Quality Assurance Project Plan (Draft)

For

Visibility Improvements for States and Tribal Associations for the Southeastern States (VISTAS)

Emissions and Air Quality Modeling

Revision 0
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1.0 INTRODUCTION

This Quality Assurance Project Plan (QAPP) describes the quality management functions and activities performed by the Visibility Improvements for States and Tribal Associations in the Southeast (VISTAS) Phases I and II Emissions and Air Quality Modeling performed by ENVIRON International Corporation (Prime Contractor), Alpine Geophysics, LLC (Subcontractor) and the University of California at Riverside College of Engineering – Center for Environmental Research and Technology (UCR/CE-CERT; Subcontractor).

VISTAS 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 Regional Haze Rule (RHR) visibility SIPs/TIPs due in 2007/2008. VISTAS modeling results will also likely 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 VISTAS Emissions and Air Quality Modeling Team is comprised of staff from ENVIRON International Corporation (ENVIRON), Alpine Geophysics, LLC (Alpine) and the University of California, Riverside (UCR). The ENVIRON/Alpine/UCR Team performs the emissions and air quality modeling simulations for states and tribes within the VISTAS region, providing analytical results used in developing implementation plans under the EPA Regional Haze Rule.

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/Alpine/UCR Team and is documented in the VISTAS Phase I and II Modeling Protocols (ENVIRON, 2003; 2004a) and in UCR’s Quality Management Plan (QMP; UCR, 2003). The VISTAS Modeling Protocols and UCR’s QMP formed the basis for much of the content in this VISTAS 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 particularly 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 making.

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 Southeastern US are required to submit visibility SIPs under Section 308 of the Regional Haze Rule (RHR).

Through the Southeastern States Air Resource Managers (SESARM), the Visibility Improvement State and Tribal Association of the Southeast (VISTAS) has implemented a regional air quality planning process to provide the necessary technical and policy tools needed by states and tribes to comply with the Section 308 of the RHR requirements. As part of this effort, VISTAS has funded modeling studies to support the development of SIPs and TIPs. In March 2003, VISTAS contracted with ENVIRON International Corporation, with Alpine Geophysics, LLC (Alpine) and University of California at Riverside (UCR) as Subcontractors, to perform Emissions and Air Quality Modeling.

The results of the modeling studies performed by VISTAS 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

The VISTAS 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 southeastern 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 VISTAS 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 VISTAS Two-Phased Approach

The VISTAS Emissions and Air Quality Modeling activities are being performed in two Phases. Phase I, which occurred primarily during the 2003 calendar year, consisted of emissions and regional haze modeling for three episodes to identify the optimal model configuration(s) for simulating regional haze in the southeastern US. Phase II, initiated in 2004, consists of operating the emissions and air quality models for the 2002 calendar year to develop the regional haze modeling databases needed to address the requirements of the Section 308 RHR SIPs and TIPs.

2.2.1 VISTAS Phase I

The objective of VISTAS Phase I was to determine the optimal modeling configuration for use in the subsequent Phase II visibility assessment. Accordingly, Phase I entailed a comprehensive literature review of recent relevant visibility studies using various photochemical/aerosol modeling platforms in order to assess and identify appropriate model configurations, data bases, and model testing methodologies that were appropriate for use in conducting the VISTAS Phase I emissions and PM modeling assessment. Key elements of Phase I included:

- Review all relevant air quality model simulations that have been completed related to regional haze and $PM_{2.5}$ modeling and document the relevant sensitivity analyses, model configuration testing, and performance evaluations that have been performed (ENVIRON, 2003b);

- Review the current science in regional emissions modeling (e.g., EPS, EMS and SMOKE) and PM air quality modeling (e.g., CMAQ, CMAQ-MADRID, CMAQ-AIM, REMSAD, UAM-V/PM, CAMx4 and PMCAMx) to determine the most appropriate model(s) for use by VISTAS (ENVIRON, 2003b);

- Review available ambient data for evaluating one-atmosphere PM/ozone models (ENVIRON, 2003c);

- Develop and implement a plan or Modeling Protocol for testing and evaluating alternative science configurations of the recommended Phase I model(s) and document the results (ENVIRON, 2003a); and

- Prepare a Task 6 report prescribing the model set-up, data base development, performance testing, and control strategy evaluation procedures to be implemented in VISTAS Phase II (ENVIRON, 2004a).

VISTAS formed three standing workgroups to plan and direct the project. These included: (a) the Technical Analysis (emissions and modeling) Workgroup; (b) the Data (monitoring) Workgroup; and (c) the Planning Workgroup. Under Phase I, the VISTAS Technical Analysis Workgroup (TAWG) managed the comprehensive model configuration testing program aimed, as noted above, at evaluating the capabilities of current state-of-science regional emissions, prognostic meteorological and PM/visibility models. The resultant modeling system (models and databases) identified and tested in Phase I were intended to be applied in Phase II (discussed below) following the procedures set forth in the Phase II Modeling Protocol (ENVIRON, 2004a).

For the meteorological component of the Phase I modeling, SESARM contracted with Baron Advanced Meteorological Systems (BAMS) to apply the PSU/NCAR Mesoscale Model (MM5) in multiple configurations and to evaluate its performance against surface and aloft meteorological observations (Olerud, 2003a-f). The emissions modeling component of VISTAS Phase I was carried out by the research team of ENVIRON/Alpine/UCR with staff at Alpine Geophysics taking the lead role in setting up, testing, and applying the emissions modeling system. The air quality modeling component was performed by the team at the ENVIRON/Alpine/UCR modeling centers. A dominant theme during Phase I was the exchange of modeling codes, databases, and evaluation software between the three modeling centers as the air quality modeling was carried out.

2.2.2 VISTAS Phase II

The Phase II modeling includes annual PM/regional haze simulations plus potentially additional shorter duration episodes. After detailed performance testing, the modeling system will then be exercised with a variety of emissions control scenarios aimed at enabling VISTAS to assess the effects of future year emission control strategies on visibility and other air quality issues. The modeling system will also allow VISTAS to track reasonable progress toward regional haze goals. More specifically, the VISTAS Phase II program will focus on the use of the CMAQ modeling system for calendar year 2002 over the same 36/12 km horizontal grid system used in Phase I. A potentially large number of annual (and episodic) model simulations will be performed; the list below reflects current plans:

- **<u>2002 Initial Annual Run</u>.** The initial annual model simulations and performance evaluations using the 2002 inventory for VISTAS and non-VISTAS states, Canada and Mexico. Multiple iterations of the 2002 annual simulation will be required to confirm the appropriateness of the model science configuration(s) recommended by the Phase I work, to evaluate updates to the model and model inputs and to refine model performance.

- **2002 Revised Annual Run.** A subsequent annual 2002 simulation using revised 2002 modeling inventory for VISTAS and non-VISTAS states, Canada and Mexico. The primary objective of this run is model performance demonstration using updated emissions inventories and best science model configurations. Additional sensitivity tests will be conducted using the revised base case year annual run.

- **2002 Annual Run with "Typical Year" EGU/Fire Inventory.** An annual 2002 simulation representing the 2000-2004 baseline period for EGU and fire emissions and using 2002 revised inventory for all other source sectors. The primary objective of this inventory is to provide the base line modeled air quality condition against which future year modeling runs will be compared to develop relative reduction factors for each pollutant species.

- **Future Year Annual Runs.** Future year simulations involving a base case inventory of typical EGU and fire emissions for VISTAS-selected future period. Additional future year inventories may also be modeled. The objective of these future year model runs is to establish the modeled air quality basis against which the effectiveness of emissions control strategies will be evaluated.

- **Future Year Emission Control Strategies.** Prescription of the future year emissions control strategies to be performed later in Phase II (e.g., 2005) will be defined after the foregoing simulations and analyses have been completed. A combination of annual and episodic runs is anticipated.

Closely integrated with the annual (and possibly episodic) meteorological, emissions and air quality modeling will be ongoing project management, technical review, and quality assurance activities performed under the guidance of the VISTAS Contracting Officer and the TAWG. The modeling team members will participate with VISTAS management in regular monthly conference calls, as well as ad hoc topical conference calls as needed, and will attend periodic meetings with the TAWG members throughout Phase II.

Complementing the data acquisition, modeling input development activities, and project management activities, four other Phase II activities will be performed, consistent with the Quality Assurance Project Plan (QAPP):

2.2.2.1 Data Gatekeepers

The VISTAS Phase II emissions and air quality modeling team are receiving emissions, meteorological and air quality data from other VISTAS contractors or other sources. As a first line of QA, we have defined a Gatekeeper function to assure 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**. Obtain air quality data as appropriate for model input development and model performance evaluation and assure that the quality of all air quality data obtained are consistent with the approved QAPP. Provide documentation of evaluation and generate IC/BC inputs for CMAQ for all modeling runs.

- **Meteorological Gatekeeper**. Obtain meteorological data, as MM5 or MCIP files, as appropriate for annual 2002 modeling runs and other episode periods and perform data quality checks as approved in the QAPP, together with appropriate documentation of model performance evaluation activities.

- **Emissions Gatekeeper.** Obtain emissions inventory data necessary to support annual 2002 and future year modeling and recommend source of emissions data to be used for Canada and Mexico. Assure quality of all emissions data received are consistent with the approved QAPP, and develop all emissions modeling files to support modeling runs for 2002. Develop the chemical speciation files and temporal and spatial allocation files necessary to convert annual inventories into hourly and daily emissions modeling files, as appropriate. Develop all emissions modeling files for non-VISTAS states to support modeling runs for future year base case and emissions strategies as defined by VISTAS.

