APPENDIX 8-3: QUALITY ASSURANCE PROJECT PLAN FOR CENTRAL REGIONAL AIR PLANNING ASSOCIATION EMISSIONS AND AIR QUALITY MODELING

Quality Assurance Project Plan (Draft)

For

Central Regional Air Planning Association (CENRAP)

Emissions and Air Quality Modeling

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1.0 INTRODUCTION

This Quality Assurance Project Plan (QAPP) describes the quality management functions and activities performed by the Central Regional Air Planning Association (CENRAP) 2002 current and 2018 future-year annual Emissions and Air Quality Modeling, performed by ENVIRON International Corporation and the University of California at Riverside College of Engineering – Center for Environmental Research and Technology (UCR/CE-CERT). This is the third revision (Revision 3) of the CENRAP Emissions and Air Quality Modeling QAPP and updates Revision 2 of the QAPP dated December 23, 2004. Revision 3 of the CENRAP Modeling QAPP updates the QAPP to include additional modeling analysis added with the CENRAP additional Award of Work dated December 15, 2005.

CENRAP is one of five Regional Planning Organizations (RPOs) that have responsibility for coordinating development of State Implementation Plans (SIPs) and Tribal Implementation Plans (TIPs) in selected areas of the U.S. to address the requirements of the EPA Regional Haze Rule (RHR). The RHR visibility SIPs/TIPs are due in 2007/2008. CENRAP modeling results may also form the regional component for 8-hour ozone and fine particulate ($PM_{2.5}$) SIPs/TIPs that are also expected to be due in 2007/2008. The CENRAP Emissions and Air Quality Modeling Team is comprised of staff from ENVIRON International Corporation (ENVIRON) and the University of California, Riverside (UCR). The ENVIRON/UCR Team will perform 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 EPA RHR.

The quality assurance approach utilized herein is generally based on the national consensus standard (ANSI/ASQC, 1994). This standard describes the necessary management and technical elements for developing and implementing a quality system. It recommends a tiered approach to the design of the specific quality system used in each of the organization's efforts. This approach has been adopted by the ENVIRON/UCR Team and is documented in the CENRAP 2002 Annual Modeling Protocol (ENVIRON and UCR, 2004) and in UCR's Quality Management Plan (QMP; UCR, 2003). The CENRAP Modeling Protocol and UCR's QMP formed the basis for much of the content in this CENRAP Emissions and Air Quality Modeling QAPP.

This QAPP was prepared in accordance with the EPA guidelines for quality assurance project plans for modeling (EPA, 2002), for QAPPs (EPA, 2001), and 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/policy applications. In order to utilize 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 guidance document for modeling:

- 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 problem; and
- Output data that can be used to help inform decision makers.

The purpose of this QAPP is to establish and encourage a continuous improvement process that will result in clearly defined data quality objectives, documentation, procedures, and requirements for QA benchmarks and reports. A rigorous quality system will assist in ensuring that the quality of the project products are known, defensible, and meet the user's data quality objectives. This system will also enable the modeling team to systematically plan to accommodate the additional work that will be required to ensure high-quality results.

1.1 Problem Definition

The 1990 Amendments to the Clean Air Act and the 1999 U.S. EPA Regional Haze Rule establishes special goals for visibility in 156 national parks, wilderness areas, and international parks. Through these amendments, Congress set a national goal for visibility as "the prevention of any future, and the remedying of any existing, impairment of visibility in mandatory Class I Federal areas which impairment results from manmade air pollution" (40 CFR 51.300). States are required to develop State Implementation Plans (SIPs) to attain visibility standards, and Tribes also may opt to assume responsibility for visibility programs under 40 CFR Part 49 by developing Tribal Implementation Plans (TIPs). States, and potentially Tribes, in the Central States are required to submit visibility SIPs under Section 308 of the Regional Haze Rule (RHR).

The Central Regional Air Planning Association (CENRAP) has implemented a regional air quality planning process to provide the necessary technical and policy tools needed by states and tribes to comply with Section 308 of the RHR. As part of this effort, CENRAP has funded modeling studies to support the development of SIPs and TIPs. In October 2004, CENRAP retained ENVIRON International Corporation and the University of California at Riverside (UCR) to perform Emissions and Air Quality Modeling of the 2002 annual period.

The results from these modeling studies will help determine the proper mitigation measures that will be necessary to comply with Section 308 of the RHR.

2.0 PROJECT DESCRIPTION

2.1 Background

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 governing body of CENRAP is the Policy Oversight Group (POG) that is made up of 18 voting members representing the 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 see Table 3-1 for contact information):

- 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 has been formed).

The RHR requires the states (the tribes may elect) to submit the first SIPs and TIPs in 2007/2008 that address progress toward natural conditions at federally mandated Class I areas. 40 CFR 51.308 (Section 308) discusses the following five 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. Long-term strategy for regional haze;
4. 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 manmade effects on visibility impairment at Class I areas. One component of this support is performing emissions and air quality modeling to obtain a better understanding of the causes of regional haze and potential mitigation measures for visibility impairment at Class I areas, to evaluate the effects of alternative control strategies for improving visibility, and for projecting future-year air quality and visibility conditions. In October 2004, CENRAP selected a team of ENVIRON and UCR to perform their initial current and future year Emissions and Air Quality Modeling for the 2002 annual period. In December 2005 CENRAP awarded additional work to ENVIRON and UCR to perform 2018 control strategy evaluation, PM source apportionment and prepare a Technical Support Document (TSD) for the modeling as part of the RHR visibility SIP due in December 2007.

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 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 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.

2.2 CENRAP Long Range Plan

CENRAP adopted an initial Long Range Plan in October 2003 (CENRAP, 2003) and will review this plan each spring and fall and update it as needed. The CENRAP Long Range Plan is organized into four primary tiers of work efforts: (1) Tasks; (2) Activities; (3) Projects; and (4) Deliverables. The CENRAP long-range plan was updated in the spring 2005 and was approved by the CENRAP POG on March 2-3, 2005 (http://www.cenrap.org/organization.asp#).

2.2.1 Tier One: Tasks

The first tier of the CENRAP Long Range Plan consists of a series of work efforts or Tasks that comprise the statuary requirements of the Regional Haze Rule (RHR):

- Develop reasonable progress goals;
- Establish baseline and natural conditions;
- Develop a long term strategy for reducing regional haze;
- Develop a monitoring strategy and other SIP/TIP requirements; and
- Establish BART requirements.

Each of these Tasks must be accomplished to achieve the goal of providing states and tribes the information upon which supportable and effective RHR SIPs and TIPs will be developed.

2.2.2 Tier Two: Activities

The second tier (Activities) consists of broad, categorized work efforts that must be completed in order to complete a Task. For example, the 2002 annual Emissions and Air Quality Modeling effort is an Activity that needs to be completed in order to perform the “develop reasonable progress goals” and “develop a long term strategy for reducing regional haze” Tasks.

2.2.3 Tier Three: Projects

The third tier consists of specific Projects aimed at completing an Activity. For example, to perform the 2002 annual modeling, 2002 emissions are needed, thus a specific project would be to compile 2002 emissions for the CENRAP states and to provide them to the Emissions and Air Quality Modeling Team. Details on specific projects are identified in the Attachments to the Updated CENRAP Long Range Plan (CENRAP, 2005).

2.2.4 Tier Four: Deliverables

The fourth and final tier is the Deliverables that consist of the individual components of the work effort necessary to complete a given Project. Deliverables for the 2002 Annual Emissions and Air Quality Modeling activities will include a Modeling Protocol, a QAPP, Base Case Modeling and Model Performance Evaluation Report, PowerPoint presentations of future-year base case modeling, control strategy evaluations and PM source apportionment modeling and a draft and final technical Support Document (TSD) that describes the modeling and is suitable for including with the visibility SIP due December 2007.

2.2.5 Critical Milestones Dates

The Updated CENRAP Long Range Plan (CENRAP, 2005) contains a series of milestone dates by which critical decisions must be made to address a regulatory or statutory deadline. Critical milestone dates were assigned to the following activities:

- SIP submittal;
- SIP and TIP drafting and approval;
- Conducting future-year modeling; and
- Conducting base case modeling.

The Updated CENRAP Long Range Plan back-calculated critical milestone dates from the date that the RHR SIPs/TIPs are required to be submitted and developed the following timeline (see Attachment 2 of Updated CENRAP Long Range Plan):

> SIP/TIPs Adopted and States Submit SIP to EPA – December 17, 2007: Although SIP/TIP may be submitted later with the $PM_{2.5}$ SIP due April 2008, CENRAP is adopting the December 2007 submittal date in developing their critical milestone dates to assure that CENRAP obtains the information necessary to develop the RHR SIP/TIPs in a timely fashion.
>
> States and Tribes Begin to Draft and Adopt SIPs and TIPs – July 1, 2006: A survey of the timelines for SIP approval for states in the CENRAP region indicates that the states can draft and adopt a SIP as long as the technical analysis has been completed 18 months in advance.
>
> Future-Year Modeling Begins – May 1, 2005: States are to provide BART reduction estimates and/or market trading estimates for their BART sources.
>
> Base Case Modeling Begins – February 1, 2005: The CENRAP Modeling Workgroup has estimated that it will take six months to perform base year base case modeling and model performance evaluation.

2.2.6 Role of Emissions and Air Quality Modeling in CENRAP Long Range Plan

As seen above, the 2002 Annual Emissions and Air Quality Modeling is a critical part of the overall CENRAP efforts and is an essential component for the development of the RHR SIPs and TIPs. The modeling information must be of high quality and reliability in order to develop effective RHR control strategies. Thus, comprehensive and exhaustive quality assurance (QA) and quality control (QC) techniques are necessary.

2.3 Quality Assurance of the CENRAP 2002 Annual Emissions and Air Quality Modeling

The CENRAP 2002 annual Emissions and Air Quality Modeling includes annual emissions and PM/regional haze simulations using a 36 km grid covering the continental US and adjacent regions, plus simulation of additional shorter duration episodes using a 12 km grid covering the Central States. After detailed performance testing, the modeling system will then be exercised with a variety of emissions control scenarios aimed at enabling CENRAP to assess the effects of future year emission control strategies on visibility and other air quality issues. The modeling system will also allow CENRAP to track reasonable progress toward regional haze goals. More specifically, the CENRAP Emissions and Air Quality Modeling effort will focus on the use of the SMOKE emissions and CMAQ and CAMx air quality modeling systems for calendar year 2002 over the Inter-RPO continental US 36 km horizontal grid, as well as potentially the CENRAP Central States 12 km grid.

2.3.1 Past Related Regional Modeling Studies

The CENRAP 2002 annual Emissions and Air Quality Modeling activities are built off of previous regional emissions, photochemical PM and visibility modeling efforts performed in the Central States and across the United States. The procedures used in these previous studies provide a guide to the modeling and QA approach for the CENRAP 2002 annual Emissions and Air Quality Modeling:

> Big Bend Regional Aerosol sand Visibility Observational Study (BRAVO): The BRAVO study examined the causes and sources of regional haze at the Big Bend National Park, the most southwesterly Class I area in the CENRAP states. It performed data collection activities, modeling and used numerous techniques to estimate PM source apportionment (Pitchford et al., 2004).
>
> CENRAP Scoping Study: CENRAP commissioned a scoping study to identify the causes of visibility impairment at Class I areas in the CENRAP states and identify the analytical tools that are available to investigate regional haze (Green et al., 2002).
>
> CENRAP Ammonia Emissions Inventory Study: CENRAP sponsored a study to develop an improved ammonia emissions inventory for the CENRAP states (Coe and Reid, 2003).

CENRAP Agricultural and Prescribed Burns Study: In this study improved emissions inventories for prescribed burns and agricultural burning were developed for the CENRAP states (Reid et al., 2004a).

Evaluation of CMAQ and CAMx Models Over the CENRAP States for Three Episodes: CMAQ and CAMx model simulations of a January 2002, July 1999 and July 2001 episodes were evaluated using measurement data in the CENRAP states (Tonnesen and Morris, 2004).

Development of Enhanced Mobile Source and Agricultural Dust Emissions for CENRAP: This study developed on-road and non-road mobile source and agricultural dust emission inventories for the CENRAP states (Reid et al., 2004b).

Development of 2002 Base Case Modeling Inventory for CENRAP: CENRAP sponsored this study to prepare a 2002 Base Case emissions inventory for the CENRAP states that can be used in emissions and photochemical modeling of the 2002 annual period (Strait, Roe and Vukovich, 2004).

Preliminary PM and Visibility Modeling for CENRAP: Under this study preliminary regional PM and visibility modeling was conducted focused on the CENRAP region using the CMAQ and CAMx models (Pun, Chen and Seigneur, 2004).

VISTAS Phase I Model Sensitivity and Evaluation Study: This study, sponsored by VISTAS, performed extensive model sensitivity testing and evaluation analysis using the CMAQ and CAMx models and three episodes, January 2002; July 1999 and July 2001 (Morris et al., 2004a).

WRAP Section 309 SIP/TIP Modeling Analysis: The WRAP performed a study to generate the necessary modeling data needed to develop Section 309 SIP/TIP for states that opt-in to this program (Tonnesen et al., 2003).

VISTAS Phase II 2002 Annual Modeling: VISTAS is performing annual modeling of 2002 using a continental US 36 km domain and eastern US 12 km domain with attendant model evaluation and sensitivity analysis (Morris et al., 2004b).

Many of the above studies are providing data (e.g., emissions) that will be used in the CENRAP Emissions and Air Quality Modeling Study. Consequently, the quality assurance (QA) and quality control (QC) procedures employed are directly relevant to this QAPP. Others are companion modeling studies (e.g., BRAVO, VISTAS and WRAP) that provide information used in the development of this QAPP and the CENRAP Emissions and Air Quality Modeling Protocol (ENVIRON and UCR, 2004).

2.3.2 QA for the CENRAP 2002 Annual Emissions and Air Quality Modeling

The CENRAP 2002 annual Emissions and Air Quality Modeling Study will use 36km MM5 meteorological data provided by the Iowa Department of Natural Resources (IDNR) (Johnson,

2004), 12km MM5 meteorological data provide by other CENRAP participants and emissions data provided by CENRAP contractors (Strait, Roe and Vukovich, 2004) and EPA. These data will be used to perform emissions and air quality modeling of the 2002 annual period on a 36 km grid and for episodes of shorter duration using a 12 km grid. Additional annual 12 km modeling may also be performed.

Closely integrated with the annual (and possibly episodic) meteorological, emissions and air quality modeling will be ongoing project management, technical review, and QA activities performed under the guidance of the CENRAP Project Manager, CENRAP Administrative Project Manager and the CENRAP Modeling Workgroup. The modeling team members will conduct regular monthly conference calls with CENRAP management, as well as ad hoc topical conference calls as needed, and will attend periodic meetings with the CENRAP Modeling Workgroup as needed.

Complementing the data acquisition, modeling input development activities, and project management activities, the following four other CENRAP Emissions and Air Quality Modeling activities/functions will be performed, consistent with the QAPP and CENRAP's Long Range Plan:

2.3.2.1 Data Gatekeeping

The CENRAP Emissions and Air Quality Modeling Team are receiving emissions, meteorological and air quality data from other CENRAP contractors, participants, or other sources. As a first line of QA, we have defined a Gatekeeping function to assure that the data have been received correctly, the quality of the data has been evaluated, and that the data received have been documented. Separate air quality, meteorological and emissions Gatekeepers have been identified whose roles are defined below. In addition, a Data Management Gatekeeper has been defined who will post data, reports and results to the project website and archive all key data generated in the project.

- **Air Quality Data Gatekeeper**. Obtains air quality data as appropriate for model input development and model performance evaluation and assures that the quality of all air quality data obtained are consistent with the approved QAPP. Provides documentation of evaluation and generate IC/BC inputs for CMAQ and CAMx for all modeling runs.

- **Meteorological Gatekeeper**. Obtains meteorological data as MM5 files for annual 2002 modeling runs (36 km) and other episode periods (12 km) and performs data quality checks as approved in the QAPP, together with the appropriate documentation of model performance evaluation activities.

- **Emissions Gatekeeper.** Obtains emissions inventory data for CENRAP states from the CENRAP emissions contractor (Strait, Roe and Vukovich, 2004) necessary to support annual 2002 and future year modeling and recommend source of emissions data to be used for non-CENRAP states, Canada and Mexico. Assures quality of all emissions data received are consistent with the approved QAPP, and develops all emissions modeling files to support modeling runs for 2002. Develops the chemical speciation files and

temporal and spatial allocation files necessary to convert annual inventories into hourly and daily emissions modeling files, as appropriate. Develops all emissions modeling files for non-CENRAP states to support modeling runs for future year base case.

- **Data Management Gatekeeper**: Maintains the CENRAP Modeling Website including posting modeling input and output files, reports, interpretation of results, and other documents as requested by CENRAP. This includes, for example, the storage of model inputs and outputs for annual (and episodic) runs and the transfer (via fire wire or alternative media) of electronic files to CENRAP states, other regional planning organizations, EPA, other contractors, and stakeholders.

2.3.2.2 Emissions QA/QC

Emissions Quality Assurance (QA) and Quality Control (QC) are some of the most critical steps in performing air quality modeling studies. Because emissions processing is tedious, time consuming and involves complex manipulation of many different types of large data sets, errors are frequently made in emissions processing and, if rigorous QA measures are not in place, these errors may remain undetected. In the CENRAP Emissions and Air Quality Modeling effort we will perform a multistep emissions QA/QC approach that was developed under WRAP and VISTAS. This includes the initial emissions QA/QC by the Emissions Gatekeeper described above, as well as QA/QC by the Emissions Modeler during the processing of emissions, and then additional QA/QC by the air quality modeler of the processed model ready emission files. This multistep process with three separate groups involved in the QA/QC of the emissions is designed to detect and correct errors prior to the air quality model simulations.

