visibility impairment with episodic events (e.g., wildfires and wind blown dust) confounding the analysis.

1.4 Organization of the Report

Chapter 1 of this TSD presents background, an overview of the approach and summary of the results of the CENRAP meteorological, emissions and air quality modeling. Appendix A contains more details on the meteorological model evaluation discussed in Chapter 1. Details on the emissions modeling are provided in Chapter 2 and Appendix B. The model performance evaluation is given in Chapter 3 and Appendix C. The 2018 visibility projections and comparisons with the 2018 URP point are provided in Chapter 4 with more details given in Appendix D. Chapter 5 contains additional supporting analysis with details on the PM source apportionment modeling and alternative projections provided in Appendices E and F, respectively. Chapter 6 lists the references cited in the report.

2.0 EMISSIONS MODELING

2.1 Emissions Modeling Overview

For the emissions modeling work conducted in support of CENRAP air quality modeling, we used updated 2002 emissions data for the U.S., 1999 emissions data for Mexico, and 2000 emissions data for Canada to generate a final base 2002 Base G Typical (Typ02G) annual emissions database. Numerous iterations of the emissions modeling were conducted using interim databases before arriving at the final Base G emission inventories. The 2002 and 2018 emissions inventories and ancillary modeling data were provided by CENRAP emissions inventory contractors (Pechan and CEP, 2005c,e; Reid et al., 2004a,b; Coe and Reid, 2003), other Regional Planning Organizations (RPOs) and EPA. Building from the CENRAP preliminary 2002 database (Pechan and CEP. 2005e) and 2018 projections (Pechan, 2005d), we integrated several updates to the inventories and ancillary data to create final emissions input files; the final simulations are referred to as 2002 Typical and 2018 Base G, or Typ02G and Base18G. We used the Sparse Matrix Operator Kernel Emissions (SMOKE) version 2.1 processing system (CEP, 2004) to prepare the inventories for input to the air quality modeling systems. The SMOKE simulations documented in this report include emissions generated for annual CMAQ and CAMx simulations at a 36-km model grid resolution, and a short-term CMAQ test simulation at a 12-km model grid resolution. We performed the modeling and quality assurance (QA) work based on the CENRAP modeling Quality Assurance Project Plan (QAPP; Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a).

The Typ02G and Base18G emission inventories represent significant improvements to the preliminary emissions modeling performed by CENRAP (Morris et al., 2005). While the preliminary 2002 modeling served its purpose to develop the infrastructure for modeling large emissions data sets and producing annual emissions simulations, much of the input data (both as inventories and ancillary data) were placeholders for actual 2002 data that were being prepared through calendar year 2005. As these actual 2002 data sets became available, they were integrated into the SMOKE modeling and QA system that was developed during the preliminary modeling, to produce a high-quality emissions data set for use in the final CMAQ and CAMx modeling. The addition of entirely new inventory categories, like marine shipping, added complexity to the modeling. By the end of the emissions data collection phase, there were 23 separate emissions processing streams covering a variety of sources categories necessary to general model-ready emission inputs for the 2002 calendar year.

2.1.1 SMOKE Emissions Modeling System Background

The purpose of SMOKE (or any emissions processor) is to process the raw emissions reported by states and EPA into gridded hourly speciated emissions required by the air quality model. Emission inventories are typically available as an annual total emissions value for each emissions source, or perhaps with an average-day emissions value. The air quality models, however, typically require emissions data on an hourly basis, for each model grid cell (and perhaps model layer), and for each model species. Consequently, emissions processing involves (at a minimum) transformation of emission inventory data by temporal allocation, chemical speciation, spatial allocation, and perhaps layer assignment, to achieve the input requirements of the air quality model. For the CENRAP modeling effort, all of these steps were needed. In addition, CENRAP processing requires special MOBILE6 processing and growth and control of emissions for the future-year inventories. Finally, the biogenic emission processing using BEIS2 includes additional processing steps. SMOKE formulates emissions modeling in terms of sparse matrix operations. Figure 2-1 shows an example of how the matrix approach organizes the emissions processing steps for anthropogenic emissions, with the final step that creates the model-ready emissions being the merging of all the different processing streams of emissions into a total emissions input file for the air quality model. Figure 2-1 does not include all the potential processing steps, which can be different for each source category in SMOKE, but does include the major processing steps listed in the previous paragraph, except the layer assignment. Specifically, the inventory emissions are arranged as a vector of emissions, with associated vectors that include characteristics about the sources such as its state and county or source classification code (SCC). SMOKE also creates matrices that will apply the gridding, speciation, and temporal factors to the vector of emissions. In many cases, these matrices are independent from one another, and can therefore be generated in parallel. The processing approach ends with the merge step, which combines the inventory emissions vector (now an hourly inventory file) with the control, speciation, and gridding matrices to create model-ready emissions.