- **Data Management Gatekeeper**: Maintain the VISTAS Modeling Website including posting modeling input and output files, reports, interpretation of results, and other documents as requested by VISTAS to support all Phase II tasks. 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 VISTAS states, other regional planning organizations, EPA, other contractors, and stakeholders.

2.2.2.2 Emissions QA/QC

Emissions Quality Assurance (QA) and Quality Control (QC) are the single 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 Phase II we will continue with the multistep emissions QA/QC approach applied in the Phase I modeling. This includes the initial emissions QA/QC by the Emissions Gatekeeper described above, as well as QA/AC 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:

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

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

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

Once 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 objective of this step is to identify errors in spatial distribution of emissions.

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

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

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

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

2.2.2.3 Meteorology QA/QC

The VISTAS meteorological modeling contractor (BAMS) will have primary responsibility in the QA/QC of the MM5 meteorological fields. However, the emissions and air quality modeling team will also perform some QA/QC of the meteorological data to assure that it has 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 VISTAS Phase II Meteorological Gatekeeper will perform the following:

- Analyze the MM5 data to assure it has been transferred correctly.
- Evaluate the MM5 using METSTAT and the surface meteorological network.
- Evaluate upper-air MM5 meteorological estimates by comparison them to upper-air observations and satellite images.
- Compare the VISTAS 2002 MM5 simulation with the one generated by WRAP.
- Generate the CMAQ-ready meteorological inputs using the MCIP2.2 processor.

2.2.2.4 Air Quality Modeling QA/QC

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

- Verification that correct configuration and science options are used in compiling and running each model of the in the CMAQ modeling system, where these include the MCIP, JPROC, ICON, BCOM and the CCTM.
- Verification that correct input data sets are used when running each model.
- Evaluation of CCTM 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 results against concurrent observations.
- Backup and archiving of critical model input data.

The most critical element for CMAQ 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 the CMAQ model we employ a system of naming conventions using environment variables in the compile and run scripts that guarantee that correct inputs and science options are used. We also employ a redundant naming system so that the names of key science options or inputs are included in the name of the CMAQ executable program, in the name of the CMAQ 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 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 output files. In the case of model sensitivity studies, the animated gifs will be prepared as difference plots for the sensitivity case minus the base case. Often, errors in the emissions inputs can be discovered by viewing the animated GIFs. Finally, we will produce 24 hour average plots for each day of the CMAQ simulations. This provides a summary that can be useful for quickly comparing various model simulations.

2.2.2.5 Overview of Data Flow and Quality Assurance Process

Figure 2-1 displays an overview of the data flow and quality assurance process in the VISTAS Emissions and Air Quality Modeling study. The VISTAS Modeling Team receives different types of data from various VISTAS contractors and other sources that have performed their own Quality Assurance (QA) and Quality Control (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. Once the Gatekeeper has conducted a QA check of the data it is passed on to the modeler who performs their QA of the data. The data are then used in the modeling and resultant output (e.g., model-ready emissions or meteorological files) are then subjected to another round of QA to assure the integrity of the data is retained.

Once the model-ready inputs have been developed and subjected to QA/QC, the models (e.g., CMAQ and/or CAMx) are applied using Base Case emissions and the modeling results subjected to a model performance evaluation. The model performance evaluation (MPE) represents an extensive QA effort and is the most time consuming component 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 VISTAS Modeling Team performs the MPE/QA process using as many different tools and analysis as possible in order to fully understand the accuracy and reliability of the model simulation. As seen in Figure 2-1b, the MPE process in VISTAS 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.

MAPS Analysis Tools: Alpine Geophysics (Alpine) has a MAPS Analysis Tool that also runs under Linux and is based on Fortran and NCAR Graphics. It was originally developed for evaluating ozone models and has been extended to treat PM species as well. In addition to calculating similar statistics, scatter plots and time series plots as the UCR Analysis Tools, it also can generate spatially averaged time series plots of concentrations, bias and error, performs analysis of peak concentrations and includes a Flying Data Grabber (FDB) for comparing modeling results with aircraft data.

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.

GA DNR Analysis Plots: Dr. James Boylan of the Georgia Department of Natural Resources has extended the concept in EPA's draft PM fine particulate and regional haze modeling guidance that model performance for species that make up a major contribution to visibility impairment be subjected to more stringent goals than species that are minor contributors by developing concentration-dependent performance goals and "Bugle Plots" to display them.

The evaluation of the VISTAS Phase II initial 2002 CMAQ Base Case simulation used each of the analysis tools listed above demonstrating their descriptive and complimentary nature.

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 mean 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, that 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 precise 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 VISTAS 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 intercomparison 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 are greater than 2.5 ug/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**	**Comment**
#∀15%	#35%	Ozone model performance goal[8] 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.

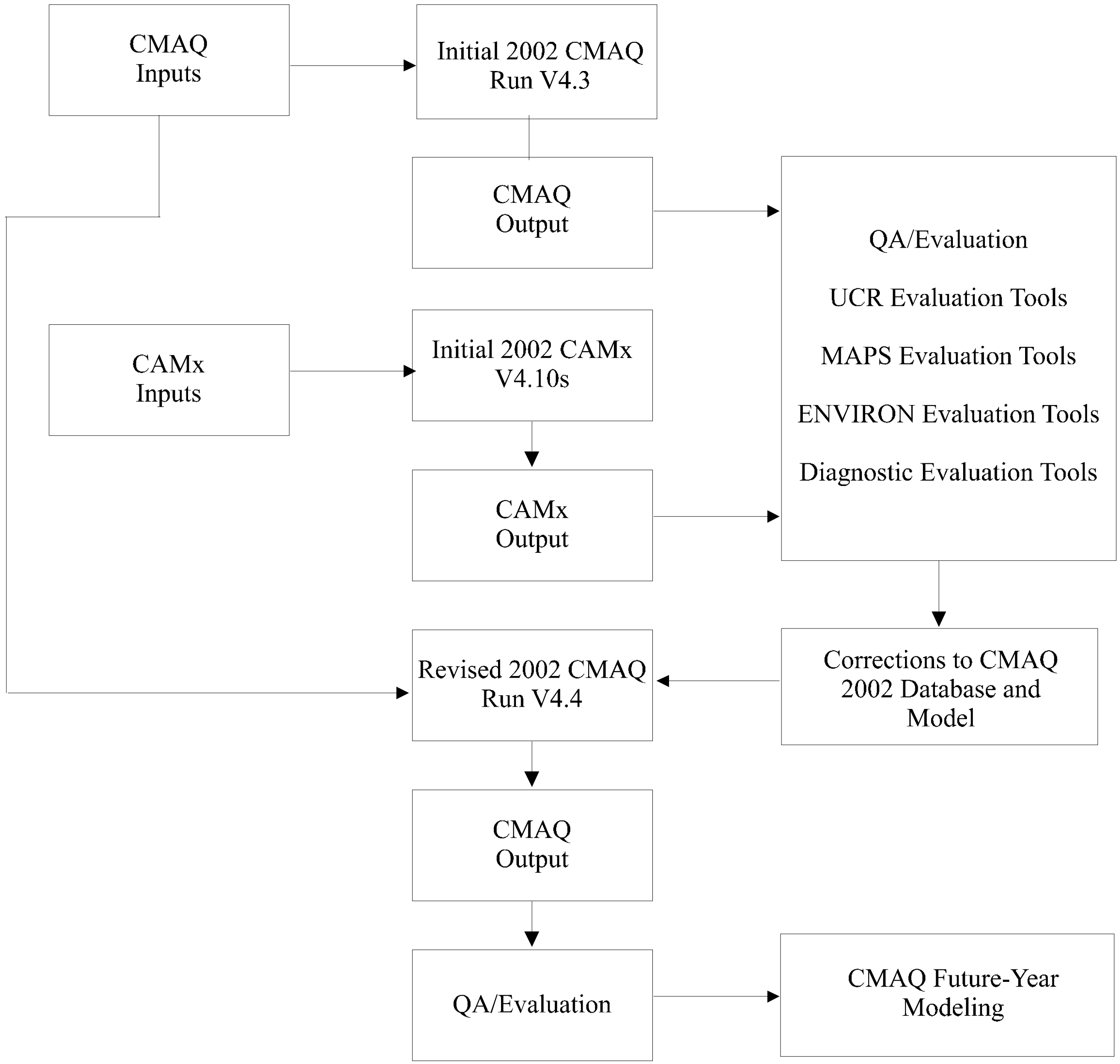

Figure 2-1a. Data flow and quality assurance steps in the VISTAS Emissions and Air Quality Modeling.