Emissions QA/QC performed as part of the emissions modeling includes:

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

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

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

After the CMAQ-ready emission inputs have been prepared, we will perform additional emissions QA/QC as follows:

Spatial Summary: We will sum the emissions for all layers and for all 24 hours that is used to prepare a PAVE plot showing the daily total emissions spatial distribution. For a 20-day simulation, this produces approximately 20 days x 20 species x 5 emissions categories = 2,000 plots. In our base case simulations these plots will be presented as tons per day. The 5 emission categories typically used are biogenic, fires, on-road mobile, other low-level anthropogenic (area plus non-road) and point sources. If possible, separate spatial QA plots will be generated for low-level and elevated point sources. The objective of this step is to identify errors in spatial distribution of emissions.

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

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

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

Control Strategy Spatial Displays: Spatial summary plots of the daily total emissions differences between a control strategy and base case emissions scenarios will be generated. These plots can be used to immediately identify a problem in a control strategy. For example, if a CENRAP state's SO_2 emissions control strategy is being analyzed and there are changes in emissions for other pollutants or for SO_2 outside of the CENRAP state, problems in emissions processing can be identified prior to the air quality model simulation.

The emissions QA/QC displays are made available to CENRAP participants for review through the project website (see: http://pah.cert.ucr.edu/aqm/cenrap/emissions.shtml).

2.3.2.3 Meteorology QA/QC

Participants performing the 36 km annual and 12 km MM5 modeling will conduct their own QA/QC and evaluation of the meteorological fields. For example, Johnson (2004) and Baller (2004) have performed an initial evaluation of the 36 km MM5 results. In addition, the Emissions and Air Quality Modeling Team will also perform some QA/QC of the meteorological

data to assure that it has been transferred correctly, to obtain an assessment of the quality of the data, and to assist in the interpretation of the air quality modeling results.

The CENRAP Emissions and Air Quality Modeling Meteorological Gatekeeper will perform the following:

- Analyses of the MM5 data to assure that it has been transferred correctly.
- Evaluation of the MM5 data using METSTAT and the surface meteorological network.
- Evaluation of upper-air MM5 meteorological estimates by comparison them to upper-air observations and satellite images.
- Comparison of the CENRAP 2002 36 km MM5 simulation with the ones generated by WRAP and VISTAS.
- Generation of the CMAQ-ready meteorological inputs using the MCIP2.3 processor.

In October 2005 EPA released a new version of the CMAQ modeling system (V4.5) that included a new version of MCIP (MCIP3.0). In order to take full advantage of the new features of CMAQ V4.5 (e.g., Sea Salt emissions, AE3 aerosol module and spatially varying minimum Kz), the MCIP3.0 processor needs to be used. A new version of CAMx is also available (V4.3) that requires use of a new version of MM5CAMx to process ice-phase water. Thus, the following additional work was added to the Meteorological Gatekeepers with the December 2005 contract update:

- Process 36 km and 12 km MM5 data for 2002 using the latest MCIP3.0 and MM5CAMx processors for CMAQ V4.5 and CAMx V4.3.

The Meteorological Gatekeeper report evaluation of the CENRAP 36 km MM5 results and comparison with the VISTAS and WRAP 36 km MM5 runs can be found on the project website (http://pah.cert.ucr.edu/aqm/cenrap/ppt_files/CENRAP_VISTAS_WRAP_2002_36km_MM5_eval.ppt).

2.3.2.4 Air Quality Modeling QA/QC

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

- Verification that correct configuration and science options are used in compiling and running each model in the CMAQ modeling system, where these include the MCIP, JPROC, ICON, BCOM and the CCTM. Same procedures for the CAMx modeling system that includes MM5CAMx and TUV.
- Verification that the correct configuration and science options are used in running each model in the CAMx modeling system where these include MM5CAMx, TUV, CAMx, and the CMAQ-to-CAMx emissions and IC/BC processors.

- Verification that correct input data sets are used when running each model.
- Evaluation of CCTM and CAMx results to verify that model output is reasonable and consistent with general expectations.
- Processing of ambient monitoring data for use in the model performance evaluation.
- Evaluation of the CCTM and CAMx results against concurrent observations and each other.
- Backup and archiving of critical model input data.

The most critical element for CMAQ and CAMx simulations is the QA/QC of the meteorological and emissions input files, which is discussed above. The major QA issue specifically associated with the air quality model simulations is verification that the correct science options were specified in the model itself and that the correct input files were used when running the model. For CMAQ modeling we have employed a system of naming conventions using environment variables in the compile and run scripts that guarantee that correct inputs and science options are used. Similar procedures are used in CAMx modeling using file and directory naming conventions. We also have employed a redundant naming system so that the names of key science options or inputs are included in the name of the CMAQ and CAMx executable program, in the name of the CMAQ and CAMx output files, and in the name of the directory in which the files are located. This is accomplished by using the environment variables in the scripts to specify the names and locations of key input files.

A second key QA procedure is to never "recycle" run scripts, i.e., we always preserve the original runs scripts and directory structure that were used in performing a model simulation.

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

2.3.2.5 Overview of Data Flow and Quality Assurance Process

Figures 2-1a and 2-1b display an overview of the data flow and quality assurance process in the CENRAP Emissions and Air Quality Modeling study. The CENRAP Modeling Team receives different types of data from various CENRAP participants and contractors and other sources that have performed their own QA and QC. Whenever data are received by the Modeling Team, it is

first subjected to a QA check by a Gatekeeper who assess the accuracy and quality of the data and prepares a summary presentation on the QA check. Figure 2-1a lists the Gatekeepers in the Modeling Team for emissions, boundary conditions, meteorological, ozone column (TOMS) and air quality data. If the Gatekeeper identifies any problems with the data, the provider of the data is contacted and asked to correct the data. After the Gatekeeper has conducted a QA check of the data it is passed on to the modeler who performs their own QA of the data. The data are then used in the modeling and resultant output (e.g., model-ready emissions or meteorological files), and are then subjected to another round of QA to assure the integrity of the data is retained.

After the model-ready inputs have been developed and subjected to QA/QC, the models (e.g., CMAQ and/or CAMx) will be applied using Base Case emissions and the modeling results will be subjected to a model performance evaluation. The model performance evaluation (MPE) represents an extensive QA effort and is one of the most time consuming components of the study. EPA has developed draft guidance for evaluating regional PM and haze models that includes performance goals (EPA, 2001). In addition, the Modeling Team has adapted EPA MPE approaches and goals for 1-hour (EPA, 1991) and 8-hour (EPA, 1999) ozone modeling. The CENRAP Modeling Team will perform the MPE/QA process using as many different tools and analyses as possible in order to fully understand the accuracy, uncertainty and reliability of the model simulation. As seen in Figure 2-1b, the MPE process in CENRAP is a multistep process using several different techniques:

UCR Analysis Tools: The University of California at Riverside (UCR) Analysis Tools were used extensively in Phase I and are run on a Linux platform separately for each network. Graphics are automatically generated using gnuplot and the software generates the following:

- Tabular statistical measures;
- Time Series Plots; and
- Scatter Plots by allsite_allday, allday_onesite and allsite_oneday.

ENVIRON Analysis Tools: ENVIRON has developed specialized evaluation tools to analyze visibility model performance for the Best and Worst 20% visibility days that are used in visibility projections for the Section 308 SIPs/TIPs. ENVIRON has also developed "Soccer Plots" that displays model performance across networks, episodes, species, models and sensitivity tests and compare them with performance goals. As part of VISTAS, the Georgia DNR has developed "Bugle Plots" that display model performance as a function of observed concentration that have been integrated with ENVIRON's evaluation tools.

CENRAP Model Evaluation Tool: CENRAP has developed a model evaluation tool that includes the observations in a MySQL database for ease of manipulation of the observation database. The CENRAP model evaluation tool can interface with Excel and/or gnuplot to generate the usual set of scatter plots, time series plots and similar visual tools.

The evaluation of the CENRAP 2002 CMAQ Base Case simulation will use each of the analysis tools listed above to take advantage of their different descriptive and complimentary nature. The use of multiple model evaluation tools is also a useful QA/QC procedure to assure that errors are not introduced in the model evaluation process.

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

In the CENRAP 2002 CMAQ Base Case modeling, we have adopted three levels of model performance goals for bias and gross error, as listed in Table 2-1, that are used to help evaluate model performance. Note that we are not suggesting that these performance goals be generally adopted or that they are the most appropriate goals to use. Rather, we are just using them to frame and put the PM model performance into context and to facilitate model performance intercomparisons across episodes, species, models and sensitivity tests.

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

- Asymptotically approaching proposed performance goals or criteria when the mean of the observed concentrations is greater than 2.5 $\mu g/m^3$.
- Approaching 200% error and ±200% bias when the mean of the observed concentrations are extremely small.

Dr. Boylan uses bias/error goals and criteria of ±30%/50% and ±60%/75% and plots bias and error as a function of average observed concentrations. As the mean observed concentration approaches zero the bias performance goal and criteria flare out to ±200% creating a horn shape, hence the name "Bugle Plots."

Table 2-1. Model performance goals used in Phase I to help interpret modeling results.

Fractional Bias	Fractional Error	Comments
#±15%	#35%	Ozone model performance goal for which PM model performance would be considered good.
#±30%	#50%	A level of model performance that we would hope each PM species could meet
#±60%	#75%	At or above this level of performance indicates fundamental problems with the modeling system.

Model performance evaluation statistical measures will be calculated separately for each monitoring network and also stratified temporally and geographically. Because different monitoring networks may use different measurement techniques it is important not to mix them when calculating statistical measures so that the results can be interpreted correctly. For example, the IMPROVE and STN Organic Carbon (OC) measurements contain significant differences. In addition, the calculation of statistical measures by network also allows comparison of model performance at the more urban STN sites versus the more rural IMPROVE and CASTNet sites. The CENRAP region will be divided up into several subdomains for the model evaluation. At a minimum this would include north and south subdomain, but there may also be advantages to further geographic stratifications (e.g., southern CENRAP subdomain could be split into west and east subdomains). Finally, temporal stratifications will be at a minimum by month, but further stratifications will also be performed, including separate evaluation for the Best 20% and Worst 20% visibility days at the Class I areas (i.e., IMPROVE sites).

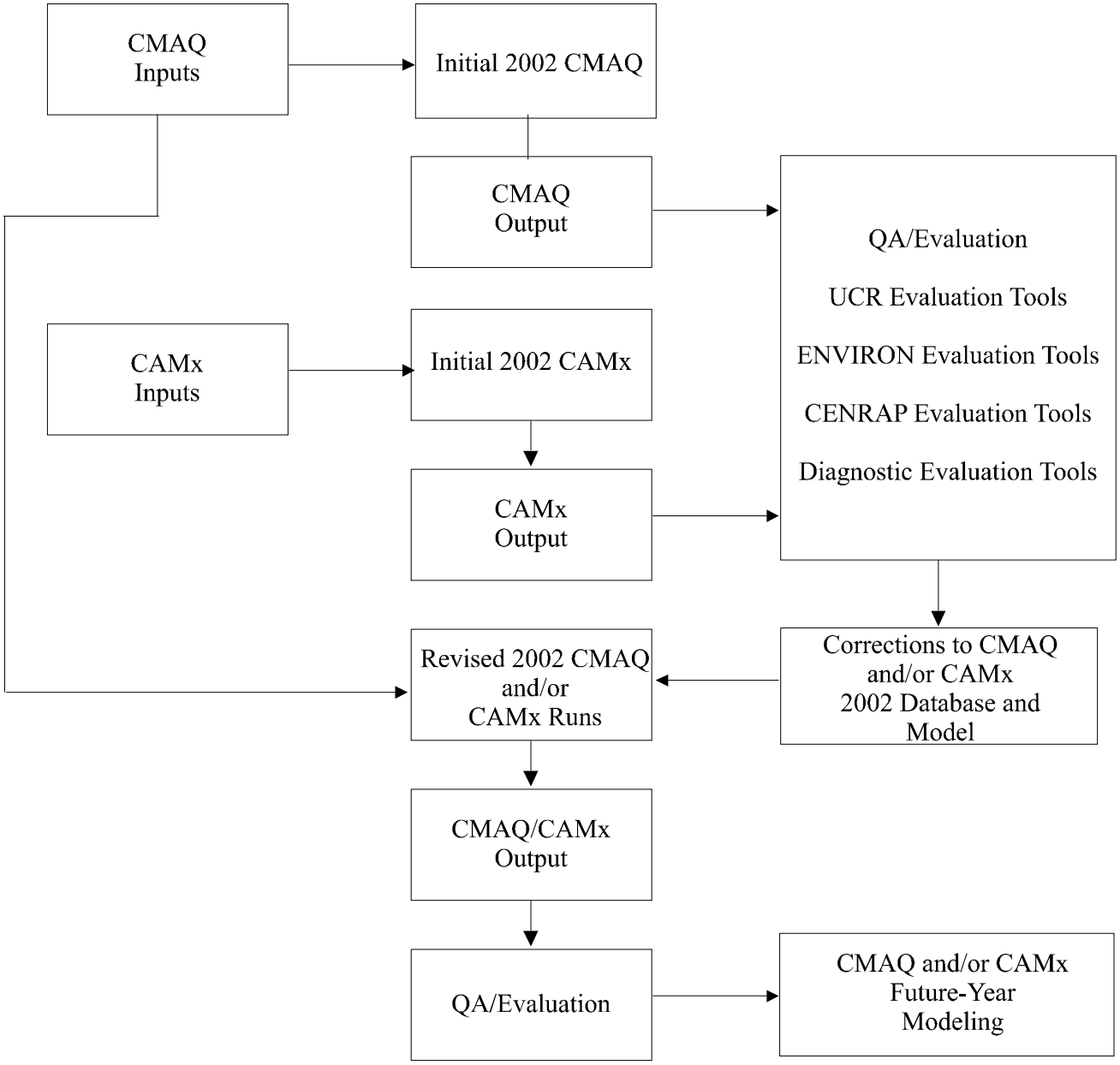

Figure 2-1a. Data flow and quality assurance steps in the CENRAP Emissions and Air Quality Modeling.

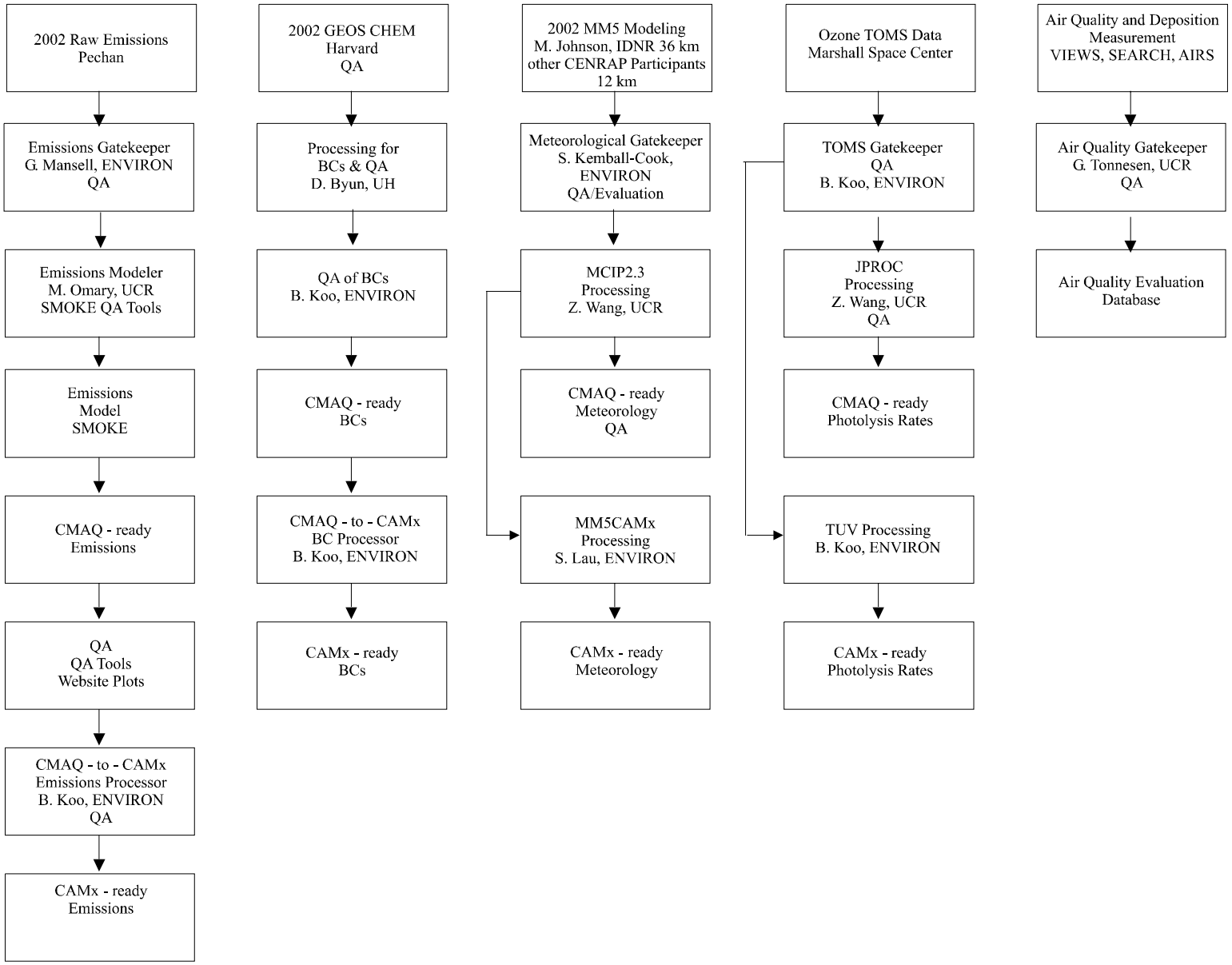

Figure 2-1b. Concluded. Data flow and quality assurance steps in the CENRAP Emissions and Air Quality Modeling.