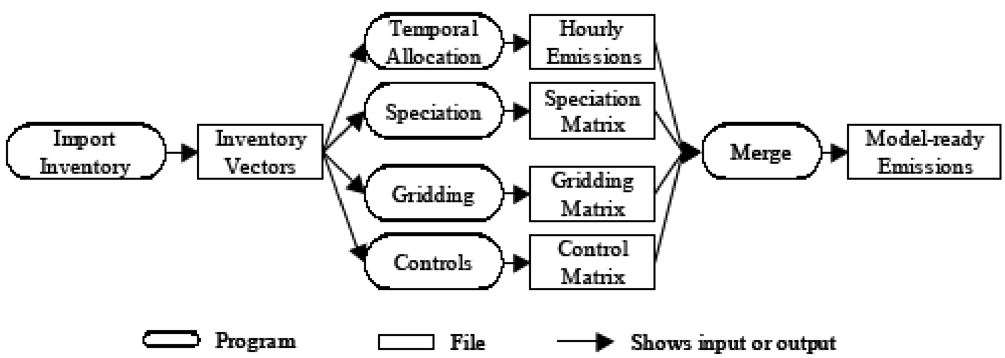

Figure 2-1. Flow diagram of major SMOKE processing steps needed by all source categories.

Temporal processing includes both seasonal or monthly adjustments and day-of-week adjustments. Emissions are known to be quite different for a typical weekday versus a typical Saturday or Sunday. For the day-of-week temporal processing step, emissions may be processed using representative Monday, weekday, Saturday, and Sunday for each month; we refer to this type of processing here as MWSS processing (note that because SMOKE operates in Greenwich Mean Time [GMT] then Monday would include some of local time Sunday so needs to be processed separately from the typical weekday). This approach significantly reduces the number of times the temporal processing step must be run. In the sections below, we have identified the cases in which we have used the MWSS processing approach. Figure 2-2 provides a schematic diagram of SMOKE/BEIS2 processing steps used in this project to generate biogenic emissions rates for Volatile Organic Compounds (VOCs) and oxides of nitrogen (NOx). Because biogenic emissions are temperature sensitive, they are generated for each day of 2002 using day-specific meteorological conditions from the MM5 meteorological model.

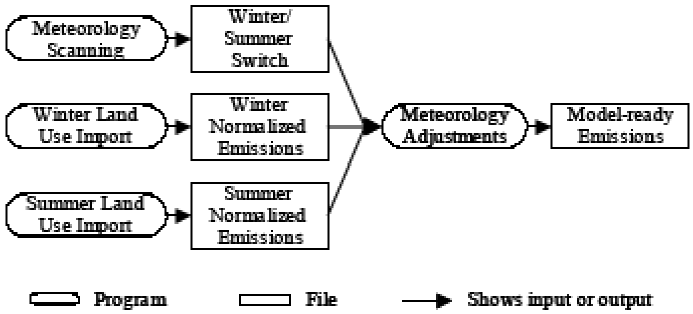

Figure 2-2. Flow diagram of SMOKE/BEIS2 processing steps.