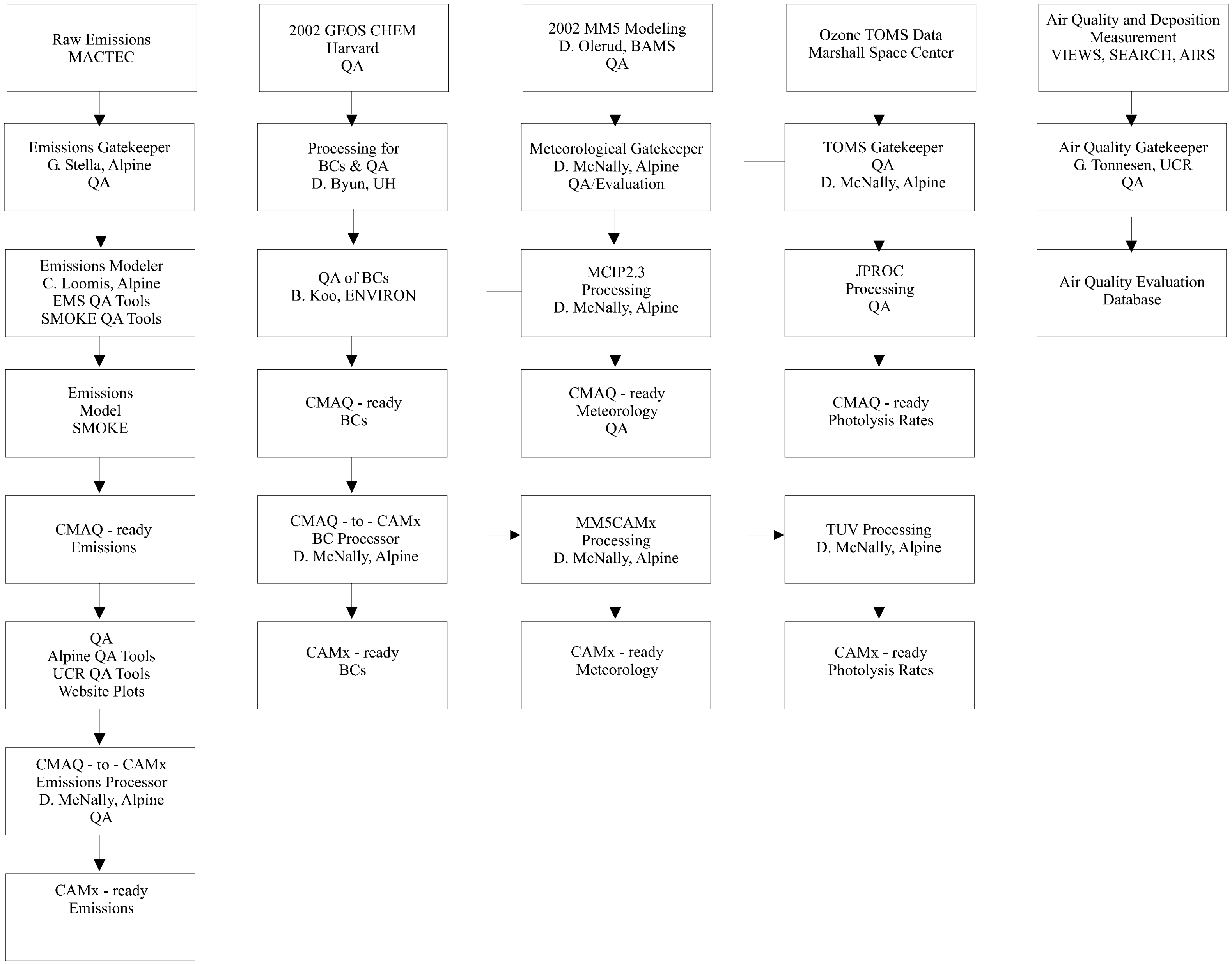

Figure 2-1b. Concluded. Data flow and quality assurance steps in the VISTAS Emissions and Air Quality Modeling.

2.3 VISTAS Phase I and II Modeling Protocols

As recommended in EPA's draft regional haze modeling guidance (EPA, 2001), the VISTAS Phase I and II modeling efforts were initiated by developing Modeling Protocols that described the procedures to be used to conduct, quality assure and quality control (QA/QC), evaluate and use the modeling results (ENVIRON, 2003a; ENVIRON, 2004a). These Modeling Protocols were reviewed and commented on by the VISTAS TAWG and others and are updated accordingly.

2.4 VISTAS Phase I Activities

The VISTAS Phase I Emissions and Air Quality Modeling work was carried out mainly during 2003 with some final deliverables provided in early 2004. The Phase I activities formed the basis for the Phase II modeling and was the foundation of the Phase II quality assurance (QA) and quality control (QC).

2.4.1 Phase I Task 1: Project Management

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

Project Management: The Project Manager, Co-Principal Investigators (Co-PIs), and Task Managers had frequent communications with the VISTAS technical and project management group through regular conference calls, e-mails and meetings as needed. The ENVIRON, Alpine and UCR Modeling Centers were headed by each of the three Co-PIs (Ralph Morris, T.W. Tesche and Gail Tonnesen, respectively) with clear lines of communication.

Technical Management: The three Co-PIs are responsible for the management of the technical work within each of their respective research groups. With responsibility comes accountability.

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

Deliverables under this task were continuous project management and conference calls, plus two project meetings held in Research Triangle Park, North Carolina (see Table 2-2). The project meetings were attended by the three Co-PIs and additional staff from the Emissions and Air Quality Modeling Team.

Table 2-2. Phase I Task 1 Project Management task deliverables and due dates.

Item	Description	Due Date
1	VISTAS TAWG Modeling Meeting September 29-30, 2003 at the Solution Center in Research Triangle Park, North Carolina	09/29-30/03
2	VISTAS TAWG Modeling Meeting February 12-13, 2004 in Research Triangle Park, North Carolina	02/12-13/04

2.4.2 Phase I Task 2: Develop Model Configuration Evaluation Plan

The first activity under the VISTAS Phase I Emissions and Modeling Study was the development a detailed plan, or Modeling Protocol (ENVIRON, 2003a), outlining the data analysis procedures and statistical/graphical tools to be used in evaluating the core and alternative CMAQ configurations in Task 4. This plan identified the procedures used in producing internally consistent observational and modeling data sets for individual particulate species and species groupings. The main purpose of this plan is to provide a consistent set of procedures to be used in the early portion of the Phase I activities when the various CMAQ model configurations are being tested. The draft plan was submitted to VISTAS TAWG who provided comments that were incorporated in the final Phase I modeling plan (see Table 2-3).

Table 2-3. Phase I Task 2 Phase I Modeling Plan task deliverables and due dates.

Item	Description	Due Date
1	Draft Report "VISTAS Emissions and Air Quality Modeling—Phase I Task 2 Report: Recommended Model Configurations and Evaluation Methodology For Phase I Modeling"	06/03/03
2	Revised Draft Report "VISTAS Emissions and Air Quality Modeling— Phase I Task 2 Report: Recommended Model Configurations and Evaluation Methodology For Phase I Modeling" Available at: http://pah.cert.ucr.edu/vistas/reports/VISTAS_Task2-REPORT.pdf	08/04/03

2.4.3 Phase I Task 3: Acquisition and Development of Modeling Data Bases

Under this task we assembled the databases needed to operate and evaluate the CMAQ model for the three Phase I episodes.

Subtask 3a: Assemble/QA Air Quality Data. Under this Subtask we assembled a comprehensive database of ambient measurements to evaluate model performance. As part of the WRAP model performance evaluation our team had previously assembled data from the CASTNet (weekly wet and dry deposition of SO4, NO3, NH4, pH, base cations) and IMPROVE (daily fine particulate mass composition as SO4, NO3, NH4, OC, EC, and soils). Additional processing of data was needed to include ambient data from the SEARCH and STN networks in the analysis. Several issues must be addressed to use these data to evaluate model performance. In many cases there is not a 1-to-1 correspondence to model species. Accordingly, formulas must be developed to correctly map the data to the model species (for details, see the IMPROVE and CASTNET links at: http://pah.cert.ucr.edu/rmc/ambient/ambient.shtml. Moreover, model predictions are hourly while some ambient data are daily or weekly averages, so algorithms were developed to correctly treat averaging periods including correct representation of the time zone used for each monitoring site. QA of ambient data is a key step; we reviewed all data for reasonableness and completeness and flagged apparent outliers for exclusion from the model evaluation. We processed the AIRS data including O3, NOx and CO to convert it to the IO/API data format so that it can be used with PAVE for visualization of model and ambient data. For long term modeling (monthly to annual) it is essential that the QA'd ambient databases be designed to work with our model performance evaluation software. This will facilitate rapid model evaluation for multiple sensitivity simulations or repeats of base case simulations.

Subtask 3b: Assemble/QA Emissions Data. CMAQ emissions inputs were prepared using data supplied by the VISTAS emissions contractors, the EPA NEI version 2 databases and the SMOKE emissions modeling system. The study team is currently working with the NEI formats and has developed the necessary QA tools to make effective use of these data. The NEI database, while the best available national inventory, must be examined for local modeling, particularly in point source locations and stack parameters. The QA tools developed as part of the EMS-2001 are a useful adjunct to the tools currently available in SMOKE.

The study team has also developed a suite of tools designed to QA and evaluate episode specific emissions prior to inclusion into the modeling inventory. Since the magnitude of the day-specific emissions for large stationary source is often significant in the modeling inventory, special attention is placed on the QA of these emissions data. The study team has processed the spatial surrogates and BELD-3/BEIS-3 databases over the Unified RPO grid under contract to the Midwest RPO. These data are currently under review and revision and the version most current will be used.

Subtask 3c: Assemble/QA Meteorological Data. The meteorological model (MM5) output data was acquired from the VISTAS meteorological modeling contractor. While we recognize that the MM5 data will already have been validated by the meteorological modeling contractor, it has been our Team's experience that an independent review is both time and cost effective. As part of our quality assurance activities, a full operational model evaluation was performed on the MM5 data sets. This operational evaluation covered surface and aloft wind direction, temperature, mixing ratio, and planetary boundary layer depths on both a domain-wide and subregional basis. The techniques used will follow the model performance protocol prepared for EPA for annual MM5 modeling (McNally and Tesche, 2002).

Table 2-4 summarizes the VISTAS Phase I Task 3 deliverables.

Table 2-4. Phase I Task 3 Phase I Acquisition and Development of Model Databases task deliverables and due dates.