2.4 Scope of Work for CENRAP 2002 Annual Emissions and Air Quality Modeling

The CENRAP 2002 annual Emissions and Air Quality Modeling work has been funded in two Phases. The first Phase was authorized in a CENRAP Award of Work for ENVIRON/UCR dated October 22, 2004 and revised November 16 and December 16, 2004 and was initially divided up into eight tasks. A ninth task and additional work in other tasks was added to the Phase I work effort in a Change Work Order dated June 8, 2005. The Phase I work effort covers the period of October 2004 through April 2006. The nine Phase I tasks are as follows:

CENRAP Phase I Modeling Tasks

- Task 1-1: Develop Quality Assurance Project Plan (QAPP)
- Task 1-2: Develop Modeling Protocol/Plan for Performing 2002 Base Case Modeling for the CENRAP Region
- Task 1-3: Develop Model-Ready Meteorological Inputs
- Task 1-4: Develop Base Case Model-Ready 2002 Emission Inputs
- Task 1-5: Perform 2002 Base Case Modeling and Model Performance Evaluation
- Task 1-6: Develop Future-Year Base Case Model-Ready Emission Inputs
- Task 1-7: Perform 2018 Modeling, Sensitivity Analysis and Control Strategy Evaluation
- Task 1-8: Reports and Recommendations
- Task 1-9: Processing, Reformatting and Quality Assurance Check of Midwest RPO Emissions Inventory Data

In December 2005 CENRAP issued ENVIRON/UCR an Award of Work dated December 15, 2005 for the Phase II 2002 annual modeling efforts. The Phase II CENRAP 2002 annual Emissions and Air Quality Modeling work is divided up into six tasks and covers the period of December 15, 2005 through December 31, 2006. The six Phase II tasks are as follows:

CENRAP Phase II Modeling Tasks

- Task 2-1: Develop and Update Quality Assurance Project Plan (QAPP) and Modeling Protocol
- Task 2-2: Develop and Update Model-Ready Meteorological Inputs
- Task 2-3: Generate Model-Ready Emissions
  - Subtask 3a: Develop 2018 36 km SMOKE Emissions Modeling for CMAQ and CAMx
  - Subtask 3b: Develop 2018 12 km Emissions for CAMx using Flexi-Nesting
- Task 2-4: Perform 2018 Base Case Modeling
  - Subtask 2-4a: 2018 Base Case Modeling using CMAQ
  - Subtask 2-4b: 2018 Base Case modeling using CAMx
  - Subtask 2-4c: Up to 8 Sensitivity Runs with CMAQ
  - Subtask 2-4d: Up to 8 Sensitivity Runs with CAMx
    - Subtask 2-4e1: 2018 PM Source Apportionment (CAMx/PSAT) for SO4, NO3, NH4 and Primary PM

        - Subtask 2-4e2: 2018 PM Source Apportionment (CAMx/PSAT) for SOA
    - Subtask 2-4f: 2018 12 km "Flexi-Nesting" CMAQ and CAMx Model Runs
    - Subtask 2-4g: Generate a Report on Model Results
- Task 2-5: Refine Perform 2002 Base Case Modeling and Model Performance Evaluation
- Task 2-6: Generate a Final Report for inclusion in the CENRAP Technical Support Document (TSD)

The previous studies discussed in Section 2.3.1 form the foundation for the CENRAP modeling and associated model QA/QC procedures. An important component of the QA/QC process is strong project management and project direction, which is discussed next.

2.4.1 Project Management

There are three aspects of Project Management that are being performed under this task: (a) Project Management of the project's resources and technical progress keeping CENRAP informed of progress; (b) Technical Management of the day-to-day technical activities of the ENVIRON/UCR Team keeping clear lines of communication, and (c) Communication Management of the data flow and expectations among the other CENRAP contractors.

Project Management: The Modeling Team Project Manager, Co-Principal Investigators (Co-PIs), and Task Managers have frequent communications with the CENRAP Project Manager and Administrative Project Manager through regular conference calls, e-mails and meetings as needed. The ENVIRON and UCR Modeling Centers are headed by the two Co-PIs (Ralph Morris and Gail Tonnesen, respectively) with clear lines of communication and authority.

Technical Management: The two Co-PIs will be responsible and accountable for the management of the technical work within each of their respective research groups.

Communication Management: Key to the communications management will be weekly internal conference calls among the two Co-Principal Investigators and the regular conference calls between the two Co-PIs and the CENRAP Project Manager, Administrative Project Manager and Modeling Workgroup and other CENRAP contractors and participants. When data are received from CENRAP contractors or other sources, the CENRAP Modeling Team's meteorological or emissions Gatekeeper will subject the data to extensive QA screening. Any problems identified will be reported to the two Co-PIs who will then immediately relay that information to the CENRAP Project Manager and Administrative Project Manager and the relevant contractor/participant with the issue addressed in a conference call so that it can be resolved. List servers related to emissions, meteorology, and modeling issues will be set up for prompt communication among the Modeling Team, CENRAP, and other CENRAP contractors.

2.4.2 PHASE I MODELING TASKS

2.4.2.1 Task 1-1: Develop and Update Quality Assurance Project Plan (QAPP) and Modeling Protocol

The objective of this task is to prepare a Quality Assurance Project Plan (QAPP) and Modeling Protocol that documents the procedures for developing all model inputs, identifying sources of databases, identifying procedures for QA model inputs, developing model performance metrics and methodologies and is approvable by EPA. A QAPP will be prepared in accordance with EPA's Quality Assurance Manuals including the "Guidance for Quality Assurance Project Plans for Modeling – EPA QA/G-5M" (EPA, 2002). EPA has developed specific format and content for QAPPs that will be followed. The steps that will be carried out to accomplish this task are as follows:

- A preliminary draft CENRAP modeling QAPP and Modeling Protocol will be prepared following EPA guidelines using a preliminary CENRAP Modeling Protocol developed under Task 1-2, CENRAP SOW and the CENRAP Long Range Plan.
- The two Co-PIs will review and update the QAPP.
- A final review of the draft QAPP will be performed to assure it adheres to EPA guidance.
- The draft QAPP will be submitted to CENRAP. If comments are received from CENRAP, the draft QAPP will be revised and submitted to CENRAP who will then submit the QAPP to EPA.

Table 2-2 summarizes the Task 1-1 deliverables and schedule.

Table 2-2. Task 1-1: Develop Quality Assurance Project Plan (QAPP) and Modeling Protocol.

Item	Description	Due Date
1	Draft QAPP	11/19/04
2	Draft Final QAPP	Within 1 week of comments

2.4.2.2 Task 1-2: Develop Modeling Protocol/Work Plan for Performing 2002 Base Case Modeling for the CENRAP Region

The objective of this task is to develop a Modeling Protocol/Work Plan (MP/WP) that describes the CENRAP modeling approach including a review of recent relevant regional modeling studies, sources of data, modeling approach, model evaluation approach and criteria, and schedule for completion.

A Modeling Protocol/Work Plan (MP/WP) will be prepared that summarizes current regional modeling studies, proposed modeling domain and grid selection, proposed model configurations, details model input preparation, design of model evaluation and sensitivity runs, discussions of model performance evaluation criteria, an assessment of uncertainties and actions needed to obtain better performance, and recommendations for future control strategy modeling. The

MP/WP will also describe the procedures that will be used to complete each task in this project. The MP/WP will also identify a list of input files and resource needs that will be used for the model assessment, as well as the suite of modeling systems (i.e. air quality, emissions, and meteorological modeling platforms) that it intends to evaluate. The Task 1-2 draft MP/WP will be prepared concurrently with the QAPP and be submitted to CENRAP for approval before initiating Tasks 1-3 through 1-9. CENRAP may provide comments on the draft MP/WP and ENVIRON/UCR will revise the MP/WP and submit a revised draft MP/WP to CENRAP within one week of receipt of comments. The MP/WP will be updated during the study as needed.

Specific steps in the development of the CENRAP modeling MP/WP are as follows:

- The two Co-PIs will be responsible for developing the MP/WP.
- A preliminary draft CENRAP modeling MP/WP will be prepared by adapting and enhancing the VISTAS Phase II Modeling Protocol to include CENRAP-specific issues and incorporating additional information from the CENRAP SOW, Long Range Plan and preliminary QAPP.
- We will then discuss the CENRAP MP/WP contents with the CENRAP Project Manager and representatives with the results integrated into the draft MP/WP.
- The draft MP/WP will be prepared following EPA guidance for preparing Modeling Protocols for 1-hour ozone (EPA, 1991) and 8-hour ozone (EPA, 1999) and $PM_{2.5}$ and regional haze (EPA, 2001) modeling.

Table 2-3 summarizes the task deliverables and schedule for this task. The draft MP/WP will be submitted to CENRAP within 3 weeks of authorization to proceed with the study. If comments are received from CENRAP, then a revised draft MP/WP will be submitted within one week of receiving comments. The modeling team will continue to update the MP/WP during the project as necessary and in consultation with CENRAP.

Table 2-3. Task 1-2: Develop Modeling Protocol/Plan for Performing 2002 Base Case Modeling for the CENRAP Region.

Item	Description	Due Date
1	Draft Modeling Protocol/Workplan	11/19/04
2	Draft Final Modeling Protocol/Workplan	Within 1 week of comments

2.4.2.3 Task 1-3: Develop Model-Ready Meteorology Inputs

The objective of this task is to develop 2002 meteorological inputs for emissions and air quality modeling. CENRAP Participants (Iowa Department of Natural Resources, IDNR for the 36 km MM5 data, others for the 12 km MM5 data) has conducted MM5 runs to develop 2002 meteorological fields for CENRAP 36 km modeling grid and will conduct 12 km MM5 modeling for episodic periods. The ENVIRON/UCR Team will acquire the CENRAP 2002 36 km and 12 km MM5 outputs and process them using the latest versions of the Models-3 MCIP and MM5CAMx processors to generate hourly 2002 meteorological fields for the CMAQ and CAMx models. Note that EPA has a new version of MCIP (Version 2.3) that includes some improvements (e.g., graupel pass through) and corrections (e.g., correction to errors in the Pleim-

Xiu variables). MCIP version 2.3 will be used in this analysis. There is also a new version of the MM5CAMx processor that includes a new treatment of subgrid-scale cloud processes that will be used in the CENRAP study; this version is currently available on the CAMx website (www.camx.com). We anticipate that MCIP and MM5CAMx will be operated using the PBL pass through option, although if TKE output data are available we may consider using it. Specific steps to be undertaken to complete this task are as follows:

- Acquisition of the 2002 36 km and 12 km MM5 output from CENRAP;
- QA of the MM5 output through the Gatekeeper including running through the existing set up of METSTAT and comparison of model performance with the 2002 MM5 simulations performed by WRAP and VISTAS.
- Processing of the MM5 output using the latest version of the Models-3 MCIP processor to generate 2002 36/12 km meteorological inputs for CMAQ.
- Processing of the MM5 output using the latest version of MM5CAMx to generate 2002 36/12 km meteorological inputs for CAMx.
- QA/QC of the CMAQ and CAMx meteorological inputs.

Assuming receipt of the 2002 MM5 36 km and some of the 12 km model output during November 2004, this task will be completed in December 2004. A PowerPoint presentation on the summary evaluation and comparison of the CENRAP MM5 model performance with WRAP and VISTAS 2002 MM5 runs and QA/QC results will be ready by December 20, 2004. The CMAQ and CAMx 36 km meteorological inputs will be ready no later than December 31, 2004. At this time it is unclear when CENRAP will provide the episodic 12km MM5 output. We anticipate that the Gatekeeper and processing into model-ready inputs will be accomplished within 3 weeks of receiving the 12 km MM5 output. Table 2-4 summarizes the deliverables under this task.

Table 2-4. Task 1-3: Develop Model-Ready Meteorological Inputs.

Item	Description	Due Date
1	Presentation (in electronic form) of Meteorological Gatekeeper evaluation and MCIP/MM5CAMx processing of 2002 36 km MM5 data	12/20/04
2	Model-ready 2002 36 km meteorological inputs for CMAQ and CAMx	12/31/04
3	Model-ready 12km meteorological inputs for CMAQ and CAMx and episodes in 2002	12/31/05

2.4.2.4 Task 1-4: Develop Base Case Model-Ready 2002 Emissions Inputs

The objective of this task is to develop 2002 Base Case model-ready hourly speciated gridded emissions inputs on the 36 km and 12 km grid for the CMAQ and CAMx models. The CENRAP emissions contractors will provide emissions data files for the CENRAP states necessary to develop a model-ready emissions inventory for the 2002 base case. Emissions for the other states, Mexico and Canada will be acquired from EPA and other sources. These data will be

compiled and subjected to QA/QC by the Emissions Gatekeeper using the procedures described previously.

The SMOKE emissions model will be used to process the CENRAP emissions data. The existing WRAP and VISTAS SMOKE setups will be used as the starting point for the SMOKE emissions modeling and be augmented by emissions for CENRAP states and other information provided by CENRAP. There are two 2002 Base Case inventories that need to be developed, an "Actual Base Case" to be used for model performance evaluation and a "Typical Base Case" that is used for future year projections. These and other details (e.g., source data for fire emissions) will be worked out with CENRAP during the development of the Task 2 MP/WP. The provisional steps to be taken to generate the CENRAP CMAQ-ready 2002 Base Case emission inputs will be the following; more details and refinements will be provided to the Task 2 MP/WP after consultation with the CENRAP participants:

1. Yearly, seasonal, monthly or daily ASCII emissions inventories in IDA format for the area and point sources including fire sources.
    a. Area sources will include non-road mobile sources, area sources, wind blown dust, and road dust.
    b. Point sources will include stationary sources with large emissions, and fire sources.
2. Yearly, seasonal, or monthly ASCII vehicle miles traveled (VMT) inventory for on road mobile sources.
3. NetCDF files for gridded land use as input for BEIS3 and the emission factors.
4. Ancillary files which include:
    a. Surrogate files for spatially allocating the area sources emissions,
    b. Temporal and cross reference files for temporal allocation,
    c. Speciation profiles and cross-reference files for chemical allocation.
5. Fire emissions: Will have prescribed burns and agricultural burns for CENTRAP state from CENRAP. WRAP and VISTAS will have prescribed burns, agricultural burns and wildfires for their states.
6. Wind Blown Fugitive Dust: Use data provided by CENRAP, the new ENVIRON/UCR 2002 EI already prepared for WRAP or leave out.
7. Ammonia: Use data provided by CENRAP and the new ENVIRON/UCR 2002 EI already prepared for WRAP.

<u>Emissions for the Entire 36 km Unified Grid Domain:</u>

To process the emissions for CENRAP:

1. All the inventories provided by CENRAP will replace any default CENRAP emissions in the current 2002 emissions inventory that was prepared for WRAP.
2. Any new specific temporal profiles (if provided by CENRAP) will be added to the current EPA temporal profiles and cross-reference files (or default to the values currently being used for WRAP).
3. The EPA spatial surrogate data will be used for area sources (as in WRAP and VISTAS inventories).

4. The EPA Model speciation profiles and cross reference file, which were distributed with SMOKE, will be used for chemical speciation.
5. For the biogenic emissions, the netCDF gridded land use inventory will be used.
6. All the emissions that are meteorology dependent will be processed using the MCIP2.3 files created using MM5 output to be provided by CENRAP.

Emissions Processing QA:

The following QA steps will be performed:

1. Use SMOKE reports to:
    a. QA the inventory for total emissions per state and/or county for spatial allocation.
    b. Check for irregularities in the temporal allocation.
    c. Check for other irregularities, such as vertical allocation, inventory per SCC, etc.
2. Use RMC Post processing QA to create and review:
    a. Spatial vertical daily total emissions,
    b. Daily domain total emissions,
    c. Diurnal domain total emissions, and
    d. Domain total vertical distribution.

Emissions for the 12 km CENRAP Domain:

To process the emissions for 12 km grid cell the following steps will be taken:

1. Establish domain definition.
2. Create new 12 km surrogates by extracting the surrogates for the domain from the EPA 12 km surrogates using SMOKE or a program written by the RMC.
3. Create new gridded netCDF biogenic land use inventory for 12 km cells (not yet available, we are working on a 1-km projection now of the landuse data).
4. Use the same temporal and speciation profiles and cross references as in the 36 km grid cell.
5. Perform QA as in the 36 km grid cell domain.

There are extensive QA protocols in place for emissions modeling that were developed as part of the WRAP and VISTAS modeling efforts. These included both internal SMOKE QA procedures and post-SMOKE QA summaries. A variety of QA summary plots will be posted to the project webpage providing easy access to emissions QA results. In addition, the complete set of QA/QC results will be archived as well as made available to the CENRAP project participants through ftp transfer or CD.

Emissions modeling for the 2002 Base Case will be performed during the December 2004 through February 2005 time period. The deliverables will be a technical memorandum suitable for inclusion as a chapter in the final report and PowerPoint presentation summarizing the 2002 emissions modeling and QA/QC results and the 2002 CMAQ-ready emission inputs for the 36 km domain. Table 2-5 summarizes the deliverables and schedule for the Task 1-4 emissions modeling.

Table 2-5. Task 1-4: Develop Base Case Model-Ready 2002 Emission Inputs.