2.1.2 SMOKE Scripts

The scripts are the interface that emissions modelers use to run SMOKE and define the set up and databases used in the emissions modeling so are important for anyone wishing to reproduce the CENRAP SMOKE emissions modeling. Many iterations of the CENRAP SMOKE emissions modeling were performed using updated and corrected emissions data and assumptions resulting in the creation of numerous SMOKE modeling scripts during the course of the study. For the CENRAP annual 2002 SMOKE emissions modeling, the default SMOKE script set up, which is based on source categories, was used to configure the scripts. We made several modifications to the default SMOKE scripts to modularize them, add error checking loops, and break up the report and logs directories by source category. The result is one script for each major source category being modeled that calls all of the SMOKE programs required for simulating that source category. 16 major source categories were modeled by SMOKE for CENRAP. An addition seven SMOKE scripts were also run to set up the emissions modeling. Table 2-1 lists all of the SMOKE scripts used for the 2002 base year modeling and the SMOKE programs called by each script. In addition to the source-specific scripts listed in Table 2-1, we also listed the SMOKE utility scripts that actually call executables, manage the log files, and manage the configuration of the SMOKE simulations.

Table 2-1. Summary of SMOKE scripts.

Source Category	Script Name	SMOKE Programs/Functions
Area	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_ar_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Area fire	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_arf_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Offshore Area	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_ofsar_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Non-road* Mobile	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_nr_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Fugitive dust	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_fd_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Road dust	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_rd_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Ammonia*	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_nh3_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
On-road Mobile (non-VMT-based)	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_mb_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
On-road non-US Mobile (non-VMT-based)	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_nusm_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
On-road Mobile (VMT-based)	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_mbv_base02f.csh	smkinev, mbsetup, grdmat, spcmat, premobl, emisfac, temporal, smkmerge, smkreport
WRAP Oil and Gas	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_wog_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Point	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_pt_base02f.csh	smkinev, grdmat, spcmat, laypoint, temporal, smkmerge, smkreport
Offshore point	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_ofs_base02f.csh	smkinev, grdmat, spcmat, laypoint, temporal, smkmerge, smkreport
Canadian Point fires	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_bsf_base02f.csh	smkinev, grdmat, spcmat, laypoint, temporal, smkmerge, smkreport
All point fires	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_alf_base02f.csh	smkinev, grdmat, spcmat, laypoint, temporal, smkmerge, smkreport
Biogenec	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_bg_base02f.csh	Normbies3, tmpbies3, smkmerge
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/make_invdir.csh	builds output file names and directories
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/smk_run.csh	Calls SMOKE executables for everything but projection, controls, and QA
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/qa_run.csh	Calls the SMOKE executables for running QA program & names the input/output directories for reports
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smoke_calls.csh	Calls smk_run.csh, qa_run.csh, configuration and management
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/Assignes/ASSIGNES.cenrap_base02f.cmaq.cb4p25	Sets up the environment variables for use of SMOKE
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/Assignes/smk_mkdir	Creates the input/output directories
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/Assignes/setmerge_files.scr	Sets up the output environment variables for the smkmerge program

* The nr and nh3 where farther divided to nrm and nry and nh3m and nh3y for the monthly/seasonal and yearly inventories

2.1.3 SMOKE Directory Structures

The SMOKE directories can be divided into three broad categories:

1. Program Directories: These directories contain the model source code, assigns files, scripts and executables needed to run SMOKE.
2. Input Directors: These directories contain the raw emissions inventories, the meteorological data and the ancillary input files.
3. Output Directories: These directories contain all of the output from the model. Also, the output directories contain the MOBILE6 input files.

The directories are described in the Table 2-2. The final pre-merged emission file names and sources of the data re provided in Appendix B.

Table 2-2. Summary of SMOKE directories.