Item	Description	Due Date
1	Draft Report "VISTAS Emissions and Air Quality Modeling— Phase I Task 3a Report: Review and Assessment of Available Ambient Air Quality Data to Support Modeling and Model Performance Evaluation for the Three VISTAS Phase I Episodes" Available at: http://pah.cert.ucr.edu/vistas/reports/VISTAS_Task_3_072203.pdf	07/22/03
2	Draft Report "VISTAS Emissions and Air Quality Modeling— Phase I Task 3b Report: CMAQ Emissions Inventory Development and Emissions QA/QC Summary Report for Episodes 1, 2 and 3" Available at: http://pah.cert.ucr.edu/vistas/reports/VISTAS_subtask_3b_QA_report.pdf	09/25/03
3	Subtask 3c-1 Report: "VISTAS Emissions and Air Quality Modeling— Phase I Task 3c-1 Report: MM5 Meteorology QA/QC Summary Report for Episode 1: 2-20 January 2002" Available at: http://pah.cert.ucr.edu/vistas/reports/met_episode_1_report.pdf	09/10/03
4	Subtask 3c-2 Report: "VISTAS Emissions and Air Quality Modeling— Phase I Task 3c-2 Report: MM5 Meteorology QA/QC Summary Report for Episode 2: 13-22 July 1999" Available at: http://pah.cert.ucr.edu/vistas/reports/met_episode_2_report.pdf	09/15/03
5	Subtask 3c-3 Report: "VISTAS Emissions and Air Quality Modeling— Phase I Task 3c-3 Report: MM5 Meteorology QA/QC Summary Report for Episode 3: 11-27 July 2001" Available at: http://pah.cert.ucr.edu/vistas/reports/met_episode_3_report.pdf	09/16/03

2.4.4 Phase I Task 4: Develop Optimal VISTAS Modeling Configuration

Under VISTAS Phase I Task 4, we developed plans for the initial testing and sensitivity modeling of the SMOKE and CMAQ modeling systems in order to identify the optimal model configurations) for simulating regional PM, ozone and visibility in the eastern US. We first reviewed and assessed recent relevant regional modeling studies from which we identified an initial configuration and list of sensitivity tests. We then performed the sensitivity tests to identify the optimal model configuration(s).

Subtask 4a: Recent Literature Review. Initiating Task 4 we performed a literature review to identify and critically evaluate recent relevant fine particulate/regional haze modeling studies, field programs and related scientific investigations that shed light on: (a) the selection and evaluation of CMAQ model configuration options, (b) the availability and adequacy of gas-phase and PM data sets for model set up and performance testing, (c) the suitability of operational and diagnostic procedures for evaluating the performance of CMAQ, and (d) any pertinent information of future year emissions control evaluations (ENVIRON, 2003b).

Subtask 4b: Recommend Initial SMOKE/CMAQ Configurations. Drawing from the Team's experience with SMOKE and CMAQ, we identified a suite of initial model configurations to be evaluated with the three test episodes. These alternative configurations included definition of: (a) vertical and horizontal grids, (b) gas-phase chemistry mechanism, (c) secondary aerosol mechanisms, (d) advection algorithms, (e) diffusion algorithms, (f) cloud and surface removal processes, (g) numerical integration scheme(s), and so on (ENVIRON, 2003b).

Subtask 4c: Evaluate Approved SMOKE/CMAQ Configurations. The ENVIRON, Alpine, and UCR team collaboratively evaluated the various model configurations recommended in Subtask 4b. These evaluations employed internally consistent statistical and graphical procedures and display software (Morris et al., 2004a).

Subtask 4d: Perform Diagnostic/Sensitivity Experiments**.** Paralleling and supporting Subtask 4c, the study team conducted a series of diagnostic/sensitivity experiments aimed at identifying the most technically sound and reliable chemistry, transport, removal, and numerical algorithms available (Morris et al., 2004a).

Subtask 4e: Recommend Optimal Model Configuration. The culmination of the literature review, CMAQ configuration testing and module sensitivity/diagnostic studies was the identification of a final, optimal configuration for the VISTAS modeling platform to be used in Phase II (Morris et al., 2004a).

Subtask 4f: Technical Documentation. Thorough documentation was performed for all aspects of Task 4 (Morris et al., 2004a). In addition, many of the findings in this task were relevant to VISTAS and other RPO's and warranted publication of the technical findings at scientific conferences or in journals (Morris et al., 2004b,c,d; Tesche et al., 2004).

Table 2-5. Phase I Task 4 Develop Optimal VISTAS Modeling Configuration task deliverables and due dates.

Item	Description	Due Date
1	"VISTAS Emissions and Air Quality Modeling— Phase I Task 4a/b Report: Review of Model Sensitivity Simulations and Recommendations of Initial CMAQ Model Configurations and Sensitivity Tests" Available at: http://pah.cert.ucr.edu/vistas/reports/VISTAS_Task4a_Report.pdf	07/25/03
2	Final Report "VISTAS Emissions and Air Quality Modeling— Phase I Task 4cd Report: Model Performance Evaluation and Model Sensitivity Tests for Three Phase I Episodes" Available at: http://pah.cert.ucr.edu/vistas/reports/Final_Phase1/VISTAS_Task4cd_FinalReport_ExcSum-Sec3_only.pdf	09/07/04

2.4.5 Phase I Task 6: Phase II Modeling Protocol

The VISTAS Phase II Modeling Protocol describes in detail the work to be performed and the specific quality assurance (QA) procedures to be used in performing, evaluating, and archiving the annual model simulations performed in Phase II. Particular emphasis in the protocol was given to: (a) model configurations, (b) specific science issues to be addressed, (c) model improvements, (d) model input preparation, (e) model applications (base year, future year, and strategies), (f) model evaluation and sensitivity analyses, (g) documentation, (h) data transfer, backup and archiving, and (i) schedule and deliverables. As shown in Table 2-6, under this task a First Draft Modeling Protocol was prepared and submitted to the VISTAS TAWG for review and comment. Based on these comments a Revised First Draft Modeling Protocol was prepared and distributed to the entire group for review and comment.

Table 2-6. Phase I Task 6 Phase II Modeling Protocol task deliverables and due dates.

Item	Description	Due Date
1	First Draft Report "VISTAS Emissions and Air Quality Modeling — Phase I Task 6 Report: Modeling Protocol for the VISTAS Phase II Regional Haze Modeling"	03/03/04
2	Revised First Draft Report "VISTAS Emissions and Air Quality Modeling — Phase I Task 6 Report: Modeling Protocol for the VISTAS Phase II Regional Haze Modeling." Available at: http://pah.cert.ucr.edu/vistas/reports/VISTAS_PhaseII_Protocol_Mar12_2004.pdf	03/12/04

2.4.6 Phase I Task 7: Website Development

We developed a technical web site that served as the primary means for distributing emissions and air quality modeling to the VISTAS TAWG. The website included model results, analyses, presentations and reports. We maintained 4 list-servs (all participants, general project management, emissions QA, and modeling results) for the VISTAS project that can be accessed from the website that provides a permanent archive for all email communications for the project. Separate list-servs provides better organization of communications and allow for detailed discussions of specific topics such as emissions QA.

Table 2-7. Phase I Task 6 Develop Website task deliverables and due dates.

Item	Description	Due Date
1	VISTAS Phase I Emissions and Air Quality Modeling Project Website: http://pah.cert.ucr.edu/vistas/index.shtml	2003-2004

2.5 VISTAS Phase II Activities

Below we discuss the project and QA activities for the currently planned VISTAS Phase II Modeling work effort.

2.5.1 Phase II Task 1: Project Management

The objective of this task is to manage project activities, participate in conference calls, attend 3 VISTAS meetings in the southeastern United States (US), project management with VISTAS contacts, subcontractor management and general oversight, and overall quality assurance.

The VISTAS Phase II management structure for Emissions and Air Quality Modeling is the same as used in Phase I with Ralph Morris of ENVIRON serving as Project Manager and Ralph Morris, T.W. Tesche and Gail Tonnesen serving as Co-Principal Investigators (Co-PIs) and managing the activities in each of the ENVIRON, Alpine and UCR modeling centers, respectively. Under this task we are performing all management activities for the VISTAS Phase II modeling study, including:

- Attendance of two scientists of the ENVIRON/Alpine/UCR Team at 3 VISTAS meetings to be held in the southeastern US.

- Participation in scheduled conference calls to be held approximately once per month as well as expected ad hoc conference calls to be held as needed.

- Refine Draft Phase II annual modeling protocol due early March 2004. Final initial Phase II annual modeling protocol incorporating review comments as directed by Contract Officer due two weeks after direction received. The modeling protocol follows EPA guidance and includes the specific task descriptions, data quality and assurance plan, and model performance evaluation plan for VISTAS Phase II 2004 work. The VISTAS Phase II modeling protocol is a living document that will be updated as tasks are added to project work scope and to document revisions in the technical approach.

- Develop and refine the Scope of Work and conduct contract discussions with the VISTAS modeling team and the VISTAS technical and project representatives.

- Preparation of subcontracts, invoicing and payments.

- Internal project conference calls and discussions among the ENVIRON/Alpine/UCR project team.

- Develop and implement the Quality Assurance Project Plan (QAPP).

- Model performance evaluation report using revised 2002 inventories. Report of model response to changes in inventory from 2002 revised to 2002 base year with “typical” EGU and fire.

- Executive Summary report summarizing key findings and results from the task summary reports.

Table 2-8. Phase II Task 1 Project Management task deliverables and due dates.