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	Technical Memorandum on development of 2002 Base Case emissions (Actual and Typical)	02/21/05
3	Presentation (electronic format) on development of 2002 Base Case emissions	02/21/05
4	Model-ready 2002 Actual Base A emissions completed	01/31/05
5	Model-ready 2002 Typical Base A emissions completed	02/28/05
6	Revised model-ready Actual Base Case emissions completed	TBD
7	Revised model-ready Typical Base Case emissions completed	TBD

2.4.2.5 Task 1-5: Perform 2002 Base Case Modeling and Model Performance Evaluation

The objective of this task is to perform 2002 Base Case modeling using the CMAQ and CAMx models and to conduct a model performance evaluation. The first step in this task will be to set up a webpage for the project to disseminate information and post documents and modeling results. The ENVIRON/UCR Team has already set up a CENRAP modeling webpage for the initial modeling analysis work conducted previously at:

http://pah.cert.ucr.edu/aqm/cenrap/index.shtml

We will use the meteorological inputs developed in Task 1-3 and the emissions files developed in Task 1-4 as inputs to the CMAQ model, and perform an initial 2002 Actual Base Case simulation and model evaluation on the 36 km grid. CAMx 2002 emissions and ICBC inputs will be prepared using the CMAQ-to-CAMx processors that will be used along with the meteorological inputs developed in Task 1-3 to perform a 2002 CAMx Base Case simulation. The CMAQ and CAMx model performance evaluation and diagnostic sensitivity tests will be conducted following the procedures in the Task 1-2 MP/WP, along with additional diagnostic tests that are identified during the course of the study. We will conduct 12 km sensitivity tests for several 2002 episodes and the compare model performance with that using a 36 km grid. Our experience with 36/12 km modeling in the southeastern US for VISTAS is that although there can be large differences in model performance at a given time and location, at most times and locations and in general, the performance attributes overall (both good and bad) are very similar.

Based on the model evaluation and diagnostic tests, an optimal model configuration(s) will be identified and, after approval from the CENRAP Project Manager, revised 2002 Actual Base Case simulation(s) and model performance evaluation will be performed. We will also conduct sensitivity analyses and use available probing tools to conduct sensitivity and source apportionment analyses following the procedures in the MP/WP.

Model performance evaluation will be completed using the UCR model performance evaluation (MPE) software, the CENRAP evaluation tool and ENVIRON's performance tools for the AQS, IMPROVE/IMPROVE Protocol, CASTNet, STN, and NADP networks. Data from the St. Louis PM supersite will be analyzed individually taking advantage of the high time, size and species resolved measurements. Standard performance evaluation plots will include time-series and scatter plots for individual and collective CENRAP and nearby sites for each network, and over 20 different model performance metrics will be calculated including several different formulas for estimating bias and error. A variety of summary plots will also be developed including stacked bar plots for individual sites and bugle and soccer plots summarizing performance at all sites in the CENRAP region. We will also examine performance in other subregions.

Specific steps to be taken under this task include:

- Preparation of CMAQ IC/BC and other inputs (e.g., photolysis rates) for 2002 and the CENRAP 36 km and 12 km grids.
- Development of CAMx emissions and IC/BC inputs using the CMAQ-to-CAMx processors and the CMAQ-ready emissions and IC/BC inputs, prepare remainder CAMx 2002 inputs.
- Performance of initial 2002 CMAQ and CAMx 36 km Actual Base Case simulations and 12 km runs for available time periods; conduct model performance evaluation and diagnostic sensitivity tests.
- Performance of diagnostic sensitivity tests, sensitivity analyses and limited source apportionment aimed at correcting potential flaws in the modeling system.
- Identification of optimal model configuration(s) and make recommendations to CENRAP Project for revised 2002 Base Case simulation(s).
- After approval from CENRAP Project Manager, performance of a revised 2002 Actual and Typical Base Case simulation with approved model configuration(s) and conduct a model performance evaluation (MPE).
- Performance of sensitivity analysis using either brute force (i.e., emission reduction) or DDM sensitivities following procedures in Task 2 MP/WP.
- Performance of limited source apportionment modeling using TSSA (CMAQ) and/or PSAT (CAMx), as available.
- Performance of typical 2002 CMAQ and CAMx Base Case runs.
- Preparation of Monthly Progress Reports.
- Preparation of Draft Final and, after receiving comments from CENRAP, preparation of Final Reports.

Table 2-6 summarizes the deliverables and schedule for Task 1-5.

Table 2-6. Task 1-5: Perform 2002 Base Case and Model Performance Evaluation.

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	Recommendations on model configuration	03/15/05
3	Draft Report on 2002 Base Case modeling and model performance evaluation	04/30/05
4	2002 Base Case model simulations completed	04/30/05
5	Second Draft Report on Revised 2002 Base Case modeling and model performance evaluation	TBD

2.4.2.6 Task 1-6: Develop Future Base Case Model-Ready Emission Inputs

The Task 1-6 objective is to develop model-ready 2018 Base Case emission inputs. CENRAP will provide 2018 point, area and non-road emissions data files and/or growth and control factors for CENRAP states necessary to develop a model-ready emissions inventory for the 2018 future case. 2018 emissions for non-CENRAP states will be acquired from the other RPOs (e.g., WRAP and VISTAS). The 2018 mobile emissions will be developed using SMOKE to produce the model-ready emissions data files for 36km/12km modeling grids. The 2002 biogenic emissions prepared under Task 1-3 will be used in the 2018 modeling. It is important that the 2018 emission scenarios be constructed in a consistent fashion to the 2002 Typical Base Case emissions in order to make reliable visibility projections. The steps to be taken to complete this task include:

- Acquisition of 2018 point, area and non-road emissions or projection factors from CENRAP.
- Processing of 2018 point, area and non-road emissions with SMOKE.
- Acquisition of fire emissions and processing by SMOKE.
- Review of 2018 on-road mobile source modeling assumptions, and application of SMOKE to generate 2018 on-road mobile source emissions.
- Merging of 2018 Base Case emissions to generate CMAQ-ready 2018 emissions for the 36 km and 12 km grids.
- Preparation of quality assurance and quality control (QA/QC) plots of the 2018 Base Case emissions.
- Preparation of technical memorandum documenting the development of the 2018 Base Case emissions.
- Preparation of Monthly Progress Reports.

The types of QA/QC plots generated for the 2018 Base Case emissions scenario would be similar to those prepared for the 2002 Base Case discussed previously. In addition, we would generate difference plots of total emissions by major source category (e.g., on-road mobile, fires, point and other anthropogenic) between the 2018 Base Case and 2002 Typical Base Case emissions scenarios. Animations of differences in hourly emissions between the 2018 Base Case and 2002

Typical Base Case emissions scenarios would also be examined to investigate potential errors in temporal allocation.

Table 2-7 summarizes the deliverables under Task 1-6. The 2018 model-ready Base Case emissions and technical memorandum on their development will be provided to CENRAP by April 30, 2005.

Table 2-7. Task 1-6: Develop Future Base Case Model-Ready Emissions Inputs.

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	Technical Memorandum on Future-Year Base Case emissions development	04/30/05
3	Model-ready 2018 Base A emission inputs	04/30/05
4	Model-ready Revised 2018 Base Case emission inputs	TBD

2.4.2.7 Task 1-7: Perform 2018 Modeling, Sensitivity Analysis and Control Strategy Evaluation

The objective of Task 1-7 is to perform 2018 sensitivity and control strategy modeling to support the development of the visibility SIPs/TIPs. Under this task we will conduct 2018 sensitivity and control strategy modeling using the Task 3 meteorological inputs and the Task 6 2018 Base Case emissions inputs. Depending on the results of Tasks 1-1 through 1-5, either the CMAQ model or the CAMx model or both will be used in the 2018 sensitivity and control strategy analysis (decision to be made by CENRAP).

We will recommend model configuration(s), sensitivity tests, model diagnostic tests and source apportionment modeling to the CENRAP Project Manager. Unique features/options of the alternative models will be considered and employed if appropriate. A 2018 modeling approach will be developed with approval of the CENRAP Project Manager. Results will be compared with the annual Base Case simulation and provide a means for corroborative analysis and diagnostic evaluation.

The exact scope of work for the 2018 modeling analysis cannot be completely defined at this time. It is expected that a combination of SMOKE emissions control strategy modeling, CMAQ and/or CAMx emissions sensitivity modeling and use of Probing Tools, such as Decoupled Direct Method (DDM) sensitivity; Process Analysis (PA) and PM Source Apportionment (PSAT and/or TSSA) will be used. At this time it is difficult to speculate which of these Probing Tools will be operational in the PM portions of CMAQ and/or CAMx models at the initiation of this Task in May 2005.

We will provide a Draft Report to the CENRAP Project Manager and Administrative Project Manager summarizing the sensitivity analysis and source apportionment analysis that can be

used to help design effective emissions control strategies. A Final Report on the sensitivity/source apportionment analysis will be submitted to CENRAP within one week of receiving comments.

CENRAP will then provide a list of the control strategy evaluations to be conducted based on the results of the sensitivity and source apportionment analyses that will be modeled using SMOKE and CMAQ and/or alternative models as directed by CENRAP. The control strategy results will be documented as they are performed with final documentation in the Task 1-8 report.

The Draft Report on 2018 sensitivity and source apportionment modeling will be submitted to CENRAP in April 2006, with the Final Report on the sensitivity/apportionment modeling being submitted a week after receiving comments from CENRAP. Results of the 2018 control strategy simulations will be provided to CENRAP as they became available and incorporated into the Task 1-8 report. The Task 1-7 deliverables and their due dates are given in Table 2-8.

Table 2-8. Task 1-7: Perform 2018 Modeling, Sensitivity Analysis and Control Strategy Evaluation.

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	Draft sensitivity and source apportionment report	04/01/06
3	Final sensitivity and source apportionment report	Within 1 week of comments
4	2018 model simulations completed	04/30/06

2.4.2.8 Task 1-8: Reports and Recommendations

The original intent of Task 1-8 was to document the work performed under Tasks 1-3 through 1-7 in reports and develop portions of a Technical Support Document (TSD) for the CENRAP states RHR SIPs/TIPs. However, because of the need to perform emission updates for CENRAP States and other RPOs, the development of the CENRAP RHR SIP/TIP TSD covering the modeling will now be performed in Phase II under Task 2-6.

Table 2-9. Task 1-8: Reports and Recommendations.

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	Draft Technical Support Document (TSD)	See Task 2-6
3	Final Technical Support Document (TSD)	See Task 2-6

2.4.3 PHASE II MODELING TASKS

2.4.3.1 Task 2-1: Revise and Update the CENRAP Modeling Quality Assurance Project Plan (QAPP)

The current CENRAP draft QAPP for Emissions and Air Quality Modeling (Revision 2 dated December 23, 2004) will be updated to include the work to be undertaken under Phase II of the modeling effort and any changes to the Phase I work. A Draft Revision 3 QAPP will be submitted to CENRAP and finalized within one week of receipt of CENRAP comments. Table 2-10 summarizes the Task 2-1 deliverables.

Table 2-10. Task 2-1: Revise and Update CENRAP Modeling QAPP

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	Draft Updated Revision 3 QAPP	March 31, 2006
3	Final Updated Revision 3 QAPP	Within one week of receipt of CENRAP comments

2.4.3.2 Task 2-2: Develop Model-Ready Meteorological Inputs

Since the development of the CMAQ and CAMx meteorological inputs using 36 km MM5 data for the annual 2002 period and 12 km MM5 data for several 2002 episodes under the Phase I Task 1-3, several changes have occurred that require the reprocessing of the MM5 data:

- A new version of CMAQ (V4.5) has been released along with a new version of the CMAQ meteorological processor (MCIP3.0). In order to take advantage of all the features of the new version of CMAQ (e.g., the AE3 aerosol module with Sea Salt and the spatially varying minimum Kz), the MM5 data must be reprocessed using MCIP3.0.
- A new version of CAMx (V4.3) has been released that includes treatment of solid phase precipitation not previously treated and a new MM5CAMx processor is needed to process the MM5 frozen cloud water and precipitation.
- The MM5 model has now been run for 2002 using both a 36 km and 12 km resolution. At the February 6-8, 2006 CENRAP Workgroup meetings it was decided to perform most of the model simulations at 36 km resolution, but process the 12 km MM5 data so that annual 12 km runs could also be made to corroborate the 36 km runs.

Based on these new events, the 2002 MM5 36/12 km annual data will be reprocessed using MCIP3.0 and the latest MM5CAMx to generate new meteorological inputs that can be used to run the latest versions of the CMAQ (V4.5) and CAMx (V4.3) models. Also under this task we will evaluate the 12 km MM5 model and compare its performance with the 36 km MM5 results that were evaluated under Task 1-3 in Phase I.

Table 2-11 summarizes the deliverables and schedule for Tasks 2-2.

Table 2-11. Task 2-2: Develop Model-Ready Meteorological Inputs

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	PowerPoint Presentation on MM5 12 km Evaluation and Comparison with 36 km Results	April 30, 2006
3	Model-ready 36 km and 12 km 2002 annual meteorological inputs for CMAQ and CAMx processed with the latest MCIP3.0 and MM4CAMx processors.	April 20, 2006

2.4.3.3 Task 2-3: Generate Model-Ready Emissions

Under this task we use the SMOKE emissions model to generate CMAQ-ready emissions for the revised 2018 Base Case emissions scenario at 36 km and 2002. CAMx-ready emissions for 2018 Base Case would be generated using the 36 km CMAQ emissions results as was done for 2002. In addition, CAMx 12 km emissions would be generated using flexi-nesting. Table 2-12 lists the deliverables and schedule for Tasks 2-3.

Table 2-12. Task 2-3: General Model-Ready Emissions.

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	Revised 2018 36 km Base Case Model-Ready Emission Inputs for CMAQ and CAMx	Within 6 weeks of receipt of 2018 growth and control factors (estimated March 31, 2006)
3	2018 12 km Emissions for CAMx using Flexi-Nesting	April 15, 2006

2.4.3.4 Task 2-4: Perform 2018 Base Case Modeling

Under this task 2018 Base Case, Sensitivity and Source Apportionment modeling would be conducted. There would be several Subtasks performance as part of this task:

- Subtask 2-4a: 2018 Base Case Modeling with CMAQ
- Subtask 2-4b: 2018 Base Case Modeling with CAMx
- Subtask 2-4c: Conduct up to 8 Sensitivity Runs with CMAQ
- Subtask 2-4d: Conduct up to 8 Sensitivity Runs with CAMx
- Subtask 2-4e: Conduct 2018 36 km CAMx PM Source Apportionment Technology (PSAT) runs for: 2-4e1 – SO4, NO3, NH4 and primary PM; and 4e2 -- SOA.
- Subtask 2-4f: Conduct 2018 12 km "flexi-nesting" CMAQ and CAMx modeling
- Subtask 2-4g: Generate report on modeling results that can be included as part of the TSD (Task 6)

Table 2-13 summarizes the deliverables and schedule for Task 2-4.

Table 2-13. Task 2-4: Perform 2018 Base Case Modeling.

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	2018 Base Case Modeling with CMAQ	May 15, 2006
3	2018 Base Case Modeling with CAMx	May 15, 2006
4	Conduct up to 8 Sensitivity Runs with CMAQ	June 15, 2006
5	Conduct up to 8 Sensitivity Runs with CAMx	June 15, 2006
6	2018 36 km PSAT Runs	May 30, 2006
7	2018 12 km flexi-nesting runs using CMAQ/CAMx	July 15, 2006
8	Draft Report on Modeling Results	July 15, 2006

2.4.3.5 Task 2-5: Refine 2018 Base Case Modeling and Conduct Control Strategy Evaluations

Under this task ENVIRON/UCR would refine the 2018 emissions and air quality modeling. 2018 control strategy modeling will be conducted using information provided by the CENRAP Implementation and Controls Strategies (ICS) Workgroup. The exact control strategies to be evaluated are to be determined (TBD). Table 2-14 summarizes the deliverables and schedule for Task 2-5.

Table 2-14. Task 2-5: Refine 2018 base case modeling and conduct control strategy evaluations.

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	Control strategy evaluations completed	Within 6 weeks of receipt of control strategy definitions from ICS

2.4.3.6 Task 2-6: Final Report for Inclusion as CENRAP Technical Support Document

Under this task ENVIRON/UCR would document all of the modeling results conducted in Phase I and II in a report that would be suitable for inclusion with the CENRAP Regional Haze SIPs/TIPs as the modeling Technical Support Document (TSD). A draft final report (TSD) would be submitted to CENRAP in MSWORD format. Based on comments received from CENRAP, the TSD would be updated and resubmitted. CENRAP and/or CENRAP States and Tribes may make further updates and modifications to the document prior to submission to EPA as part of each State's SIP or Tribe's TIP.

Also under this task we would archive all model inputs and scripts and selected model outputs on USB drives supplied by CENRAP and transfer the data to CENRAP.

Table 2-15. Task 2-6: Final report/Technical Support document (TSD).

Item	Description	Due Date
1	Monthly Progress Reports	2nd week of following month
2	Draft Report/TSD submitted to CENRAP	July 15, 2006
3	Final Report/TSD Submitted to CENRAP	Within 2 weeks of receipt of comments on draft report
4	Disk drives with model inputs and selected outputs	June-July 2006

3.0 PROJECT MANAGEMENT

3.1 Project Organization

This project is being performed by the ENVIRON International Corporation and the University of California at Riverside (UCR), with input from the CENRAP Project Manager, CENRAP Administrative Project Manager, CENRAP Modeling Advisor and CENRAP Modeling Workgroup and other CENRAP Workgroups (e.g., ICS). Organizational commitment is an essential element for developing and implementing a successful research project. Ralph Morris of ENVIRON will be the CENRAP Emissions and Air Quality Modeling Project Manager (PM). The CENRAP Modeling Team has two Co-Principal Investigators that coordinate activities at each of the modeling centers, Ralph Morris of ENVIRON and Gail Tonnesen at UCR. The PM and two Co-PIs will be kept apprised of all project activities, from identifying the need to develop sound experimental and project designs to delivering reports. Commitments to research and project activities, such as those described in this QAPP are made only after the activities are thoroughly reviewed and approved by the PM, Co-PIs and CENRAP Project Manager. Figure 3-1 presents the organizational chart that shows the lines of responsibility and information flow for activities under this project. Table 3-1 lists the project responsibilities for participants in the CENRAP Emissions and Air Quality Modeling study, with more details on their roles provided next.