Category	Directory Location	Directory Contents
Program	/home/aqm2/edss2/ cenrap02f/subsys/smoke/src	SMOKE source code
	/home/aqm2/edss2/ cenrap02f/subsys/smoke/assigns	SMOKE assigns files
	/home/aqm2/edss2/ cenrap02f/subsys/smoke/scripts	SMOKE make and run scripts
	/home/aqm2/edss2/ cenrap02f/subsys/smoke/Linux2_x86pg	SMOKE executables
Input	/home/aqm2/edss2/ cenrap02f/data/met	MCIP out metrology files
	/home/aqm2/edss2/ cenrap02f/data/ge_dat	SMOKE ancillary input files
	/home/aqm2/edss2/ cenrap02f/data/inventory/cenrap2002	Raw emissions inventory files
Output	/home/aqm2/edss2/ cenrap02f/data/run_base02f/static	Non-time dependent SMOKE intermediate outputs and MOBILE6 inputs
	/home/aqm2/edss2/ cenrap02f/ data/run_base02f/scenario	Time dependent SMOKE intermediate outputs
	/home/aqm2/edss2/ cenrap02f/data/run_base02f/outputs	Model-ready SMOKE outputs
	/home/aqm2/edss2/ cenrap02f/data/reports	SMOKE QA reports

2.1.4 SMOKE Configuration

SMOKE was configured to generate emissions for all months of 2002 on the 36-km unified RPO modeling domain (Figure 1-2). For the anthropogenic emissions sources that use hourly meteorology and daily or hourly data (i.e., on-road mobile sources, point sources with CEM data, point source fires and biogenic sources) we configured SMOKE to represent the daily emissions explicitly. For the non-meteorology dependent emissions, we used a representative Saturday, Sunday, Monday, and weekday for each month as surrogate days for the entire month's emissions (we refer to this as the MWSS processing approach). For these non-meteorology dependent emissions sources we explicitly represented the holidays as Sundays. Table 2-3 lists the days that we modeled as representative days in the months that we simulated for the 2002 base year modeling. Table 2-4 lists the holidays in 2002 that were modeled as Sundays.

Table 2-3: Representative model days for 2002 base year simulation.

Saturday	Sunday	Monday	Weekday
January 5	January 6	January 7	January 4
February 2	February 3	February 4	February 5
March 2	March 3	March 4	March 5
April 6	April 7	April 8	April 2
May 4	May 5	May 6	May 7
June 8	June 9	June 3	June 4
July 6	July 7	July 8	July 3
August 3	August 4	August 5	August 6
September 7	September 8	September 9	September 10
October 5	October 6	October 7	October 8
November 2	November 3	November 4	November 5
December 7	December 8	December 9	December 10

Table 2-4: 2002 modeled holidays.

Holiday	Date
New Years	January 1, 2002 January 2, 2002
Good Friday	March 29, 2002 March 30, 2002
Memorial Day	May 27, 2002 May 28, 2002
Independence Day	July 4, 2002 July 5, 2002
Labor Day	September 2, 2002 September 3, 2002
Thanksgiving Holiday	November 28-30, 2002
Christmas Holiday	December 24-26, 2002

We used the designations in Table 2-5 to determine which months fell into each season when temporally allocating the seasonal emissions inventories. Some of the inventories for the Electrical Generating Units (EGUs) were received for Winter and Summer. Table 2-6 determines which months fell into each season

Table 2-5. Assignments of months to four seasons for use of seasonal inventory files in SMOKE.

Month	Season
January	Winter
February	Winter
March	Spring
April	Spring
May	Spring
June	Summer
July	Summer
August	Summer
September	Fall
October	Fall
November	Fall
December	Winter

Table 2-6. Assignments of months to two seasons for use of seasonal inventory files in SMOKE.

Month	Season
January	Winter
February	Winter
March	Winter
April	Winter
May	Summer
June	Summer
July	Summer
August	Summer
September	Summer
October	Winter
November	Winter
December	Winter

2.1.5 SMOKE Processing Categories

Emissions inventories are typically divided into area, on-road mobile, non-road mobile, point, and biogenic source categories. These divisions arise from differing methods for preparing the inventories, different characteristics and attributes of the categories, and how the emissions are processed through models. Generally, emissions inventories are divided into the following source categories, which we refer to later as "SMOKE processing categories."

- Stationary Area Sources: Sources that are treated as being spread over a spatial extent (usually a county or air district) and that are not movable (as compared to non-road mobile and on-road mobile sources). Because it is not possible to collect the emissions at each point of emission, they are estimated over larger regions. Examples of stationary area sources are residential heating and architectural coatings. Numerous sources, such as dry cleaning facilities, may be treated either as stationary area sources or as point sources.