Item	Description	Due Date
1	Second Draft Report "VISTAS Emissions and Air Quality Modeling — Phase I Task 6 Report: Modeling Protocol for the VISTAS Phase II Regional Haze Modeling." Available at: http://pah.cert.ucr.edu/vistas/vistas2/reports/vistasII_Final_Protocol_05_10_2004.pdf	05/06/04
2	Conference Calls with VISTAS among Modeling Team and with TAWG	2004-2005
3	National Inter-RPO Modeling Meeting in Denver, Colorado May 25-26, 2004	05/25-26/04
4	VISTAS TAWG Meeting in Atlanta, Georgia September 22-23, 2004	09/22-23/04
5	VISTAS TAWG meeting to be determined (TBD)	TBD
6	Quality Assurance Project Plan (QAPP)	November 2004
7	Draft VISTAS Phase II Executive Summary Report	12/31/04
8	Final VISTAS Phase II Executive Summary Report	01/15/05

2.5.2 Phase II Task 2: Develop IC/BCs for 2002 Annual Run

The objective of this task is to analyze the need for a high time resolution (e.g., 3-hourly) global climate model (e.g., GEOS-CHEM) output for generating Boundary Conditions (BCs) for 2002 annual modeling of the 36 km national RPO grid.

Under this task we are recommending a source of initial and boundary conditions (IC/BC) for 2002 annual and 2003 episodic CMAQ modeling. We would analyze in more detail the VISTAS Phase I July 2001 episode CMAQ simulations using the BCs generated from GEOS-CHEM 2001 3-hour concentrations outputs. The CMAQ model performance and output for the July 2001 episode using BCs generated from GEOS-CHEM seasonal/monthly vs. 3-hour output performed under Phase I would be analyzed and compared with a run using the EPA CMAQ default BCs. This is followed by interaction with investigators at Harvard University and University of Houston to evaluate temporal and spatial variability between BC based on 3-hour average and monthly average GEOS-CHEM outputs for 2001. Based on these results we would recommend whether GEOS-CHEM 2002 day-specific outputs are justified to capture daily variability in BC concentrations.

Table 2-9. Phase II Task 2 GEOS-CHEM Boundary Conditions Analysis task deliverables and due dates.

Item	Description	Due Date
1	PowerPoint Presentation: "VISTAS Phase I and II Modeling Boundary Condition Sensitivity" presented at February 12-13, 2004 VISTAS Modeling Meeting in RTP, NC	02/12-13/04

2.5.3 Phase II Task 3: 2002 Data Preparation and Model Inputs

The development of the VISTAS Phase II 2002 annual CMAQ model inputs is being performed in several Subtasks as follows.

2.5.3.1 Subtask 3a: Air Quality Data Gatekeeper

The objective of Subtask 3a is to acquire, process and QA/QC air quality data, deposition data and other data that can be used to evaluate CMAQ and other air quality models for the 2002 annual cycle and the 36 km national RPO grid with particular emphasis on the VISTAS southeastern US region.

Under this Subtask the Air Quality Gatekeeper would perform the following activities:

- Obtain air quality data as appropriate for model input development and model performance evaluation. At a minimum, the same data bases as used in Phase I should be used in Phase II.
- Identify if any special aircraft (or other) measurements are available within the VISTAS 12-km domain for the 2002 modeling year.
- Assure quality of all air quality data obtained, are consistent with the approved QA/QC plan.
- Provide documentation of evaluation.
- Generate IC/BC inputs for CMAQ for all 2002 modeling runs described in Task 4 below.

2.5.3.2 Subtask 3b: MM5 Meteorological Model Gatekeeper

The objectives of this Subtask is to acquire the 2002 MM5 data from the VISTAS Meteorological Contractor (BAMS) and perform QA/QC, an independent evaluation, and process the data using MCIP for input into CMAQ.

The Meteorological Gatekeeper's function for the VISTAS Phase II 2002 MM5 modeling results would be the similar as was done in Phase I, only we would leverage off of the 2002 MM5 model evaluation infrastructure set up at ENVIRON for WRAP. The MM5 output would be acquired from BAMS and subjected to an initial quality check. Any issues associated with the 2002 MM5 output would be reported immediately back to BAMS and VISTAS. After an initial quality check is performed, a more thorough QA/QC and an independent evaluation would be conducted. Results would be compared with other 2002 MM5 simulations (e.g., WRAP). The CMAQ-ready meteorological inputs would also be generated under this subtask. The MM5 data would be provided in two installments of 8 months and 4 months, respectively.

2.5.3.3 Subtask 3c: Emissions Gatekeeper and Emissions Development for Non-VISTAS States, Canada, and Mexico

Under this Subtask we would coordinate activities with the VISTAS emissions contractor and perform initial QA/QC of emissions. We would also develop emissions for non-VISTAS States, Canada, and Mexico for the 2002 annual modeling period. The Emissions Gatekeeper would coordinate activities with the VISTAS emissions contractors and technical advisors to assure that data are provided in the correct format and that there are no holes in the emissions inventory. They would also coordinate with EPA and other RPOs to determine the best sources of data for non-VISTAS States as well as Canada and Mexico. Once data are received from the VISTAS emissions contractor the Emissions Gatekeeper would perform a preliminary QA/QC and immediately report back to VISTAS and the emissions contractor any issues that are uncovered. These results would be documented in the Emissions Gatekeeper report.

Under this task we would also develop emissions inventories for non-VISTAS States, Canada, and Mexico consistent with the RPO data exchange protocol, using existing national or regional modeling inventories, state CERR submittals, EPA National Emissions Inventories, or other sources, as appropriate

2.5.3.4 Subtask 3d: Emissions Modeling

The objective of this Subtask is to generate base- and future-year CMAQ-ready gridded, hourly, speciated, three-dimensional emission inputs for 2002. The SMOKE emissions processing system would be used along with the 2002 MM5 data to process the 2002 emissions for VISTAS states from the VISTAS emissions contractor and emissions from the non-VISTAS states, Canada and Mexico provided under Subtask 3c Emissions Gatekeeper. CMAQ emission modeling files would be generated to support four rounds of emissions modeling runs using the 2002 meteorological conditions:

1. An initial 2002 Base Case run of CMAQ-ready emission inputs using VISTAS States emissions data received by January 31, 2004, and MM5 meteorological data received by March 31, 2002 would be ready by May 30, 2004.
2. Revised 2002 Base Case and 2002 Typical Year emission runs using the emissions submitted by September 15, 2004 that would be ready by October 15, 2004.
3. Future-year emission scenarios using 2002 meteorology and emissions data submitted by October 15, 2004 would be ready by November 15, 2004.

The initial 2002 Base Case emissions modeling would use the existing Phase I SMOKE emissions modeling set up. For the revised 2002 Base Case, 2002 Typical Year and Future-Year emissions modeling, the existing Phase I SMOKE emissions modeling set up would be updated and enhanced as follows:

- Process emissions with SMOKE version 2
- Implement EPA’s new spatial surrogate distributions
- Implement EPA’s revised PM speciation profiles and SCC cross-references
- Implement revised temporal profiles as collected and converted from data provided by VISTAS’ emissions contractors or other sources

Biogenic emissions will be processed using SMOKE and the 2002 MM5 day-specific temperatures and held constant for all the 2002 and future-year emission scenarios (i.e., the effects of climate change and land cover changes will not be accounted for in the future-year biogenic emission estimates).

On-road mobile sources comprise a major computational component of the SMOKE emissions modeling. If day-specific adjustments are required using day-of-week and daily MM5 temperature estimates that would increase the SMOKE processing time considerably and potentially impact the schedule.

Currently, other RPOs are modeling the motor vehicle emissions using average monthly temperature data, or by modeling one weekday, Saturday and Sunday from each quarter. To better represent the day-of the-week variability typical to motor vehicle emissions, and to make the best possible use of the meteorological data available, we propose to model one full week from each month of the annual episode, for a total of 84 episode days modeled. Note that this approach will allow us to expand the number of motor vehicle days modeled, if particular periods of the annual episode warrant additional refinement in the modeling inventory.
Area source and non-road mobile source emissions will also be modeled for one week per month, using seasonal, monthly and day-of-week adjustments available in the current SMOKE configuration.

EGU emissions will be supplied by the VISTAS emissions contractor in an annual file. To temporally allocate the EGU point sources, heat input data from the 2002 CEM datasets will be used to develop facility or unit-level temporal distributions. The day-specific and facility-specific temporal profiles will be used in conjunction with the emissions contractor supplied emissions data to calculate hourly EGU emissions by facility.

For the 2002 Typical Year and Future-Year emission scenarios the VISTAS emissions contractor would provide average emissions for EGUs for the current baseline (2000-2004) and the future-year baseline (2014-2018) periods.

Day-specific emissions for fires (wildfires, prescribed burns and agricultural fires) may be provided by the VISTAS emissions contractor and would be used in the 2002 Base Case emissions scenario. If other temporally allocated fire emissions are provided, we will generate a set of actual 2002 fire-based temporal profiles and cross-references to allocate emissions to hours in the modeled episodes. Typical year emissions for fires would be provided by the VISTAS emissions contractor and would be used in both the 2002 Typical Year and Future-Year emission scenarios.

Ammonia emissions will be modeled as provided by the emissions contractor. Supplemental ammonia modeling is not expected during the emissions modeling phase.

Wind blown dust emissions (i.e., PM10 and PM2.5 emissions from wind erosion of natural geogenic sources (SCCs 2730100000 [total] and 2730100001 [dust devils]), will be excluded from the modeling files consistent with Phase I.

Each round of emissions modeling would be documented in emission summary tables and PowerPoint presentations that would contain tables and graphs of the emissions and QA/QC summaries. A final report on the VISTAS Phase II emissions modeling would be prepared that focuses on the differences in emissions in the different emissions scenarios including documentation of the changes in emissions from the 2002 Typical Year to Future-Year emissions scenario that would assist in the interpretation of the visibility projections.

2.5.3.5 Subtask 3e: Future-Year Emissions Modeling for Three VISTAS Phase I Episodes

Under this Subtask we would develop emissions modeling files for the initial future-year base case inventory for the July 2001 and Jan 2002 Phase I episodes. These inventories will be used in emissions sensitivity modeling analyses between May 2004 and September 2004. The same SMOKE emissions set up from the Phase II Subtask 3d would be used.