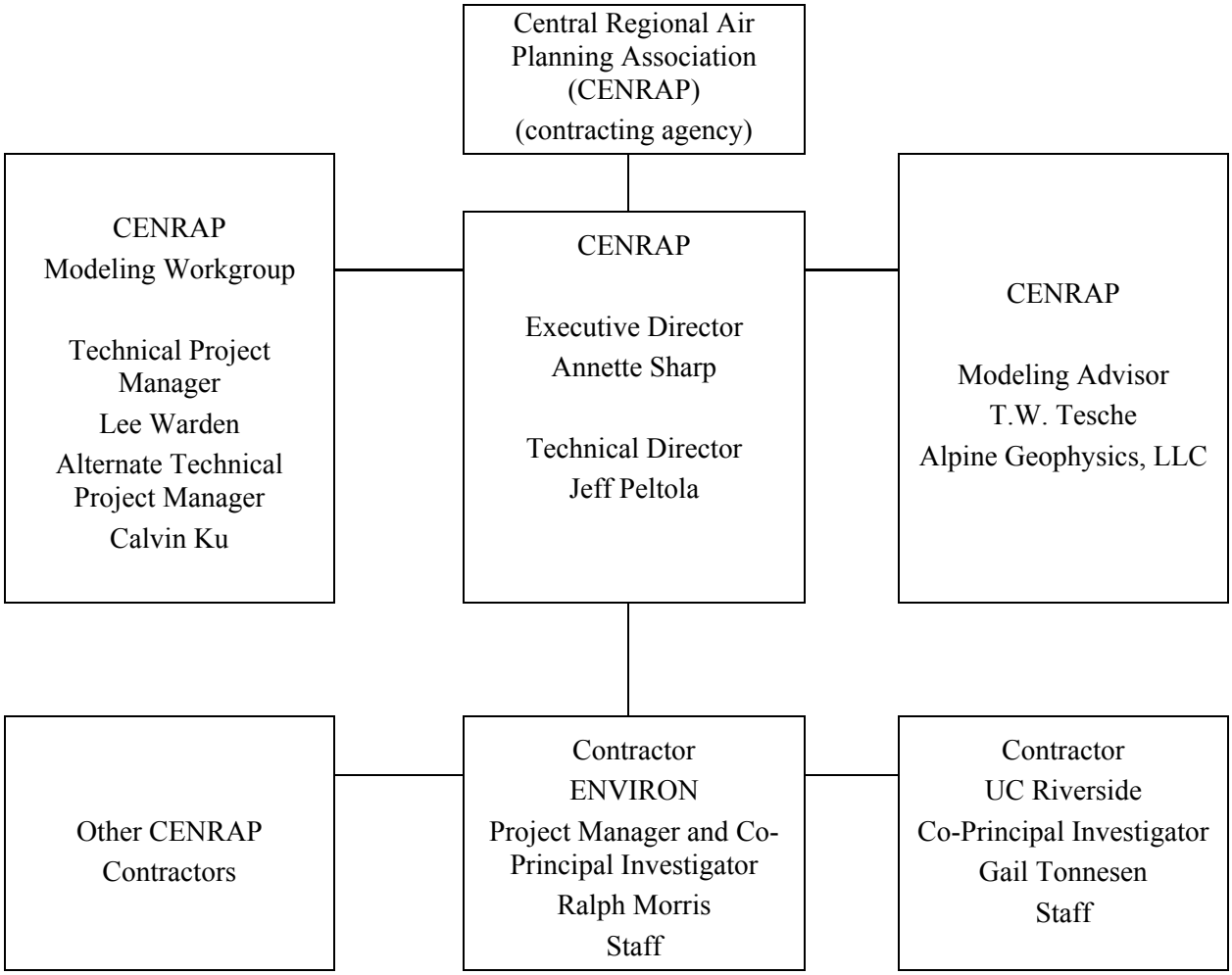

Figure 3-1. CENRAP Emissions and Air Quality Modeling Project Organizational Chart.

Table 3-1. CENRAP 2002 Annual Emissions and Air Quality Modeling project participants and contacts.

Person & Role	Affiliation/Address	Contact Information
Annette Sharp (Executive Director)	CENRAP 10005 S. Pennsylvania, Ste. C Oklahoma City, OK 73159	(405) 378-7377 asharp@censara.org
Jeff Peltola (Technical Director)	CENRAP 10005 S. Pennsylvania, Ste. C Oklahoma City, OK 73159	(405) 378-7377 or (651) 293 1295 jpeltola@censara.org
Lee Warden (Technical Project Manager)	Oklahoma DEQ 707 N. Robinson Oklahoma City, OK 73102	(405) 702-4201 Lee.Warden@deq.state.ok.us
Calvin Ku (Alternate Technical Project Manager)	Missouri DNR P.O. Box 176 Jefferson City, MO 65012	(573) 751-4817 calvin.ku@dnr.mo.gov
T.W. Tesche (CENRAP Modeling Advisor)	Alpine Geophysics, LLC 3479 Reeves Drive Ft. Wright, KY 41017	(859) 341-7502 (Fax) (859) 341-7508 twt@iac.net
Ralph Morris (Project Manager and Co-Principal Investigator)	ENVIRON 101 Rowland Way Novato, CA 94945	(415) 899-0708 (Fax) (415) 899-0707 rmorris@environcorp.com
Gail Tonnesen (Co-Principal Investigator)	UC Riverside CE-CERT 1084 Columbia Avenue Riverside, CA 92507	(951) 781-5676 (Fax) (951) 781-5790 tonnesen@cert.ucr.edu
Key ENVIRON Participants		
Gerry Mansell (Emissions Modeling Coordinator)	ENVIRON 101 Rowland Way Novato, CA 94945	(415) 899-0727 gmansell@environcorp.com
Bonyoung Koo	ENVIRON	(415) 899-0727 bkoo@environcorp.com
Edward Tai	ENVIRON	(415) 899-0725 etai@environcorp.com
Steven Lau	ENVIRON	(415) 899-0739 slau@environcorp.com
Key UCR CE-CERT Participants		
Mohammed Omary (Chief Emissions Modeler)	UC Riverside CE-CERT 1084 Columbia Avenue Riverside, CA 92507	(951) 781-5652 omary@cert.ucr.edu
Zion Wang	UC Riverside	(951) 781-5655 zsw@cert.ucr.edu
Chao-Jung Chien	UC Riverside	(951) 781-5666 chien@cert.ucr.edu
Glen Kaukola	UC Riverside	(951) 781-5630 glen@cert.ucr.edu
CENRAP Workgroup Chairpersons (www.cenrap.org)		
Brandon Krogh (Monitoring)	Minnesota Power	(218) 723-3954 bkrogh@allete.com
Ray Bishop	Oklahoma Department of	(405) 702-4218

Person & Role	Affiliation/Address	Contact Information
(Monitoring)	Environmental Quality	Ray.Bishop@deq.state.ok.us
Calvin Ku (Modeling)	Missouri Department of Natural Resources	(573) 751-8406 Calvin.Ku@dnr.mo.gov
Lee Warden (Modeling)	Oklahoma Department of Environmental Quality	(405) 702-4201 Lee.Warden@deq.state.ok.us
Ron Hoofman (Emissions)	Arkansas Department of Environmental Quality	(501) 682-0357 hoofman@adeq.state.ar.us
Lisa Brenneman (Emissions)	Eastern Shawnee Tribe of Oklahoma	estoepa@hotmail.com
John Seltz (Implementation and Control Strategy)	Minnesota Pollution Control Agency	(651) 296-7801 John.Seltz@pca.state.mn.us
Mark McCorkle (Implementation and Control Strategy)	Arkansas Department of Environmental Quality	(501) 682-0736 mac@adeq.state.ar.us
Scott Weir, Communications	Kansas Department of Health and the Environment	(785) 291-3272 sweir@kdhe.state.ks.us

3.1.1 ENVIRON/UCR Project Manager and Co-Principal Investigators

Mr. Ralph Morris of ENVIRON is the Project Manager (PM) and Co-Principal Investigator (Co-PI) for the CENRAP Emissions and Air Quality Modeling Team. He provides overall direction to the project and establishes a policy relationship with the sponsor, ensuring that all issues of importance to the CENRAP Project Manager, Executive Director and Technical Director and Workgroups are addressed. The PM is responsible for the overall conduct of the project, experimental design, reporting of the results, and interacting with the client, consultants, and project staff. The specific responsibilities of the PM include, but are not necessarily limited to, the following:

- Directs and coordinates the activities of the project team and computer facilities to conduct the test program
- Ensures that this QAPP and the Modeling Protocol are followed during the course of the project
- Guides the overall approach for performing modeling evaluations
- Keeps current on project status and delivers progress reports
- Conducts initial modeling or analysis of experiments to determine if inconsistencies or unexpected results suggest possible experimental or measurement problems
- Evaluates overall data quality, characterization results, and overall system performance with regard to meeting project objectives
- Reviews and delivers modeling and assessment reports
- Interacts with external scientific reviewers, collaborators and other external groups in their area of expertise in the development of study priorities, reporting of results, and obtaining external input
- Oversees the project team in responding to any issues raised in assessment reports and initiates corrective actions as necessary
- Serves as ENVIRON's primary point of contact for contract issues
- Establishes a project budget and monitors the effort to ensure that budget is not exceeded
- Assists in the performance of the modeling program in accordance with its contract and the Work Plan
- Provides information to assist the CENRAP Project Manager, Administrative Project Manager and Modeling Workgroup in achieving its goals as stated in its Work Plan and Long Range Plan
- Develops individual test protocols and reports as directed
- Analyzes modeling data and provides assessment reports
- Supports the CENRAP Project Manager and CENRAP in responding to any issues raised in assessment reports

3.1.2 ENVIRON and UCR Co-Principal Investigators

The two Co-Principal Investigators of Ralph Morris and Gail Tonnesen perform the following functions:

- Direct and coordinate the day-to-day project activities of the project team and computer

facilities to conduct the test program
- Ensure that this QAPP and Modeling Protocol are followed during the course of the project
- Manage the activities in each of the three modeling centers
- Directly supervise personnel working on this project
- Guide the approach for performing modeling evaluations following the direction of the Project Manager
- Keep current on project status and deliver information to Project Manager for progress reports
- Conduct initial modeling or analysis of experiments to determine if inconsistencies or unexpected results suggest possible experimental or measurement problems
- Evaluate overall data quality, characterization results, and overall system performance with regard to meeting project objectives
- Review and deliver data and sections for integration into modeling and assessment reports
- With the Project Manager, interact with external scientific reviewers, collaborators and other external groups in their area of expertise in the development of study priorities, reporting of results, and obtaining external input
- Oversee the project team in each modeling center responding to any issues raised in assessment reports and initiates corrective actions as necessary with the Project Manager
- Monitor the effort to ensure that budget is not exceeded
- Assist in the performance of the modeling program in accordance with its contract and the Work Plan
- Develop individual test protocols and reports as directed
- Analyze modeling data and provide assessment reports

3.1.3 CENRAP Technical Director and Executive Director

The CENRAP Technical Director (Jeff Peltola) and Executive Director (Annette Sharp) serve as the primary administrative contact between the Emissions and Air Quality Modeling Team and CENRAP and performs the following functions:

- Provides day-to-day oversight of CENRAP Emissions and Air Quality Modeling Team activities
- Works with the CENRAP Project Manager and Modeling Team Project Manager and Co-Principal Investigators, CENRAP Modeling Workgroup, States, Tribes oversight groups, collaborators, Stakeholders, etc. in assuring that the interests and concerns of all of the CENRAP participants are appropriately represented as project priorities are developed or modified due to external input
- Assists in organizing and conducting meetings, conference calls, and workshops where this and related projects are discussed

3.1.4 CENRAP Project Manager

The CENRAP Project Manager (Lee Warden) for the Emissions and Air Quality Modeling Team works with the CENRAP Administrative Project Manager/Project Coordinator in the day-to-day oversight and management of the modeling analysis:

- Provides day-to-day oversight of CENRAP Emissions and Air Quality Modeling Team activities
- Works with the CENRAP Administrative Project Manager and Modeling Team Project Manager and Co-Principal Investigators to assure that the study is being carried out in a technically correct fashion following the QAPP and Modeling Protocol
- Prepares and gives presentations to CENRAP groups on the activities of the Modeling team as needed.

The CENRAP Alternate Project Manager (Calvin Ku) provides backup and seamless continuation of work should the primary Project Manager be unavailable.

3.1.5 CENRAP Modeling Workgroup

The CENRAP Modeling Workgroup is responsible for overseeing the regional haze and fine particulate modeling that will be required for the CENRAP States and Tribes State Implementation Plans (SIPs) and Tribal Implementation Plans (TIPs). This workgroup provides both emissions modeling and air quality modeling technical support to CENRAP. Modeling efforts will include identification, evaluation, and application of air quality modeling tools (including emissions, meteorological and air quality models) to quantify the effects of emission management options upon air quality in Class I areas in the CENRAP region. Specific activities of the CENRAP Modeling Workgroup include:

- Oversees the activities of the CENRAP Emissions and Air Quality Modeling Team through the CENRAP Project Manager and Administrative Project Manager, conference calls, and periodic in-person meetings and workshops
- Provides the CENRAP Project Manager, CENRAP Administrative Project Manager, and Modeling Team Project Manager and Co-Principal Investigators input on the research plans and their ability to meet the needs of the various stakeholders relevant to the overall objectives of the project
- Provides input as needed to assure that the project has effective and appropriate peer review
- Makes the Modeling Team Project Manager and Co-Principal Investigators aware of other projects that may be of relevance to this project
- Reviews the QAPP and conducts critical project reviews

3.2 Project Schedule and Execution

The schedule for each of the CENRAP Emissions and Air Quality Modeling Phase I and II Tasks are presented at the end of each Task Description in Section 2.4.

3.3 Personnel Qualifications and Training

General education of all project personnel lays the foundation for successful project implementation. It is not intended to provide detailed and specific knowledge of all components of the project, but it promotes an understanding of the nature of the overall project goals, ensuring that all personnel understand the part they are to play in the project. The members of this project team include resident experts in emissions, meteorological and air quality model development and operations.

All project personnel must have extensive experience in their particular disciplines. Each team member must be familiar with the content of this QAPP and the CENRAP Modeling Protocol thus obtaining a project overview, including information on all functions of the modeling systems, from experimental design, objectives, and data validation and reporting. Where applicable, project personnel must be familiar with the SOPs applicable to their areas of responsibility. In addition, if major revisions or enhancements are made to the QAPP and/or SOPs, all affected individuals must review those revisions at that time.

3.4 Communications Plan

The CENRAP Emissions and Air Quality Modeling Team members, other CENRAP Contractors and CENRAP representatives are linked by e-mail correspondence, and also use this as a means to communicate and exchange data, either as e-mail attachments, website or by network-accessible files. A considerable amount of information is exchanged by e-mail within this project. The CENRAP Modeling Team maintains listservs to distribute information to CENRAP.

The Modeling Team members and CENRAP Project Manager, Administrative Project Manager and other members of the Modeling Workgroup will hold periodic conference calls and meetings to report results, discuss project status, and modify work plans as necessary. Unscheduled meetings or conference calls will also be held concerning specific issues as the needs arise. In addition, periodic project meetings and conference calls will be held. In these meetings detailed technical information will be exchanged, project status will be discussed, and project direction will be assessed.

Written progress reports on the CENRAP Emissions and Air Quality Modeling Team activities will be submitted to the CENRAP Project Manager and Administrative Project Manager on a monthly basis. These reports will summarize project progress, results to date, problems encountered and necessary action items, and plans for the upcoming reporting period.

Key modeling results, quality assurance reports, and related documents will be posted on the project web site.

http://pah.cert.ucr.edu/aqm/cenrap/index.shtml

3.5 Documentation and Records

After the project tasks described in Section 2.4 that require deliverables are completed, the ensuing documents will be posted on the CENRAP Modeling project website. In addition, during the project, the CENRAP participants will be provided updates by e-mail or telephone.

Document control is the system that ensures that the Modeling Team personnel engaging in project activities use only the latest revisions of the defined documents. The system includes retention of the document with original signed page(s) in a limited access storage area, a unique numbering system for all documents (typically identified by revision number and/or date), and electronic storage of documents by date so that the latest versions is clearly identifiable. Such documents are controlled documents, and can be revised only by the personnel listed within each document or the project quality document. The following is a typical list of the controlled documents within the project folder:

1. The quality documents for the project such as the Quality Management Plan, Modeling Protocol and Quality Assurance Project Plan.
2. All applicable and referenced or attached Standard Operating Procedures and/or Methods.
3. Project proposals, contracts, Work Plans, experimental designs, software documentation, and/or similar documents.

4.0 MEASUREMENT AND DATA ACQUISITION

4.1 Computer Hardware/Systems Administration

All emissions and air quality modeling will be performed on computer equipment located at either the ENVIRON or UCR modeling centers.