- On-Road Mobile Sources: Vehicular sources that travel on roadways. These sources can be computed either as being spread over a spatial extent or as being assigned to a line location (called a link). Data in on-road inventories can be either emissions or activity data. Activity data consist of vehicle miles traveled (VMT) and, optionally, vehicle speed. Activity data are used when SMOKE will be computing emission factors via another model, such as MOBILE6 (U.S. EPA, 2005). Examples of on-road mobile sources include light-duty gasoline vehicles and heavy-duty diesel vehicles.

- Non-Road Mobile Sources: These sources are engines that do not always travel on roadways. They encompass a wide variety of source types from lawn and garden equipment to locomotives and airplanes. Emission estimates for most non-road sources come from EPA's NONROAD model (OFFROAD in California). The exceptions are emissions for locomotives, airplanes, pleasure craft and commercial marine vessels.

- Point Sources: These are sources that are identified by point locations, typically because they are regulated and their locations are available in regulatory reports. In addition, elevated point sources will have their emissions allocated vertically through the model layers, as opposed to being emitted into only the first model layer. Point sources are often further subdivided into electric generating unit (EGU) sources and non-EGU sources, particularly in criteria inventories in which EGUs are a primary source of NO_x and SO_2. Examples of non-EGU point sources include chemical manufacturers and furniture refinishers. Point sources are included in both criteria and toxics inventories.

- Biogenic Land Use Data: Biogenic land use data characterize the types of vegetation that exist in either county-total or grid cell values. The biogenic land use data in North America are available using two different sets of land use categories: the Biogenic Emissions Landcover Database (BELD) version 2 (BELD2), and the BELD version 3 (BELD3) (CEP, 2004b).

In addition to these standard SMOKE processing categories, we have added other categories either to represent specific emissions processes more accurately or to integrate emissions data that are not compatible with SMOKE. Examples of emissions sectors that fall outside of the SMOKE processing categories include emissions generated from process-based models for representing windblown dust and agricultural ammonia (NH_3) sources. An emissions category with data that are not compatible with SMOKE is one with gridded emissions data sets, such as commercial marine sources. Another nonstandard emissions category that we modeled was emissions from fires. All of the emissions categories that we used to build CENRAP simulations are described in detail in the following sections.

Continuing the enhancement of the emissions source categories that we initiated during the preliminary 2002 modeling, we further refined the categories from the standard definitions listed above to include more explicit emissions sectors. The advantage of using more detailed definitions of the source categories is that it leads to more flexibility in designing control strategies, substituting new inventory or profile data into the modeling, managing the input and output data from SMOKE and conducting QA of the SMOKE outputs. The major drawback to defining more emissions source categories is the increased level of complexity and computational requirements (run times and disk space) that results from having a larger number of input data sets. Another motivation behind separating the various emissions categories is related to the size and flexibility of the input data. Some data sets, like the CENRAP on-road mobile inventory, were so large that we had to process them separately from the rest of the sources in the on-road sector due to computational constraints. We also separated the non-road mobile and ammonia sectors into yearly and monthly inventories to facilitate the application of uniform monthly temporal profiles to the monthly data. Additional details about how we prepared the emissions inventories and ancillary data for modeling are described in Sections 2.2 through 2.16. Table 2-7 summarizes the entire group of source sectors that composed simulation Typ02G. Each emissions sector listed in the table represents an explicit SMOKE simulation. As discussed in Section 2.1.2 below, after finishing all of the source-specific simulations, we used SMOKE to combine all of the data into a single file for each day for input to the air quality modeling systems. Each subsection on the emissions sectors describes each sector in terms of the SMOKE processing category, the year covered by the inventory, and the source(s) of the data.

Additional details about the inventories are also provided, including any modifications that we made to prepare them for input into SMOKE.

Table 2-7. CENRAP Typ02G emissions categories.