2.5.3.6 Subtask 3f: Interim Future-Year Emissions Modeling using 2002 Meteorology

Under this Subtask we would generate CMAQ-ready emission inputs for an interim future-year and the 2002 meteorological year. The VISTAS emissions contractors would provide interim future-year emissions estimates.

2.5.3.7 Phase II Task 3 Deliverables

The VISTAS Phase II Task 3 deliverables are summarized in Table 2-10.

Table 2-10. Phase II Task 3 2002 Data Preparation and Model Inputs task deliverables and due dates.

Item	Description	Due Date
1	Subtask 3a 2002 Air Quality and Deposition Database for Model Performance Evaluation	04/30/04
2	PowerPoint Presentation for Subtask 3b: “VISTAS 2002 MM5 Annual Run Meteorological Gatekeeper Evaluation.” Available at: http://pah.cert.ucr.edu/vistas/vistas2/ppt_files/Task3b_VISTAS_II%20_met_gatekeeper_.ppt	06/30/04
3	PowerPoint Presentation for Subtask 3c VISTAS Initial Base Year 2002 Emissions Inventory Preparation.” Available at: http://pah.cert.ucr.edu/vistas/vistas2/ppt_files/Task3c_Initial_Base_Year_EI_Preparation.ppt	08/08/04
4	PowerPoint Presentation for Subtask 3c VISTAS Future Year Emissions Inventory Preparation.” Available at: http://pah.cert.ucr.edu/vistas/vistas2/ppt_files/Task3c_Initial_Future_Year_EI_Preparation.ppt	08/08/04
5	Subtask 3d Initial 2002 Base Case CMAQ-ready Emission Inputs	05/30/04
6	Subtask 3d Revised and Typical 2002 CMAQ-ready Emission Inputs	10/15/04
7	Subtask 3d Future-Year (2018) CMAQ-ready Emission Inputs for Two Scenarios	12/15/04
8	Subtask 3e Future-Year (2018) CMAQ-ready Emission Inputs for Two Phase I Episodes	06/15/04
9	Subtask 3f Interim Future-Year (2009) CMAQ-ready Emission Inputs	12/15/04

2.5.4 Phase II Task 4: 2002 Annual CMAQ Modeling

Under Phase II Task 4 we would apply the CMAQ model using Initial and Revised 2002 Actual Base Case emissions and other inputs and perform a model performance evaluation on the results.

2.5.4.1 Subtask 4a: Initial Base Case and Model Performance Evaluation

A preliminary 2002 CMAQ Actual Base Case simulation would be performed using the initial 2002 inventory for VISTAS and Non-VISTAS states, Canada and Mexico that are to be delivered to modeling team by January 31, 2004. After subjecting the initial 2002 emissions to the Emissions Gatekeeper quality checks and QA/QC (Subtask 3c), CMAQ-ready emissions would be generated using the initial emissions for 2002 (Subtask 3d). The primary objective of this initial CMAQ run is to set up and streamline the modeling system and approach and obtain a preliminary model performance evaluation for the 2002 annual period. The focus of the analysis will be on model performance diagnostics and experience in running the annual simulations to optimize model performance both in terms of ability to estimate fine particulate matter in the southeastern US as well as optimize the ability of the modeling centers to perform 2002 annual CMAQ runs.

Once the initial CMAQ base case simulation is generated, it will be subjected to a model performance evaluation. In Phase II multiple approaches will be utilized in the evaluation process:

- Alpine will use their MAPS software to generate performance statistics and graphical displays by network and by subregion. The MAPS software generated some performance measures not supported by other software (e.g., spatial average time series) and once set up can easily generate performance measures and displays by subregion.

- Alpine will also apply the UCR statistical performance package that was used in Phase I that includes model performance metrics, scatter plots and time series plots. This package has been extended to include PAVE spatial maps with superimposed observation to provide spatial information on model performance.

- UCR will help analyze and interpret the model performance results and post them on the VISTAS modeling website.

- ENVIRON will evaluate the results using techniques they developed for WRAP that focus on model performance at Class I areas for the 20% Best and 20% Worst visibility days that are the data used to project future-year visibility improvements. This performance would include predicted and observed stacked bar charts of extinction showing the contributions of each of the for the 7 components of extinction (SO4, NO3, EC, OC, Soil, CM and Rayleigh) of extinction averaged and separately for the 20% Best/Worst days. Days from then 20% Best/Worst days and Class I areas where the modeling results deviate greatly from the observed values would be flagged for further analysis into model performance and possible exclusion for use in the visibility projections (i.e., calculating RRFs).

Use of multiple MPE approaches will allow the quick identification of potential problems in the model estimates or the model performance evaluation software. The results would be shared among the group and with VISTAS. The operational model performance evaluation would be conducted using the same “routine” ambient databases as used in Phase I (e.g., IMPROVE, CASTNet, AQS, SEARCH, STN and SEARCH).

Because the initial emissions may undergo significant changes, limited diagnostic sensitivity tests would be conducted using the initial 2002 CMAQ database. The limited sensitivity tests would be aimed at identifying and rectifying specific performance issues of the model that we don’t believe will be corrected by updated emissions. As in the VISTAS Phase I modeling, the sensitivity tests will be flexible and opportunistic to quickly identify and resolve areas of highest importance. However, the number of sensitivity tests will be limited by available funding and time constraints.

2.5.4.2 Subtask 4b: Revised Base Case Simulation

A 2002 CMAQ simulation would be conducted using the revised 2002 Base Case emissions inventory that is expected to be received from the VISTAS emissions contractor by September 15, 2004. Several components of 2002 initial CMAQ set up could change including, but not limited to, emissions, meteorology, boundary conditions, CMAQ update, CMAQ chemical module. For example, if a 2002 GEOS-CHEM simulation is performed, then the revised BCs from Optional Task 13 would be used in the revised base case simulation. The revised 2002 CMAQ simulation would be run using the “best configuration” identified in Subtask 4a. The results would be transferred to each of the modeling centers that would conduct their own operational MPE as was done under Subtask 4a. We have budgeted 8 annual 36 km and 4 annual 12 km sensitivity simulations under this task to investigate alternative configurations, options and updates on model performance. The results would be documented in a draft final report submitted to VISTAS.

2.5.4.3 Subtask 4c: Typical Year Emissions Simulation

EPA guidance recommends using models in a relative sense to project future year visibility through relative reduction factors (RRFs). Thus, for projecting changes in visibility, the current-year base case and future-year scenarios must be consistent. Thus, in this task typical emissions for fires and EGUs will be used for the 2002 Typical Year emissions scenario, instead of the episodic specific emissions used in the 2002 Base Case simulation. The 2002 typical year emissions generated under Subtask 3d would be used in this simulation. The results would be subjected to a QA/QC, compared with the 2002 Base Case simulation and a cursory evaluation would be conducted.

2.5.4.4 Subtask 4d: Future-Year Modeling for Two Scenarios

Using the CMAQ-ready emissions for the two future-year emission scenarios prepared under Subtask 3d that would be ready by November 15, 2004 and December 15, 2004, we would perform the two future-year CMAQ simulations under this subtask. New future-year boundary conditions (BCs) may be used depending on the availability of data. The future-year CMAQ results for the two scenarios and the CMAQ results for the 2002 Typical Year scenario would be used to project visibility improvements at Class I areas using EPA guidance.

2.5.4.5 Subtask 4e: Interim Future-Year using 2002 Database

Using the CMAQ-ready emissions for the interim future-year emission scenario prepared under Subtask 3f that would be ready by December 15, 2004, we would perform the interim future-year CMAQ simulation under this subtask. New future-year boundary conditions (BCs) may be used depending on the availability of data. The future-year CMAQ results for the interim future-year scenario and the CMAQ results for the 2002 Typical Year scenario would be used to project visibility improvements at Class I areas using EPA guidance.

2.5.4.6 Summary of Phase II Task 4 Deliverables

Table 2-11 summarizes the VISTAS Phase II Task 4 deliverables and due dates.

Table 2-11. Phase II Task 4 2002 CMAQ Modeling task deliverables and due dates.

Item	Description	Due Date
1	PowerPoint Presentation for Subtask 4a: "Initial Vistas 2002 CMAQ Run, Analysis of 36 km Performance for PM." Presented at July 27, 2004 VISTAS TAWG Conference Call. Available at: http://pah.cert.ucr.edu/vistas/vistas2/reports/2002_CMAQ_initial.ppt	07/27/04
2	PowerPoint Presentation for Subtask 4a: "Initial VISTAS 2002 CMAQ Run: 36/12 km Diagnostic MPE" Presented at July 27, 2004 VISTAS TAWG Conference Call. Available at: http://pah.cert.ucr.edu/vistas/vistas2/reports/2002_CMAQ_initial_AG.ppt	07/27/04
3	Revised Draft Final Report for Subtask 4a: "VISTAS Phase II Emissions and Air Quality Modeling -- Task 4a Report: Evaluation of the Initial CMAQ 2002 Annual Simulation." Dated September 27, 2004.	09/27/04
4	PowerPoint Presentation for Subtask 4a: "Initial CMAQ Diagnostic MPE for 2002: VISTAS Task 4a Results." Presented at VISTAS September 21-22, 2004 TAWG meeting in Atlanta, Georgia. Available at: files/Sept_2004_tawg/2002_CMAQ%20Diagnostic%20MPE_TWT.ppt	09/21/04
5	PowerPoint Presentation for Subtask 4a: "Initial VISTAS Phase II 2002 CMAQ Operational Model Performance Evaluation." Presented at VISTAS September 21-22, 2004 TAWG meeting in Atlanta, Georgia. Available at: http://pah.cert.ucr.edu/vistas/vistas2/docs.shtml	09/21/04
6	PowerPoint Presentation for Subtask 4a on diagnostic analysis of the Initial	11/12/04