4.1.1 ENVIRON Modeling Center Hardware

The computing facilities at the ENVIRON Novato, CA office are built on current state-of-the-art hardware and software. The networked configuration of personal computers, workstations and printers includes Linux and Window PCs, SGI, SUN and DEC Unix workstations and Linux Clusters all connected by a fast network with disk access to RAID systems. The ENVIRON computer center includes the very latest computing technology including both OMP (shared memory) and MPI (cluster) multi-processing capability. ENVIRON currently has three Linux Clusters each with > 10 CPUs and each connected to RAID disk systems. All staff also has their own state-of-the-art PCs and has access to all workstations at all times, there are no problems with computer resource availability. ENVIRON's high speed Linux and UNIX computing environment includes workstations from three top suppliers, Sun, Digital Equipment Corporation (DEC) and Silicon Graphics Incorporated (SGI). ENVIRON also uses Linux PC workstations with several different distributions of the Linux OS (e.g., Red Hat, Debian, Mandrake) and these exceed the performance of fast UNIX workstations. Using workstations from several suppliers

allows us to develop and test model codes on multiple computer platforms and means that we are experienced with most of the workstations used by our clients. The latest addition to the ENVIRON computing facilities is a 16 node Linux cluster using the Athlon MP2200 chip set with gigabit Ethernet that is configured as two 8 node MPI multiprocessing platforms.

4.1.2 UCR Modeling Center Hardware

The UCR computer laboratory is designed to process large data sets for air quality modeling. It includes over 30 high-performance, dual CPU Linux workstations configured as several small Linux clusters on a private network to facilitate parallel simulations. These systems include a 24 CPU Athlon 2000MP cluster, an 8 CPU Xeon 2.2GHz cluster and an 8 CPU 64-bit Opteron 2GHz cluster. The data storage system includes over 23 TB of disk space configured as RAID5 disk systems. All computers and disk systems are networked using high speed Gigabit Ethernet for efficient simulation and analysis of large datasets. To provide maximum data security the systems are located behind the UCR firewall and an additional firewall is used internally within the laboratory so that only project team members have access to project computers and data.

Data are also routinely transferred from the UCR systems to other organizations using a variety of tape formats and portable hard drives. The data backup/archiving system include 8mm tape drives and DLT and Super DLT auto loading cartridge system capable of performing unattended archive/backups of over 1 TB (uncompressed). Key disk systems have hot-swappable hard drives with stand-by spare drives and redundant power supplies. The compute clusters and disk systems are located in a locked, secure room with a dedicated climate control system and with backup air conditioning. UCR also uses the computer laboratory for air pollution modeling classes for graduate students and for professional staff from State and Tribal air pollution agencies. The laboratory has a full time systems administrator to perform system backups, maintenance and updates and Dr. Tonnesen's group includes a second full time systems administrator.

4.1.3 Backup Procedures

Different back-up procedures are applied to three different sets of computers that include (1) file servers; (2) user desktop Windows PCs; and (3) RAID5 disks storage systems. Several different File servers are used to host systems and user information, websites and ftp sites.

1. Each server receives a full Level 0 backup at least once every 14 days, and an incremental backup at least three times per week to an independent computer. In addition, incremental backups are periodically made to tape.

2. Windows based PC's are used to for editing project documents and reports. Each PC on the LAN receives a full Level 0 backup at least once every 14 days and incremental backups every three days.

3. Most of the project data are stored on RAID5 disk systems. Because of the large volume of data (> 20 TBs) it cannot be routinely backed up. Moreover, most of the project data are output from model simulations, which can be regenerated more quickly by re-running the models than by restoring from tape. Therefore, only critical model input data are

backed-up. One 2 TB RAID5 disk system is reserved for backup of critical project data. Backups are performed weekly. In addition, critical project input data is archived to IDE drives, firewire drives or DLT tape.

All incoming electronic mail receives virus scanning using commercial software (Norton or McAffee Anti-Virus), which is updated routinely. Windows PC receives automated, weekly scans for viruses.

Three types of software are used in the project: (1) commercial software for word processing, project management, communications, and commercial software compilers; (2) compilers and computer operating systems publicly available through the GNU Public License (GPL) distribution channels; and (3) custom software used in computer simulation modeling and data analysis. All commercial software used in the CENRAP modeling project has been purchased with licenses and is installed and tested as specified by the publisher. Commercial compilers include Portland Group compilers, and Intel and IBM FORTRAN compilers. All GPL software is obtained from official distribution centers, such as Redhat, and are regularly maintained and updated with each official release from the code developers. Custom software is developed by UCR, EPA and other researchers using commercial and GPL compilers for FORTRAN, C and C++.

4.2 Sources for Data Used in Modeling

Most of the data used in the CENRAP Emissions and Air Quality Modeling will be provided by other CENRAP contractors or participants. The data will be subjected to QA/QC screening prior to delivery to the Modeling Team. In addition, the Modeling Team has formed data "Gatekeeper" functions to further screen the data prior to its use. Below the data used in the modeling and the function of the Gatekeeper roles is discussed, which are also described in Section 2.3.2.1:

- **Air Quality Gatekeeper:** The Air Quality Gatekeeper will download air quality data from the VIEWS AIRS, and St. Louis Supersite websites and subject it to QA/QC. The data will be reformatted and processed for use in the modeling.

- **Meteorological Gatekeeper:** The Meteorological Gatekeeper will evaluate the 36 km MM5 data provided by the Iowa Department of Natural Resources (IDNR), a CENRAP state, and 12 km MM5 data for 2002 episodes provided by other CENRAP participants, subjects it to QA/QC, and processes it for input to the CMAQ/CAMx air quality models.

- **Emissions Gatekeeper:** The Emissions Gatekeeper will receive emissions data from the CENRAP Emissions Contractors (Pechan and STI) for CENRAP states and other sources for non-CENRAP states, subjects them to a comprehensive QA/QC, and will reject data that doesn't pass the QA/QC and reformats the data for input into the SMOKE emissions model.

- **Data Management Gatekeeper:** The Data Management Gatekeeper will maintain the project website, keep backups of data, respond to data requests and will update reports and files on the website.

5.0 EMISSIONS MODELING

The project objective is to integrate mesoscale emissions and transport modeling efforts so that predictions of regional haze in Class I areas can be performed under different emissions and meteorological transport scenarios. Meeting this objective means that modeling outputs must be of known quality. This section addresses emissions modeling, Section 6.0 addresses meteorological modeling and Section 7 addresses air quality modeling as they apply to this project.

The CENRAP Modeling Team uses the Sparse Matrix Operator Kernel Emissions (SMOKE) emissions model to simulate the anthropogenic and biogenic gas and particulate matter (PM) emissions needed for regional haze modeling. A detailed quality assurance protocol for utilizing SMOKE has been prepared as part of the CENRAP Modeling Protocol (ENVIRON and UCR, 2004) and is summarized in this section.

The purpose of SMOKE is to convert the resolution of the raw emission inventory data to the resolution needed by an air quality model. Emission inventories are typically available with 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 for this project involve transformation of emission inventory data by temporal allocation, chemical speciation, spatial allocation, and layer assignment, to achieve the input requirements of the air quality model.

SMOKE formulates emissions modeling in terms of sparse matrix operations. Figure 5-1 presents an example of how the matrix approach is used by the project team to organize the emissions processing steps for anthropogenic emissions, with the final step in creating the model-ready emissions being the merge step. This example does not include all processing steps, which can be different for each source category in SMOKE, but does include the major processing steps listed above, except for 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 (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.

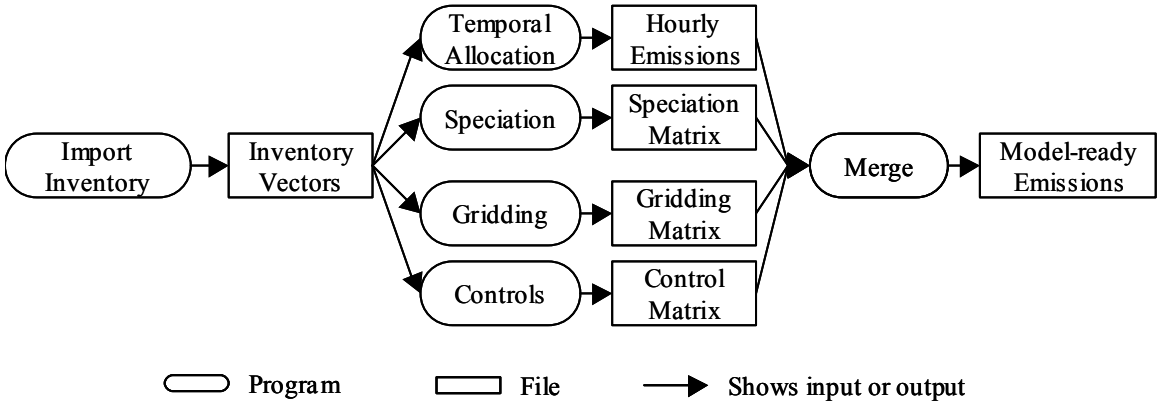

Figure 5-1. Flow Diagram of Major SMOKE Processing Steps

5.1 Quality Assurance Components of Emissions Modeling

The quality assurance (QA) screening steps for the emissions modeling process has been divided into the four major classifications defined in the sections below.

5.1.1 Modeling QA

Modeling QA involves performing data quality checks, assuring simulation accuracy, and recognizing and identifying problems as they happen; it is the process of looking for glaring faults in the model input and output data (I/O) and determining whether the input data are producing the desired results. Scrutiny of the I/O using standard statistical analyses can reveal problems in the data and/or the model setup. Using a standard approach for analyzing emissions model I/O establishes reference points to use when scrutinizing the data. Seeking these indicators of correct model performance allows project personnel to determine the accuracy of the simulations and whether faults in the data or model configuration exist.

5.1.2 System QA

System QA addresses model installation and configuration issues, data accounting, and ensures that the modeling systems are producing results that are reasonable and reproducible. The first step in this process is to properly benchmark the model and assuring that the installation is complete. Confirmation of configuration settings, compile options, and other system-related parameters must then occur and be documented prior to producing any model results. Archiving the model installation at set “freeze points” in the project is also required in order to keep accurate records of the modeling installation and run scripts. A key feature of System QA is facilitating the reproduction of model results in the future and the ability to revert back to a previous configuration or installation after the model has been revised or updated. In addition to thorough documentation, version control software is required for archiving model executables, run and configuration scripts, and important data files. Combining documentation of the modeling procedures with archives of the model installation and data files will ensure that the

model installation and configuration are correct and that past simulations are sufficiently documented and archived to allow their reproduction.

5.1.3 Gatekeeping and Outside Review

Gatekeeping and outside review is the process of ensuring that the data entering and exiting the SMOKE modeling process meet a predetermined quality level. A gatekeeper screens model data before they pass from one major step of the modeling process to the next. In emissions QA, gatekeeping is applied to the emissions inventory and SMOKE input files on the front end of the modeling process, and to the SMOKE output files at the back end. A gatekeeper (or gatekeeping team) is responsible for performing a series of reasonableness checks on both the input and output data streams. Outside reviewers are emissions experts who are not part of the CENRAP Modeling Team. They periodically review the entire process—the emissions data, the modeling, and the QA steps taken—using their judgment as experts to decide what to review and how to review it.

5.1.4 Documentation

Documentation, a critical component that is common to all of the other three QA classifications, provides the record of the QA process. Establishing a detailed set of requirements for documenting every step in the QA process will ensure not only that the documentation is created as expected, but that the processes recorded by the documentation are completed correctly. In addition to records or lists of completed QA steps, documentation refers to summaries and interpretations of emissions inventory reports and analyses. Covering the entire realm of the modeling process, QA documentation includes records of model configuration, details about data files, simulation records, and final report generation.

5.2 Implementation of the QA System

5.2.1 The Emissions QA Team

The level of effort required to implement the CENRAP Emissions QA framework requires a team consisting of: a data gatekeeper(s), a production modeler(s), a QA manager, outside reviewers, and a project manager (See Section 2.3.2.5 and Figure 2-1 for data flow and QA overview). Each team member contributes a different critical perspective on the data and modeling.

- The *Gatekeeper* (or *gatekeeping team*) is responsible for reviewing the SMOKE I/O data streams for correctness. Before new datasets are used in SMOKE modeling, or new SMOKE output emissions datasets are used in air quality modeling, they must be reviewed by the gatekeeper. For all SMOKE input and output files, the gatekeeper ensures that the data are complete, are formatted correctly, and pass reasonableness checks. Checking completeness entails examining the files for the necessary data elements, spatial coverage, and temporal extent. Data formats will be confirmed using the SMOKE manual to check ASCII files and using PAVE to check binary netCDF files, such as the meteorological inputs. Reasonableness

checks consist of looking for glaring errors in the file contents and ensuring that the data make sense in the context of how they will be used and relative to similar or reference datasets. Issues that arise during the gatekeeping process are reported to the Project Manager for resolution.

- The *Production Modeler* is responsible for receiving input data, maintaining the model run scripts, running the model per the work plan, producing default QA reports, delivering model output data, and assisting with compiling QA reports into summaries for documentation purposes. A *Lead Modeler* oversees the entire modeling process, performs the majority of the SMOKE modeling, and receives and archives input and output data. *Secondary Modelers* organize the SMOKE QA reports into emissions summaries for data QA and reporting, and generate custom QA summaries and reports for troubleshooting any problems encountered during the modeling process.

- The *QA Manager* performs and documents all of the checks required for determining model accuracy and revealing errors. The QA Manager also ensures that the software is configured correctly and that the data and model are being archived consistently and correctly. Overseeing the production modelers, the QA Manager verifies that SMOKE is being applied correctly and that all QA summaries are consistent with the relevant input data. Leading the documentation efforts, the QA Manager ensures that all the necessary QA summaries are generated and certified and that they are compiled into the project report.

- The *Project Manager* is ultimately responsible for the quality of the final products of the modeling process. Providing technical assistance to the production modelers and clarifying any uncertainties about model input, configuration, and operation for the QA Manager, the Project Manager addresses any questions in the modeling process. Working with the QA Manager, the Project Manager approves the results of all QA procedures, and thoroughly scrutinizes the QA summaries for problems to determine whether the data are ready to be sent to the gatekeepers and outside reviewers for final review before delivery to the air quality modelers. For the CENRAP project the Project Manager is the liaison between the emissions modeling team and the CENRAP Modeling Workgroup and in this role communicates any issues raised during the emissions QA process.

Figure 5-2 presents the QA framework developed by the CENRAP Modeling Team for SMOKE modeling. Identifying the specific participants in the CENRAP Modeling Team for performing all of the tasks in the framework is the first step of the QA process for each new emissions modeling scenario. Two Production Modelers are shown in the diagram, with the Lead Modeler performing the SMOKE simulations and receiving the input data and the Secondary Modeler compiling the output of the SMOKE QA programs into the QA products for evaluating the quality of the simulations. Gatekeepers are positioned in the SMOKE input and output data streams to screen the data before they are used in either SMOKE or CMAQ modeling, respectively. Reviewers are solicited from outside the emissions modeling team on a volunteer basis to conduct periodic reviews/audits of the data and modeling process.

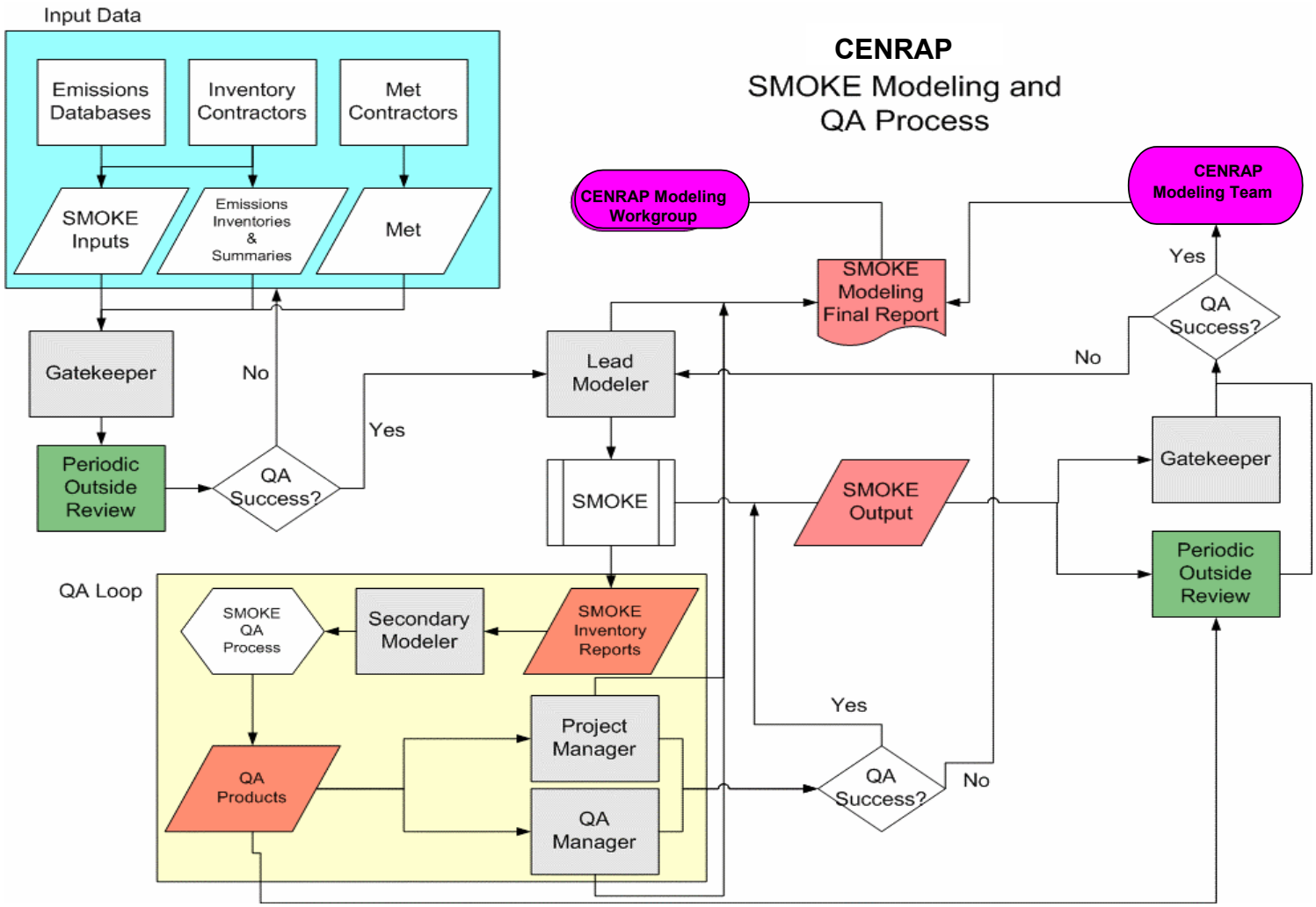

Figure 5-2. Diagram of CENRAP Modeling Team Approach to SMOKE Modeling

6.0 METEOROLOGICAL MODELING

The EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system and the Comprehensive Air-quality Model with extensions (CAMx) are the two regional ozone and particulate matter (PM) air quality models being used in the CENRAP project. Meteorological inputs for CMAQ and CAMx have been generated using output from the fifth generation Mesoscale Model (MM5). The 2002 MM5 36 km database for the continental US was developed by the Iowa Department of Natural Resources (IDNR) (Johnson, 2004). Whereas, other CENRAP participants are developing the 12 km MM5 database. The MM5 model was initial applied for the entire year of 2002 on a continental scale domain with 36 km grid spacing. Subsequent MM5 model runs were applied to a regional-scale domain with 12 km grid spacing covering the central United States for 2002. The CMAQ and CAMx models require inputs of three-dimensional gridded wind, temperature, humidity, cloud/precipitation, and boundary layer parameters. The MM5 meteorological model was developed and is maintained by the Pennsylvania State University and National Center for Atmospheric Research (PSU/NCAR).