Emissions Sector	Abbreviation*
Fires as Point Sources (WRAP, CENRAP, VISTAS)	Alf
Area Sources (All domain)	ar
CENRAP area fires	arf
Area fires, Anthropogenic (All domain, excluding WRAP and CENRAP)	arfa
Area fires, Wild (All domain, excluding WRAP)	arfw
Biogenic	b3
Ontario, Canada, point-source fires	bsf
Fugitive dust	fd
WRAP on-road mobile	mb
CENRAP on-road mobile	mbv_CENRAP
Other US on-road mobile	mbv
Monthly CENRAP/MRPO anthropogenic NH_3	nh3m
Ammonia from annual inventory (CENRAP)	nh3y
WRAP anthropogenic NH_3	nh3
Seasonal/Monthly non-road mobile (WRAP, CENRAP, MW)	nrm
Annual non-road mobile	nry
On-road Mobile (Non-US)	nusm
Offshore shipping (Gulf, Atlantic)	ofs
Offshore area (Gulf)	ofsar
Stationary point (All domain, including offshore)	pt
Road dust	rd
Windblown dust (All domain)	wb_dust
WRAP oil and gas	wog

*These abbreviations are used in the file naming of the SMOKE output files for each sector.

Emissions models such as SMOKE are computer programs that convert annual or daily estimates of emissions at the state or county level to hourly emissions fluxes on a uniform spatial grid that are formatted for input to an air quality model. For the Typ02G and Base18G emission inventories we prepared emissions for CMAQ version 4.5 using SMOKE version 2.1 on the UCR Linux computing cluster. SMOKE integrates annual county-level emissions inventories with source-based temporal, spatial, and chemical allocation profiles to create hourly emissions fluxes on a predefined model grid. For elevated sources that require allocation of the emissions to the vertical model layers, SMOKE integrates meteorology data to derive dynamic vertical profiles. In addition to its capacity to represent the standard emissions processing categories, SMOKE is also instrumented with the Biogenic Emissions Inventory System, version 3 (BEIS3) model for estimating biogenic emissions fluxes (U.S. EPA, 2004) and the MOBILE6 model for estimating on-road mobile emissions fluxes from county-level vehicle activity data (U.S. EPA, 2005a).

SMOKE uses C-Shell scripts as user interfaces to set configuration options and call executables. SMOKE is designed with flexible QA capabilities to generate standard and custom reports for checking the emissions modeling process. After modeling all of the source categories individually, including those categories generated outside of SMOKE, we used SMOKE to merge all of the categories together to create a single CMAQ input file per simulation day. Also, for use in the CAMx modeling, we converted the CMAQ-ready emissions estimates to CAMx-ready files using the CMAQ2CAMx converter. Additional technical details about the version of SMOKE used for final simulations are available from CEP (2004b). All scripts, data, and executables used to generate the Typ02G and Base18G emissions for CMAQ and CAMx are archived on the CENRAP computing cluster.

2.1.6 2002 and 2018 Data Sources

This section describes the procedures that the CENRAP followed to collect and prepare all emissions data for Typ02G and Base18G simulations. We discuss the sources of all inventory and ancillary data used for simulations. CENRAP worked with emissions inventory contractors, other RPOs, and EPA to collect all of the data that constitute the simulation. Table 2-8 lists all of the contacts for the various U.S. anthropogenic emission inventories we used. For the CENRAP inventories, this table lists the contacts for the contractors who prepared the inventories; for the non-CENRAP inventories it lists the contacts at the RPOs who provided us inventory data. We obtained the emissions inventories for Canada and Mexico from the U.S. EPA Emissions Factors and Inventory Group (EFIG) via the Clearinghouse for Inventories and Emissions Factors (CHIEF) website (http://www.epa.gov/ttn/chief/index.html).

Table 2-8. CENRAP anthropogenic emissions inventory contacts.