Item	Description	Due Date
	2002 CMAQ Base Case simulation to identify OC and NO3 performance issues.	
7	PowerPoint Presentation for Subtask 4b on Revised 2002 XCMAQ Base Case Simulation and Model Performance Evaluation	11/30/04
8	Subtask 4b Draft Report on Revised 2002 CMAQ Base Case simulation and model performance evaluation	12/15/04
9	Subtask 4b Report on Model Sensitivity Tests	01/15/05
10	PowerPoint Presentation on Subtask 4c 2002 Typical Base Case simulation	12/31/04
11	Subtask 4d Draft Report on Future-Year (2018) Base Case modeling	01/31/04
12	PowerPoint Presentation on Subtask 4e Interim Future-Year modeling	01/31/05

2.5.5 Phase II Task 5: Episodic Modeling

The VISTAS Phase II plan includes potential provisions for performing episodic modeling if needed. In particular, additional episodic modeling may be carried out to: (1) capture meteorological conditions for Worst 20% or Best 20% visibility days at Class I areas that did not occur during the 2002 annual modeling period; and (2) to obtain modeling periods during 2003 when the FOCUS sites were operating that contain enhanced speciated PM measurements. The Phase II Task 5 Episodic Modeling work effort is currently not funded. Given that the 2003 year was fairly wet and atypical and the 2002 annual modeling year appears to capture most of the meteorological conditions, additional episodic modeling may not be carried out so is not addressed in this QAPP.

2.5.6 Phase II Task 6: Data Management

2.5.6.1 Subtask 6a: VISTAS Modeling Website

Under this Subtask we would maintain the VISTAS Modeling Website including posting modeling input and output files, reports, interpretation of results, and other documents including Task Reports and PowerPoint Presentations presented during meetings and conference calls.

2.5.6.2 Subtask 6b: Data Transfer, Storage and Retrieval

Under this Subtask we would archive and store key model inputs and outputs and make them available to others. Storage of model inputs and outputs for up to 6 annual runs plus episodic runs or optional tasks to be defined. A firewire or IDE drive(s) of the key model inputs would be provided to VISTAS who could distribute it to states, stakeholders and others as desired (i.e., technology transfer). We would also perform data requests as directed by VISTAS under this Subtask.

2.5.6.3 Phase II Task 6 Data Management Deliverables

Table 2-12 summarizes the deliverables and schedule for the Phase II Task 6 Data Management. The VISTAS Phase II modeling website would be operated and maintained continuously during the 2004-2005. We expect the Initial and Revised 2002 CMAQ databases to be delivered to VISTAS in October and December 2004, respectively. Finally, as directed by VISTAS we would provide additional data to others as requested.

Table 2-12. Phase II Task 6 Data Management task deliverables and schedule.

Item	Description	Due Date
1	VISTAS Phase II Modeling Website. Available at: http://pah.cert.ucr.edu/vistas/vistas2/index.shtml	2004-2005
2	Firewire disks of Initial 2002 CMAQ annual modeling databases	10/15/04
3	Firewire disks of Revised 2002 CMAQ annual modeling databases	12/31/04
4	Disks, CD, DVD, ftp files and e-mail files of data transfer as directed by VISTAS	2004-2005

2.5.7 Phase II Task 7: Emission Reduction Sensitivity Simulations using CB4 and SAPRC Chemistry and 2 Phase I Episodes

The objective of this optional task is to investigate the sensitivity of estimated PM concentrations to emissions reductions using the CB4 and SAPRC99 chemical mechanisms. If significant differences exist and there are reasons to believe that the SAPRC99 response may be more correct, then the revised 2002 Base Case modeling starting in September would be performed using the SAPRC99 chemistry.

The CB4 and SAPRC99 emission reductions sensitivity tests would be performed using the January 2002 (winter) and July 2001 (summer) episodes. We would perform 30% emission reductions across all source categories and across the entire modeling domain for the 36 km grid for the following five precursors:

- NOx
- SO2
- VOC
- NH3
- NOx+NH3

With 2 episodes and 2 chemical mechanisms this results in 10 total CMAQ 36 km simulations. We would also perform two corroborative emissions reductions sensitivity simulations using the CAMx model for the July 2001 episode and 36 km grid. Table 2-13 summarizes the deliverables under Phase I Task 7.

Table 2-13. Phase II Task 7 CB4/SAPRC Sensitivity Modeling task deliverables and due dates.

Item	Description	Due Date
1	PowerPoint Presentation for Task 7: "VISTAS Phase II Task 7 Update: CMAQ Version 4.4beta CB4/SAPRC99 Comparisons" presented at July 27, 2004 TAWG Conference Call. Available at: http://pah.cert.ucr.edu/vistas/vistas2/reports/PhaseII_Task7_Update.ppt	07/27/04
2	PowerPoint Presentation for Task 7: "VISTAS Phase II Task 7 Results: CMAQ Version 4.4beta CB4/SAPRC99 Comparisons" presented at September 2, 2004 TAWG Conference Call. Available at: http://pah.cert.ucr.edu/vistas/vistas2/ppt_files/Task7_VISTAS_PhaseII_Task7_CB4-SAPRC_Sep02_2004.ppt	09/02/04
3	PowerPoint Presentation for Task 7: "VISTAS Phase II Task 7 Results: CB4/SAPRC99 Comparisons for Urban Sites" presented at September 14, 2004 TAWG Conference Call. Available at: http://pah.cert.ucr.edu/vistas/vistas2/ppt_files/Task7_VISTAS_PhaseII_CB4-SAPRC_Urban_Sep14_2004.ppt	09/14/04

2.5.8 Phase II Task 10: Journal Paper on VISTAS Phase I Modeling

The objective of this task is to write and submit the results of the VISTAS Phase I modeling results to a peer-review journal. An outline for a journal article on the VISTAS Phase I modeling would be prepared and distributed to VISTAS. Based on comments the outline would be updated and a draft paper written documenting the VISTAS Phase I modeling results. The draft paper would be distributed to VISTAS and updated based on their comments. In consultation with VISTAS a Journal would be selected and the paper submitted to the Journal for publication. The paper would be updated as needed to address comments of the Journal peer-reviewers and a final manuscript submitted to the Journal for publication.

Table 2-14. Phase II Task 10 Phase I Journal Article task deliverables and due dates.

Item	Description	Due Date
1	Draft Journal Article on VISTAS Phase I Modeling for VISTAS review	11/30/04
2	Journal Article for Submission	12/31/04

2.5.9 Phase II Task 13: Analysis and Processing of 2002 GEOS-CHEM Data

Under this task we would process output from a 2002 GEOS-CHEM global climate model simulation performed by Harvard University to generate 2002 day-specific 3-hourly CMAQ boundary condition (BC) inputs for 2002.

Table 2-15. Phase II Task 13 2002 GEOS-CHEM Boundary Condition Processing task deliverables and due dates.

Item	Description	Due Date
1	PowerPoint Presentation: "Documentation and Evaluation of the 2002 GEOS-CHEM Simulation." Presented during VISTAS TAWG October 4, 2004 conference call. Available at: http://pah.cert.ucr.edu/vistas/vistas2/ppt_files/2002_GEOS_CHEM_100404.ppt	10/01/04
2	CMAQ-ready Boundary Condition (BC) input files	10/15/04

3.0 PROJECT MANAGEMENT

3.1 Project Organization

This project is conducted by the ENVIRON International Corporation, Alpine Geophysics, LLC (Alpine), and the University of California at Riverside (UCR), with input from the VISTAS Technical Analysis Workgroup (TAWG). Organizational commitment is an essential element for developing and implementing a successful research project. Ralph Morris of ENVIRON would be the VISTAS Emissions and Air Quality Modeling Project Manager (PM). The VISTAS Phase II Modeling Team has three Co-Principal Investigators that coordinate activities at each of the three modeling centers, Ralph Morris of ENVIRON, T.W. Tesche of Alpine and Gail Tonnesen at UCR. The PM and three Co-PIs are 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 and Co-PIs and VISTAS TAWG. 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 VISTAS Emissions and Air Quality Modeling study, with more details on their roles provided next.