The procedures used for applying MM5 for CENRAP are based on an extensive evaluation of MM5 and a series of sensitivity tests conducted by IDNR and the Lake Michigan Air Directors Consortium (LADCO) that was consequently updated based on the MM5 sensitivity modeling conducted as part of VISTAS (www.baronams. Com/projects/VISTAS). A description of CENRAP 36 km MM5 modeling approach including the modeling domain, MM5 physical configuration, and a model application approach can be found in Johnson (2004).

MM5 has proven useful for air quality applications and has been used extensively in past local, state, regional, and national modeling efforts. MM5 has undergone extensive peer-review, with all of its components continually undergoing development and scrutiny by the modeling community. MM5 is the most widely used public-domain prognostic model. In-depth descriptions of MM5 can be found in Dudhia (1993) and Grell et al. (1994), and at the following web site:

http://www.mmm.ucar.edu/mm5.

The evaluation of the MM5 meteorological modeling will be performed primarily by the meteorological modeler. For the CENRAP 2002 36 km MM5 modeling preliminary evaluation of the MM5 model can be found at:

http://www.ladco.org/tech/photo/present/mm5v363_eval.pdf
http://www.ladco.org/tech/photo/present/rainfall_eval.pdf

In addition, the CENRAP Emissions and Air Quality Modeling Team has a Meteorological Gatekeeper role that is described in Section 2.3.2.3 that will evaluate the MM5 fields to provide an independent verification step and assure that the data have been transferred correctly to the Modeling Team. The Modeling team Meteorological Gatekeeper reports will be posted on the project website at:

http://pah.cert.ucr.edu/aqm/cenrap/mm5.shtml

7.0 CENRAP 2002/2018 AIR QUALITY MODELING

For the 2002 annual modeling on the 36 km grid, the CENRAP Emissions and Air Quality Modeling Team will apply and evaluation EPA's Models-3 Community Multiscale Air Quality (CMAQ) modeling system and the Comprehensive Air-quality Model with extensions (CAMx).

7.1 CMAQ Overview

For more than a decade, EPA has been developing the Models-3 Community Multiscale Air Quality (CMAQ) modeling system with the overarching aim of producing a 'One-Atmosphere' air quality modeling system capable of addressing ozone, particulate matter (PM), visibility and acid deposition within a common platform (Dennis, et al., 1996; Byun et al., 1998a; Byun and Ching, 1999, Pleim et al., 2003). The original justification for the Models-3 development emerged from the challenges posed by the 1990 Clean Air Act Amendments and EPA's desire to develop an advanced modeling framework for 'holistic' environmental modeling utilizing state-of-science representations of atmospheric processes in a high performance computing environment (Ching, et al., 1998). EPA completed the initial stage of development with Models-3 and released the Community Multi-Scale Air Quality model (CMAQ) in mid-1999 as the initial operating science model under the Models-3 framework (Byun et al., 1998b). The most recent rendition is CMAQ version 4.4, publicly released in October 2004, is the version that will be used in the CENRAP Emissions and Air Quality Modeling Study.

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

A number of features in CMAQ's theoretical formulation and technical implementation make the model well-suited for annual PM modeling. In CMAQ, the modal approach has been adapted to dynamically represent the PM size distribution using three log-normal modes (2 fine and 1 coarse). Transfer of mass between the aerosol and gas phases is assumed to be in equilibrium and all secondary aerosols (sulfates, nitrates and organics) are assumed to be in the fine modes. The thermodynamics of inorganic aerosol composition are treated using the ISORROPIA module. Aerosol composition is coupled to mass transfer between the aerosol and gas phases. For aqueous phase chemistry, the RADM model is currently employed. This scheme includes oxidation of SO_2 to sulfate by ozone, hydrogen peroxide, oxygen catalyzed by metals and radicals. The impact of clouds on the PM size distribution is treated empirically. For wet deposition processes, CMAQ uses the RADM/RPM approach. Particle dry deposition is

included as well. CMAQ contains three options for treating secondary organic aerosol (SOA), the latest being the Secondary Organic Aerosol Model (SORGAM) that was updated in August 2003 to be a reversible semi-volatile scheme whereby VOCs can be converted to condensable gases that can then form SOA, and then evaporate back into condensable gases depending on atmospheric conditions.

A description of the features implemented in the version of CMAQ ver 4.4 (released October 2004) used in the initial CENRAO 2002 modeling is available from the CMAS Center website (www.cmascenter.org). Many of these features are mentioned above; others pertain to details in the model's chemistry, transport, computer implementation, and model operation. In October 2005, a new version of CMAQ was released (V4.5) that included several updates and was subsequently adopted by CENRAP.

7.2 CMAQ Configuration for CENRAP Modeling

Based on preliminary modeling performed by CENRAP (Pun, Chen and Seigneur, 2004; Tonnesen and Morris, 2004), BRAVO (Pitchford et al., 2004), VISTAS (Morris et al, 2004a) and WRAP (Tonnesen et al., 2003) we have identified and justified a set of initial recommended science options for the CENRAP CMAQ modeling. In this section we briefly identify the main science options recommended for annual PM modeling with CMAQ, more details are provided in the Modeling Protocol (ENVIRON and UCR, 2004). The model will be set up and exercised on the same 36 km Inter-RPO Continental US modeling domain that is being used by WRAP and VISTAS. This domain is larger than the 36 km domain used in the preliminary CENRAP modeling (Pun, Chen and Seigneur, 2004). For the 12 km episodic modeling, the CMAQ modeling domain will be determined after receipt of the 12 km MM5 data. For the 12 km CMAQ modeling, one-way grid nesting will be used whereby the results of the 36 km simulation are used to provide hourly BCs to the 12 km simulation. A total of 19 vertical layers will be implemented, extending up to a region top of 100 mb (approximately 15 km AGL).

The latest versions of CMAQ (Version 4.4 and 4.5) will be used in the CENRAP modeling. The PPM advection solver will be used along with the spatially varying (Smagorinsky) horizontal diffusion approach and K-theory for vertical diffusion. MM5 meteorological output based on the Pleim-Xiu Land-Surface Model (LSM) and the ACM planetary boundary layer (PBL) scheme will be used and the latest CMAQ Meteorological-Chemistry Interface Processor (latest MCIP2.3) will process the MM5 data using the "pass through" option. The CB4 gas-phase, RADM aqueous-phase, and AERO3/ISORROPIA aerosol chemistry schemes are recommended for use in the CMAQ 2002 modeling. Treatment of reversible secondary organic aerosols will be simulated by the SORGAM implementation in CMAQ.

7.2.1 Updates to the CMAQ Secondary Organic Aerosol (SOA) Module

Initial simulations of the CMAQ V4.4 for the 2002 annual period revealed that Organic Carbon (OC) was underestimated in the central and eastern U.S. by approximately 80% to 100% during the summer. A review of the CMAQ model formulation and model inputs found that one potential reason the model was underestimating OC was because there are several processes

associated with SOA formation from biogenic VOCs believed important for SOA formation. These processes are not treated in the current CMAQ model. Thus, the CMAQ SOA module was enhanced to include several missing processes. The formulation and resulting model performance are discussed in detail in a manuscript that has been accepted for publication in *Atmospheric Environment* (Morris, et al., 2006). The SOA module enhancement were first added to CMAQ V4.3 and then transferred to CMAQ V4.5 when it became available in October 2005.

7.2.1.1 SOAmods Formulation

The formulation of the standard CMAQ SOA module is described in Binkowski and Roselle (2003). SOA can be formed from aromatic VOCs and biogenic terpenes. The biogenic SOA precursors were modeled with the Biogenic Emissions Information System – Version 3 (BEIS3) model (Pierce et al., 2002). BEIS3 generates three biogenic VOC species: isoprene (ISOP), monoterpenes (TERP) and other biogenic VOC (OVOC). For this study, the Carbon Bond IV photochemical mechanism was used (Gery et al., 1989) that represents VOC compounds based on their carbon bond structure. The BEIS3 ISOP, TERP and OVOC species are speciated into the CB4 species for photochemical modeling in CMAQ and CAMx as follows (molar speciation):

- ISOP = ISOP (isoprene is an explicit species)
- ALD2 = 1.5 x TERP
- OLE = 0.5 x TERP
- PAR = 6.0 x TERP
- NR = 0.5 x OVOC
- OLE = 0.5 x OVOC
- PAR = 8.5 x OVOC
- TERPB = TERP

Here, ALD2, OLE, PAR and NR are the CB4 chemical mechanism representations of the biogenic VOC emissions as high molecular weight aldehydes, olefinic carbon bond, paraffin carbon bond and non-reactive functional groups. In CMAQ, the TERPB species is specified in the emissions inputs, along with its CB4 representation of ALD2, OLE and PAR, but does not participate in the photochemical mechanism and is only used in the SOA formation module. The TERPB species forms a SGTOT species based on oxidation parameters extracted from the photochemical module. SGTOT consists of the combined gaseous condensable gas (CG) plus particle SOA that are assumed to be in equilibrium. CMAQ transports the SGTOT species and splits it to a CG gaseous and particle SOA for output.

The CMAQ TERB SOA formation rate is based on a fit to smog chamber data collected at the California Institute of Technology for several biogenic monoterpene species (Binkowski and Roselle, 2003). A review of recent literature of biogenic SOA measurements identified several processes that may be important to biogenic SOA formation that are not treated by the BEIS3 biogenic emissions and the CMAQ SOA module:

Polymerization: Recent measurements indicate that some SOA species may polymerize, resulting in species that are no longer volatile and cannot evaporate back to a CG. In this case, the equilibrium assumption between the CG and SOA will understate the amount of particle SOA present in the atmosphere (Kalberer et al., 2004; Jang et al., 2002).
Sesquiterpenes: Sesquiterpenes are not accounted for in the BEIS3/CMAQ SOA modeling system (Guenther et al., 2000; Vizuete et al., 2004).
Isoprene: More recent evidence suggests that isoprene can also form particle SOA compounds that are not accounted for in CMAQ (Claeys et al., 2004; Matsunaga et al., 2003; 2005).
Acid Catalyzation: Recent literature also suggests that some SOA formation may have acid catalyzed reactions (Claeys et al., 2004; Jang et al., 2005).
Heterogeneous Reactions: Recent evidence suggests that some SOA formation may occur during heterogeneous aqueous-phase chemical reactions (Yu et al., 2005).

A prototype module was added to CMAQ that accounted for the first three processes listed above. The last two processes were not included in this work because there are not enough quantitative experimental data yet to establish a parameterization. Modules were added to the CMAQ SOA module under the following constraints:

- The existing CMAQ SOA module for monoterpenes would remain unchanged;
- The same CMAQ model inputs would be used; and
- The basic CMAQ model formulation would remain unchanged, modules would be added to account for polymerization and SOA from sesquiterpenes and isoprene.

Figure 7-1 displays how the prototype representation of new processes to represent SOA polymerization and SOA formation from sesquiterpenes and isoprene were added to the CMAQ SOA module using the existing CMAQ structure and inputs. The new components of the SOA module are indicated in bold italic, whereas the existing CMAQ SOA components (Binkowski and Roselle, 2002) use a regular font. There are several parameters that must be defined in the new elements of the enhanced SOA module: emission factors (EF), canopy escape efficiencies for gases (EEG) and aerosols (EEA) and SOA yields (Y). Based on an analysis of recent measurements, primarily from a recent biogenic emissions field study in Duke Forest, North Carolina (Stroud et al., 2005; Matsunaga et al., 2005), a range of values for the factors in Figure 7-1 were developed as shown in Table 7-1. For the initial prototype of the enhanced SOA module, we selected the mid-point of the range values for the factors from the measurements (Table 7-1). No attempt was made to optimize the parameters in Table 7-1 for OC/TCM model performance.

The emission factors, EF1 and EF2, relate the monoterpene emissions estimated by BEIS3 to emissions of monoterpenes, EF1 (e.g., α-pinene), and sesquiterpenes (EF2). Table 2 displays the range of EF1 and EF2 factors based on recent field study data (Stroud et al., 2005). Using the midpoint of the range results in emission factors of 0.7 for EF1 and 0.4 for EF2. EF1 is assigned a value of 0.7 based on field observations that indicate that the BEIS3 terpene emission factors are likely overestimated due to a tendency of earlier measurements approaches to artificially increase the emissions due to disturbance when leaves were enclosed in the measurement system.

As an initial approach for including sesquiterpene emissions, we have assigned EF2 a value of 0.4 based on the ratio of the observed sesquiterpene emission from the Duke Forest field study (Stroud et al, 2005) to the BEIS3 monoterpene emission estimate. The net result is that BEIS3 TERP emissions are increased by 10% and split 64% as monoterpenes and 36% as sesquiterpenes. The CG yields from the sesquiterpenes are assumed to partly condense into a non-volatile SOA particle that is modeled in CMAQ using the new secondary organic carbon species (SOC2) species and only some of the gas and aerosol species associated with sesquiterpenes are assumed to escape from the canopy using the mid-range of the Escape Efficiencies (EE) estimated by Stroud et al. (2005). The fraction of BEIS3 TERP emissions that are assumed to be monoterpenes (i.e., 64% of the emissions) are treated with the standard CMAQ two-product SOA module (Binkowski and Roselle, 2003) assuming equilibrium between the CG and SOA with the SOA output in the standard AORGB species (Binkowski and Roselle, 2003). The isoprene SOA formation pathway forms a CG using the mid-point yield rate based on the range of recent measurements (Stroud et al., 2005) and a CG/SOA partitioning rate based on the mid-point of measurements from Matsunaga et al. (2003, 2005) (Table 7-1). The isoprene SOA is assumed to be volatile and is modeled as a new secondary organic carbon species in CMAQ SOAmods (SOC3). Finally, all SOA species, with the exception of the already non-volatile SOC1 (polymerized SOA) and SOC2 (sesquiterpene) species, are assumed to partially polymerize into non-volatile particles that are stored in the SOC1 species. The polymerization rate is based on the results of Kalberer et al (2004) who found that 50% of the SOA polymerized in 20 hours.

Table 7-1. Parameters use in enhanced SOA module (see Figure 7-1).

Parameter	Mid-Point	Range
EF1	0.7	0.4 ~ 1.0
EF2	0.4	0.2 ~ 0.6
EEG1	0.325	0.2 ~ 0.45
EEA1	0.2	0.05 ~ 0.35
Y2	0.875	0.75 ~ 1.0
Y1	0.11	0.06 ~ 0.16
P1	0.45	0.15 ~ 0.75

EF1 = emission factor of monoterpenes to the TERP emissions estimated by BEIS3
EF2 = emission factor of sesquiterpenes relative to the TERP emissions estimated by BEIS3
EEG1 = escape efficiency of gas phase precursor of sesquiterpenes from canopy
EEA1 = escape efficiency of SOA from sesquiterpenes from canopy
Y1 = SOA yield of oxidated isoprenes
Y2 = SOA yield of sesquiterpenes

7.2.1.2 Quality Assurance of SOAmods

Several levels of Quality Assurance and Quality Control of the enhanced SOAmods module in the CMAQ model were conducted as follows.

QA/QC of SOAmods Coding: The SOAmods implementation was conducted at ENVIRON. Staff at the University of California at Riverside performed independent QA/QC of the SOAmods code implementation and independent testing and evaluation.

QA of SOAmods Formulation: The new processes being added to the CMAQ SOA module was discussed with researchers at EPA's Office of Research and Development (ORD). Although they have not completed all the laboratory tests, the inclusion of SOA from sesquiterpene and isoprene have been observed and are supported.

Peer Review of SOAmods: The formulation of the SOAmods enhancement to the CMAQ SOA module was documented and comments were received by several parties. The results were also written up and submitted to *Atmospheric Environment* where it was subjected to peer review and will be published (Morris et al., 2006).