Source Category	Emissions Data Contact
WRAP	
All	Tom Moore, Western Governors' Association Phone: (970) 491-8837 Email: mooret@cira.colostate.edu
CENRAP	
2002 Consolidated Inventory	Randy Strait, E.H. Pechan & Assoc., Inc. Phone: 919-493-3144 Email: rstrait@pechan.com
NH3 Inventory, Prescribed and Agricultural Fires, and On-road mobile emissions	Dana Sullivan, Sonoma Technology, Inc. Phone: 707-665-9900 Email: dana@sonomatech.com
Gulf Off-shore platform and support vessel emissions	Holly Ensz, Minerals Management Service Phone: (504) 736-2536 Email: holli.ensz@mms.gov
VISTAS	
All	Greg Stella, Alpine Geophysics, LLC, Phone: 828-675-9045 Email: gms@alpinegeophysics.com
MANE-VU	
All	Megan Schuster, MARAMA, Baltimore, MD USA Phone: 410-467-0170 Email: mschuster@marama.org
MRPO	
All	Mark Janssen, LADCO, Des Plaines, IL, USA Phone: 847-296-2181 Email:janssen@ladco.org

As mentioned above, the refinement of these inventories involved splitting some of the inventory files into more specific source sectors. As the stationary-area-source emissions sector has traditionally been a catch-all for many types of sources, this is the inventory sector that required the greatest amount of preparation. Upon receiving all stationary-area-source inventories we extracted fugitive dust, road dust, anthropogenic NH_3, and for the non-WRAP U.S. inventories, stage II refueling sources. We retained the dust sources as separate categories that we would further refine with the application of transport factors (see Section 2.8).

We collected the ancillary data used for SMOKE modeling from several sources. SMOKE ancillary modeling data include:

- Temporal and chemical allocation factors by state, county, and source classification code (SCC);
- Spatial surrogates and cross-reference files for allocating county-level emissions to the model grid;
- Hourly gridded meteorology data;
- Stack defaults for elevated point sources;
- MOBILE6 configuration files;
- A Federal Implementation Standards (FIPS) codes (i.e., country/state/county codes) definition file;

- A Source Category Classification (SCC) codes definition file;
- A pollutant definition file; and
- Biogenic emission factors.

Except for the meteorology data and the MOBILE6 configuration files, we used default data sets provided by EPA as the basis for all of the ancillary data except for temporal profiles used for Electric Generating Units (EGUs). These profiles were developed based on CEM data from 2000 through 2003 (Pechan and CEP, 2005c). CENRAP provided the meteorology data for the simulations at 36-km and 12-km grid resolutions (Johnson, 2007). The inventory contractor who prepared the MOBILE6 inventories provided the MOBILE6 configuration files either directly or via an RPO representative; details about the sources of the MOBILE6 inputs are provided in Section 2.4. We made minor modifications to the chemical allocation, pollutant definition, and country/state/county codes files for new sources, pollutants, or counties contained in the inventories that we had not previously modeled. We made major modifications to the temporal and spatial allocation inputs, as described below.

2.1.7 Temporal Allocation

Temporally allocating annual, daily, or hourly emissions inventories in SMOKE involves combining a temporal cross-reference file and a temporal profiles file.

- Temporal cross-reference files associate monthly, weekly, and diurnal temporal profile codes with specific inventory sources, through a combination of a FIPS (country/state/county) code, an SCC, and sometimes for point sources, facility and unit identification codes.
- Temporal profiles files contain coded monthly, weekly, and diurnal profiles in terms of a percentage of emissions allocated to each temporal unit (e.g., percentage of emissions per month, weekday, or hour).

As a starting point for the temporal allocation data for simulations, we used the files generated by emission inventory contractors (Pechan and CEP, 2005c). Based on guidance from the developers of some of the inventory files, we enhanced the temporal profiles and assignments for some source categories (Pechan, 2005b).

We modified the temporal allocation data for the simulations to improve the representation of temporal emissions patterns for certain source categories. We implemented the adjusted profiles in SMOKE by modifying the temporal cross-reference file for the applicable FIPS and SCC combinations.

Updated temporal profiles for EGUs were made available for MRPO in the MRPO Base K inventory. Since the non-road emissions for IA and MN were monthly emissions developed by MRPO, new temporal profiles were created for all the SCCs in these emissions files for these two states only. The monthly profile was uniform and the weekly and diurnal profiles were kept the same as were modeled for the rest of the country.

An updated temporal profile, profile 485, based on NOAA 1971-2000 population weighted average heating degree days for home heating area source emissions was obtained from