Model Performance Evaluation of SOAmods: The final level of QA of the SOAmods was comparisons of CMAQ V4.4 model performance with and without including the SOAmods enhancement. Table 7-2 displays fractional bias error for Organic Carbon (OC) for regions corresponding to VISTAS, MRPO, MANE-VU and CENRAP states using the standard CMAQ Version 4.4 (V4.4) and then CMAQ V4.4 with the SOAmods enhancement. Whereas the standard CMAQ V4.4 underestimates OC across IMPROVE sites of from –76% (MRPO) to –102% (VISTAS), with the SOAmods enhancement the fractional biases centered on zero and ranges from –14% to +8%. Similar results are seen for OC fractional bias across the more urban STN sites where the CMAQ V4.4 exhibits an underestimation bias of –67% to –105%, when using SOAmods the under-prediction bias is –27% to –44%. Note that the continued underestimation of OC across the urban STN sites is likely due to missing primary OC emissions and uncertainties in the STN OC measurements.

Table 7-2. Comparison of fractional bias performance metric for Organic Carbon (OC) using the standard CMAQ Version 4.4 (V4.4) and CMAQ V4.4 with the SOAmods enhancement.

July 2002 Fractional Bias	IMPROVE OC		STN OC	
	V4.4	SOAmods	V4.4	SOAmods
Southeastern U.S.	-102%	-2%	-105%	-32%
Midwestern U.S.	-76%	+12%	-67%	-24%
Northeast U.S.	-82%	-14%	-95%	-44%
Central U.S.	-98%	+8%	-81%	-27%

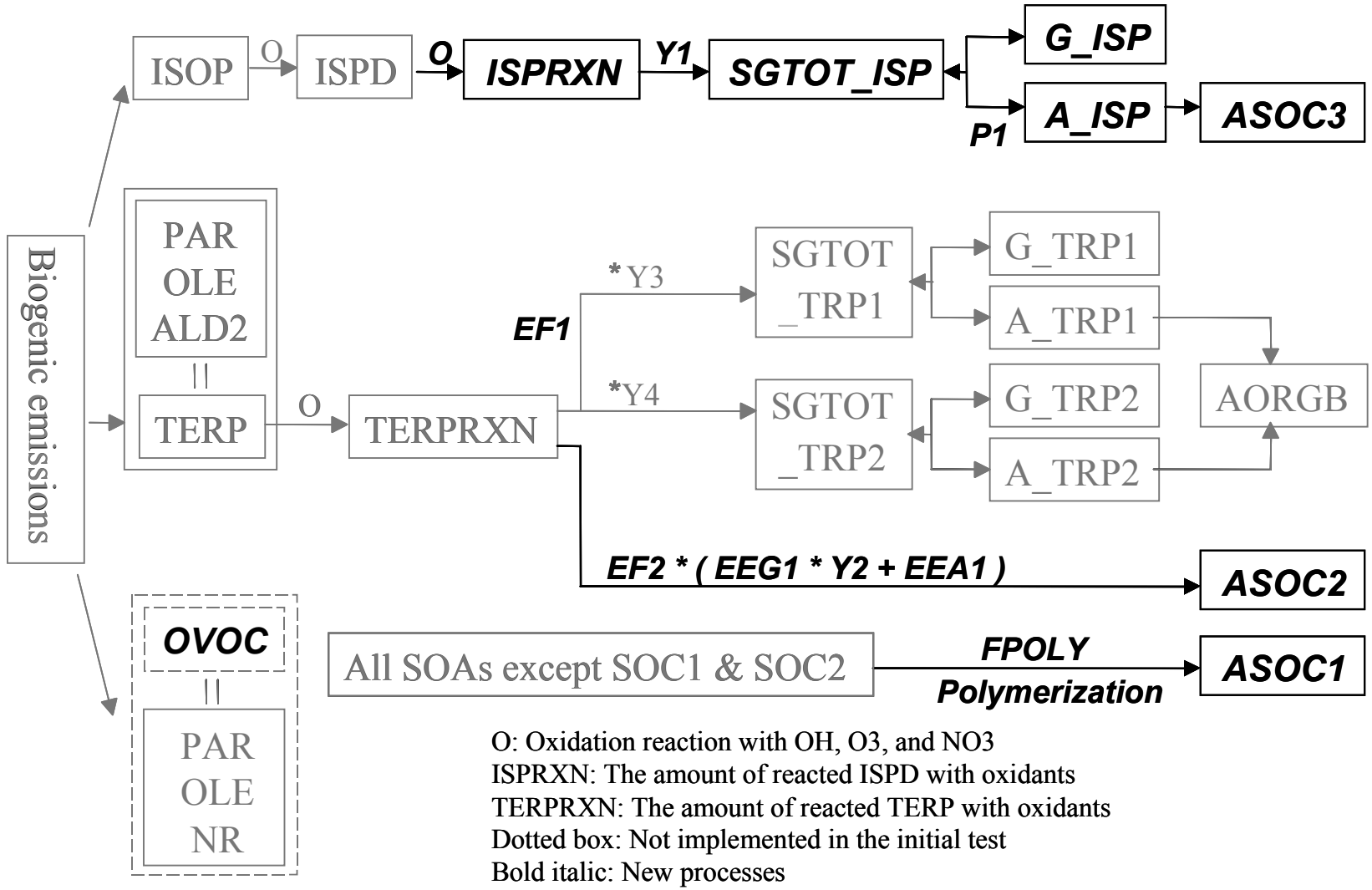

Figure 7-1. Schematic describing the addition of new SOA processes (bold italic) within the existing CMAQ SOA module (regular font) to treat polymerization and SOA from sesquiterpenes and isoprene.

7.3 CAMx Overview

The Comprehensive Model with Extensions (CAMx) modeling system is a publicly available (www.camx.com) three-dimensional multi-scale photochemical/aerosol grid modeling system that has been developed and maintained by ENVIRON International Corporation. CAMx was developed with all new code during the late 1990s using modern and modular coding practices. This has made the model an ideal platform for the extension to treat a variety of air quality issues including ozone, particulate matter (PM), visibility, acid deposition, and air toxics. The flexible CAMx framework has also made it a convenient and robust host model for the implementation of a variety of mass balance and sensitivity analysis techniques including Process Analysis (IRR and IPR), Decoupled Direct Method (DDM), and the Ozone and PM Source Apportionment Technology (OSAT and PSAT). Designed originally to address multiscale ozone issues from the urban- to regional-scale, CAMx has been widely used in recent years by a variety regulatory agencies for 1-hr and 8-hr ozone SIP modeling studies. Key attributes of the CAMx model for simulating gas-phase chemistry include the following:

- Two-way grid nesting that supports multi-levels of fully interactive grid nesting (e.g., 36/12/4/1.33 km).
- CB4 or SAPRC99 Chemical Mechanisms.
- Two chemical solvers, the CAMx Chemical Mechanism Compiler (CMC) Fast Solver or the highly accurate Implicit Explicit Hybrid (IEH) solver.
- Multiple numerical algorithms for horizontal transport including the Piecewise Parabolic Method (PPM), Bott, and Smolarkiewicz advection solvers.
- Subgrid-scale Plume-in-Grid (PiG) algorithm to treat the near-source plume dynamics and chemistry from large NO_x point source plumes.
- Ability to interface with a variety of meteorological models including the MM5 and RAMS prognostic hydrostatic meteorological models and the CALMET diagnostic meteorological model (others also compatible).
- The Ozone Source Apportionment Technology (OSAT) ozone apportionment technique that identifies the ozone contribution due to geographic source regions and source categories (e.g., mobile, point, biogenic, etc.).
- The Decoupled Direct Method (DDM) sensitivity method is implemented for emissions and IC/BC to obtain first-order sensitivity coefficients for all gas-phase species.
- Treatment of particulate matter (PM) using an empirical aerosol thermodynamics algorithm.

Culminating extensive model development efforts at ENVIRON and other participating groups, the CAMx (ver 4.10s) code was released in the autumn of 2004 as a truly "One-Atmosphere' model that rigorously integrates the gas-phase ozone chemistry with the simulation of primary and secondary fine and course particulate aerosols. This extension of CAMx to treat PM involved the addition of several science modules to represent important physical processes for aerosols. Noteworthy among these are:

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

- Size distribution is represented using the Multi-component Aerosol Dynamics Model (MADM), which uses a sectional approach to represent the aerosol particle size distribution (Pilinis et al., 2000). MADM treats the effects of condensation/evaporation, coagulation and nucleation upon the particle size distribution.

- Inorganic aerosol thermodynamics can be represented using ISORROPIA (Nenes et al, 1998; 1999) equilibrium approach within MADM, or a fully dynamic or hybrid approach can also be used.

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

- Aqueous-phase chemical reactions are modeled either using the RADM module (like CMAQ) or the Variable Size-Resolution Model (VRSM) of Fahey and Pandis (2001), which automatically determine whether water droplets can be represented by a single 'bulk' droplet-size mode or whether it is necessary to use fine and coarse droplet-size modes to account for the different pH effects on sulfate formation.

CAMx (ver 4.10s) provides two key options to users interested in simulating PM. For CPU-efficient annual PM modeling applications, CAMx may be run using Mechanism 4 (M4) with only two size sections (fine and coarse) and the efficient RADM bulk aqueous-phase module (as used in CMAQ). Alternatively, more rigorous aerosol simulations (perhaps for shorter episodes) may be addressed using the version that treats N-size sections (N is typically 10) and the rigorous, but computationally-extensive CMU multi-section aqueous-phase chemistry module.

Several updates have been made to CAMx since Version 4.10a was released. The current version is Version 4.3 that includes updates to treat frozen precipitation over Version 4.2. Version 4.3 of CAMx will be used in the CENRAP modeling.

7.4 CAMx Configuration for CENRAP Modeling

CAMx (ver 4.3) will be applied using many similar science options and input data sets to CMAQ. However, in some instances, the CMAQ and CAMx model development teams chose

different options for characterizing physical and chemical processes, or for implementing the governing equations on modern parallel computers. In these cases, we will utilize the science configurations embodied in the current release of CAMx.

The latest version of CAMx (ver 4.3 newer) will be employed and the model will be set up and exercised on the same 36/12 km grid as CMAQ. However, CAMx will be run using two-way grid nesting. The base configuration of CAMx will use 19 vertical layers to a 100 mb region (~15 km AGL) that exactly match those used by CMAQ. The PPM advection solver will be used along with the spatially varying (Smagorinsky) horizontal diffusion approach. Vertical diffusion in CAMx will be modeled by K-theory. The MM5 simulation using the Pleim-Xiu Land-Surface Model (LSM) and the ACM Planetary Boundary Layer (PBL) scheme will be used in the CAMx base configuration using the MM5CAMx processor that is similar to the CMAQ MCIP2.3 "pass through" option of the MM5 data invoked. CAMx will be exercised with the CB4 gas-phase, RADM aqueous-phase, and CMU/ISORROPIA aerosol chemistry schemes. The SOAP secondary organic aerosol scheme will be used for the base configuration in CAMx.

Note that it may be desirable to exercise CAMx using its "full-science" configuration for selected periods to investigate scientific issues that may be of interest that cannot be simulated by CMAQ, such as:

- The full sectional approach could be used to determine whether allowing secondary PM to grow into the coarse mode affects the model estimates;
- The model could be exercised with chemical active Sea Salt emissions; this could be important for fine particulate and visibility at key coastal sites in the CENRAP domain, especially when looking at clean days or natural background; and
- The full sectional aqueous-phase chemistry module may be important for sulfate formation.

7.5 Advantages of Operating Multiple Models

The use of both CMAQ and CAMx in the CENRAP 2002 annual modeling is a powerful and comprehensive diagnostic and quality assurance (QA) check of the modeling. There are numerous uncertainties in air quality models and the completely independent formulation of CMAQ and CAMx allow an independent QA check of one model against the other that will not be available if only one model was applied.

EPA's guidance on model selection for $PM_{2.5}$ SIPs and Regional Haze "reasonable progress demonstrations" do not identify a preferred photochemical grid modeling system, recognizing that at present there is "no single model which has been extensively tested and shown to be clearly superior or easier to use than several alternatives" (EPA, 2001, pg. 169). The agency recommends that models used for $PM_{2.5}$ SIPS or RH reasonable progress requirements should meet the requirements for alternative models. The CMAQ, CMAQ-AIM, CMAQ-MADRID and CAMx modeling systems all meet these requirements.

We believe that there is potentially significant value in including two or more regional modeling systems. Our testing of the CMAQ and CAMx model in some preliminary CENRAP model evaluation analysis (Tonnesen and Morris, 2004) found that their performance was generally similar for most species, with one model performing slightly better for some species and vice versa. Similar findings were obtained by VISTAS (Morris et al., 2004a). There are numerous advantages in applying both the CMAQ and CAMx models in the CENRAP 2002 annual modeling:

- **Diagnosis:** To serve as an efficient diagnostic tool addressing model performance issues that may arise in the establishment of the CMAQ and CAMx annual 2002 base cases. CAMx's suite of diagnostic probing tools plus its flexi-nesting algorithms make it an attractive tool for assisting in the diagnosis of model performance should this unexpected situation arise. CMAQ and CAMx both possess Process Analysis (PA) that can be a powerful diagnostic tool.

- **Model Evaluation Corroboration:** To provide corroboration of the base case model performance evaluation exercises and help identify any compensatory errors in the MM5/SMOKE/CMAQ or SMOKE/MM5/CAMx modeling systems.

- **Emissions Control Response Corroboration:** To provide corroboration of the response of the CMAQ or CAMx modeling system to generic and specific future year emissions changes on modeled gas-phase and particulate aerosol concentrations and resultant regional haze impacts.

- **Quantification of Model Uncertainty:** To provide one estimate of the range of uncertainty that attends statements of CMAQ and/or CAMx model performance in the annual and episodic base case simulations, and in the estimate of $PM_{2.5}$ and visibility reductions associated with future emissions change scenarios.

- **Alternative Science:** CMAQ and CAMx contain alternative science algorithms that may elucidate model performance issues in one model or the other.

- **Consistency with Other RPOs:** The Midwest RPO (MRPO) may end up using CAMx for their regional haze modeling, whereas the VISTAS and WRAP RPOs are currently using CMAQ as their primary model. As sources in the MRPO, VISTAS and WRAP likely influence visibility at Class I areas in the CENRAP region, having results from both models will be useful for reconciling any differences.

- **Backup Contingency:** To provide a 'backstop' model in the event that unforeseen difficulties with one of the models make it necessary to switch to an alternative 'One-Atmosphere' model at some point during the CENRAP modeling effort.

The benefits of employing a pair of complimentary state-of-science air quality models are thus quite significant. Especially considering that the same MM5 output (through MCIP and MM5CAMx) and SMOKE output and IC/BC files (through CMAQ-to-CAMx emissions and

IC/BC converters) can be used to operate CAMQ and CAMx without performing any additional meteorological or emissions modeling.

8.0 ASSESSMENTS AND OVERSIGHT

8.1 Assessment Responsibilities

The primary point of contact for CENRAP Modeling project assessment is that of the Modeling Team Project Manager (PM). This PM is available to the CENRAP Project Manager and Administrative Project Manager, CENRAP Modeling Workgroup, external reviewers, and internal staff by direct contact through e-mail and telephone. These links provide timely reviews of the project experimental design, implementation, and interpretation of the experimental results.

The assessments of overall project quality are provided from a number of different sources. Internal reviews of selected project components are periodically performed by the Project Manager and Co-Principal Investigators. The results of this and other routine (e.g., QC checks) and special reviews of project data quality are documented in the monthly reports.

The project team is committed to achieving and maintaining the highest level of quality possible throughout the performance of this program. The modeling information generated will be both technically sound, and, where appropriate, defensible from a regulatory perspective. The former is an obvious requirement but is not, in and of itself, sufficient to defend the data against an adversarial inquiry. The latter will address, through documentation, the level of quality achieved. The quality of the project data will be maintained not only through the development and use of data quality objectives (DQOs), which place numerical limits on the QC indicators, but also through the use of subjective science quality objectives. Science quality objectives are used to provide evaluations of the quality of the research project and goals of the study. Evaluations of all research activities by internal and external peer review will assure that the methodology, experimental processes, conclusions and recommendations provided by this project are scientifically sound.

8.2 Assessment Types and Usage

Assessments of the quality of the products generated on this project will be made by:

- Conducting internal performance reviews of the critical components of the experimental setup and data processing systems. Where applicable, adherence to SOPs will be evaluated. The results of these reviews will contain any suggested corrective actions, and be appended to the reports generated in this project.

- Independent peer reviews of thesis materials, reports, and papers resulting from this project.

The CENRAP Modeling Workgroup provides external review of all reports and plays an active role in the development of experimental matrices and to review research progress and plans for future project tasks.

8.3 Assessment Criteria

The project assessment criteria address the extent to which the modeling runs and experiments provide the quality of data needed to satisfy the objectives of this project. A major objective of this project consists of providing the data and information needed for evaluating and improving models for predicting the effects of emissions on air quality. Therefore, the evaluation process includes assessments of model uncertainties, the extent to which the proposed actions or system improvements can reduce these uncertainties, and estimates of the certainty of this work in providing the data of the type and quality needed. Criteria for assessing data utility and quality will include the following:

- Utility of the type of measurements for model evaluation. For example, are model predictions of the measurements sensitive to the uncertainties in the mechanism that are being evaluated? Are the available resources being applied to the highest priority types of measurements?

- Degree of characterization of experimental conditions for modeling. For data to be useful for model evaluation, experimental conditions must be sufficiently well characterized, so that the data can be used for model evaluation without characterization uncertainties dominating the results.

- Accuracy, precision, and sensitivity of the measurement data. The measurements in the concentration region of interest should be sufficiently accurate and precise to provide a meaningful test of model predictions.

- Procedures used to assure data quality, identify data not meeting quality objectives, and to minimize errors and other data quality problems.

- Degree to which the modeling appropriately incorporates the characterization results in the inputs, and the analysis of the modeling results appropriately take into account characterization and measurement uncertainties and biases.

- Degree to which the experimental procedures, measurement methods, and data processing and analyses, and modeling methods are documented.

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