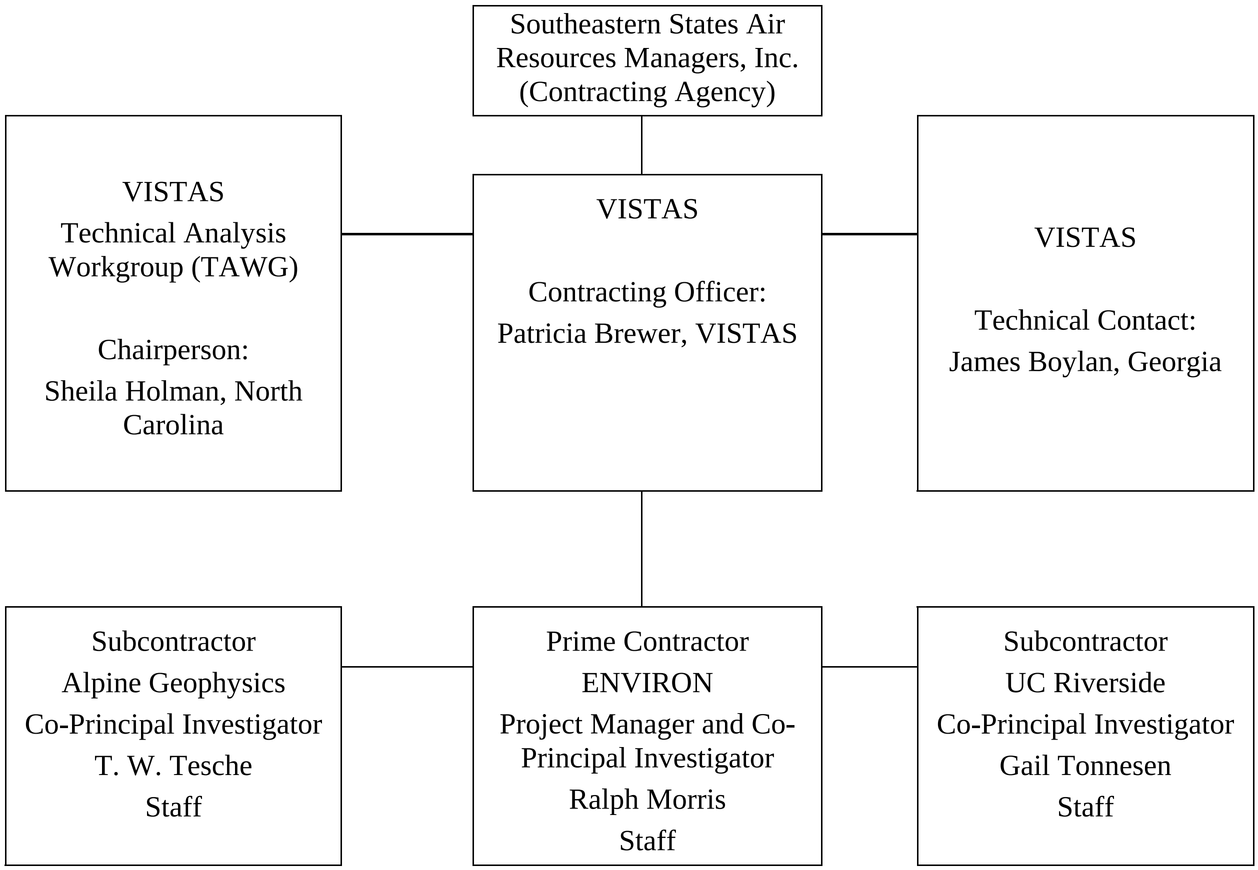

Figure 3-1. VISTAS Emissions and Air Quality Modeling Project Organizational Chart.

Table 3-1. VISTAS Phase II Emissions and Air Quality Modeling project participants and contacts.

Person & Role	Affiliation/Address	Contact Information
Patricia Brewer (Contracting Officer)	VISTAS Technical Coordinator 2090 US Highway 70 Asheville, NC 28778	(828) 296-4500 (Fax) (828) 299-7043 pat.brewer@ncmail.net
James Boylan (Technical Contact for Emissions & AQ Modeling)	Georgia DNR Air Protection Branch 4244 International Pkwy, Ste 120 Atlanta, GA 30354-3906	(404) 362-4851 (Fax) (404) 363-7100 James_Boylan@mail.dnr.state.ga.us
Michael Abraczinskas (Technical Contact for MM5 Modeling)	North Carolina DENR 1641 Mail Service Center Raleigh, NC 27699-1641	(919) 715-3743 Michael.Abraczinskas@ncmail.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
T.W Tesche (Co-Principal Investigator)	Alpine Geophysics, LLC 3479 Reeves Drive Ft. Wright, KY 41017	(859) 341-7502 (Fax) (859) 341-7502 twt@iac.net
Gail Tonnesen (Co-Principal Investigator)	UC Riverside CE-CERT 1084 Columbia Avenue Riverside, CA 92507	(951) 781-5676 (Fax) (909) 781-5790 tonnesen@cert.ucr.edu
Key ENVIRON Participants		
Bonyoung Koo	ENVIRON 101 Rowland Way Novato, CA 94945	(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 Alpine Geophysics Participants		
Dennis McNally	Alpine Geophysics, LLC 7341 Poppy Way Arvada, CO 80007	(303) 421-2211 (Fax) (303) 421-9553 dem@alpinegeophysics.com
Cyndi Loomis	Alpine Geophysics, LLC 7341 Poppy Way Arvada, CO 80007	(303) 421-2211 (Fax) (303) 421-9553 cfl@alpinegeophysics.com
Greg Stella	Alpine Geophysics, LLC 387 Pollard Mine Road Burnsville, NC 28714	(828) 675-9045 gms@alpinegeophysics.com
Key UCR CE-CERT Participants		
Zion Wang	UC Riverside CE-CERT 1084 Columbia Avenue Riverside, CA 92507	(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

3.1.1 ENVIRON Project Manager and Co-Principal Investigator

Mr. Ralph Morris of ENVIRON is the Project Manager (PM) and Co-Principal Investigator (Co-PI) for the VISTAS 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 VISTAS TAWG 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
- Serve 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
- Establishes a Subcontracts with Alpine and UCR to perform the work, and adhere to the terms and conditions of that contract
- Assists in the performance of the modeling program in accordance with its contract and the Work Plan
- Provides information to assist the VISTAS TAWG in achieving its goals as stated in its Work Plan and Strategic Plan
- Develops individual test protocols and reports as directed
- Analyzes modeling data and provides assessment reports
- Supports the Principal Investigator and VISTAS in responding to any issues raised in assessment reports

3.1.2 ENVIRON, Alpine and UCR Co-Principal Investigators

The three Co-Principal Investigators of Ralph Morris, T.W. Tesche and Gail Tonnesen perform the following functions:

- Directs and coordinates the day-to-day project activities of the project team and computer facilities to conduct the test program

- Ensures that this QAPP and Modeling Protocol are followed during the course of the project
- Manages the activities in each of the three modeling centers
- Direct supervises personnel working on this project
- Guides the approach for performing modeling evaluations following the direction of the Project Manager
- Keeps current on project status and delivers information to Project Manager for 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 data and sections for integration into modeling and assessment reports
- With the Project Manager, 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 each modeling center responding to any issues raised in assessment reports and initiates corrective actions as necessary with the Project Manager
- 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
- Develops individual test protocols and reports as directed
- Analyzes modeling data and provides assessment reports

3.1.3 VISTAS Contracting Officer

The VISTAS Contracting Officer (Patricia Brewer) serves as the primary contact between the Emissions and Air Quality Modeling Team and VISTAS and performs the following functions:

- Provides day-to-day oversight of VISTAS Phase II Emissions and Air Quality Modeling Team activities
- Works with the Project Manager, Co-Principal Investigators, TAWG, States, Tribes oversight groups, collaborators, Stakeholders, etc. in assuring that the interests and concerns of all of the VISTAS 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 VISTAS Technical Contact

The VISTAS Technical Contact (James Boylan) for the Emissions and Air Quality Modeling Team works with the VISTAS Contacting Officer in the day-to-day oversight and management of the modeling analysis:

- Provides day-to-day oversight of VISTAS Phase II Emissions and Air Quality Modeling Team activities
- Works with the VISTAS Contracting Officer, 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 VISTAS groups on the activities of the Modeling team.

3.1.5 VISTAS Technical Analysis Workgroup (TAWG)

The Technical Analysis Workgroup is responsible for overseeing the regional haze and fine particulate modeling that will be required for the State Implementation Plans (SIP's). This workgroup provides both emissions inventory and modeling technical support to VISTAS. Emissions Inventory efforts include the development of emissions inventories and forecasts to be utilized in VISTAS modeling efforts. Modeling efforts will include identification, evaluation, and application of air quality modeling tools (including meteorological and air quality models) to quantify the effects of emission management options upon air quality in Class I areas in the VISTAS region. Specific activities of the TAWG include:

- Oversees the activities of the VISTAS Emissions and Air Quality Modeling Team through the Contracting Officer, conference calls, and periodic in-person meetings and workshops
- Provides the Contracting Officer, technical Contact, 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 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 VISTAS Phase I and II Tasks are presented at the end of each Task Description in Sections 2.4 and 2.5.

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 all documents presented in Section 8.0, 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 VISTAS Emissions and Air Quality Modeling Team members, other VISTAS Contractors and VISTAS 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 VISTAS Modeling Team maintains four listservs to distribute information to different VISTAS groups as indicated in Table 3-2.

Table 3-2. VISTAS listservs maintained by the Emissions and Air Quality Modeling Team.

Listserv	Purpose
Vistas-all@cert.ucr.edu	Contacts all participants including Modeling Team, VISTAS TAWG and Stakeholders
Vistas-modeling@cert.ucr.edu	Contacts Modeling team and VISTAS TAWG Modeling Contacts
Vistas-emissions@cert.ucr.edu	Contacts emissions staff in the Modeling team and emissions people in the VISTAS TAWG
Vistas-met@cert.ucr.edu	Contacts meteorology staff in the Modeling team and meteorology people in the VISTAS TAWG

The Modeling Team members and VISTAS TAWG hold periodic conference calls and meetings to report results, discuss project status, and modify work plans as necessary. Unscheduled meetings or conference calls are also held concerning specific issues as the needs arise. In addition, periodic project meetings and conference calls are held. In these meetings detailed technical information is exchanged, project status is discussed, and project direction is assessed.

Written progress reports on the VISTAS Emissions and Air Quality Modeling Team activities are submitted to the VISTAS Contracting Officer on a monthly basis. These reports summarize project progress, results to date, problems encountered and necessary action items, and plans for the upcoming reporting period.

All modeling results, quality assurance reports, and related documents are posted on the project web site, as described in Section 3.5.

3.5 Documentation and Records

After the project tasks in Sections 2.4 and 2.5 that require deliverables are completed, the ensuing documents are posted on the VISTAS Modeling Phase I and II project websites at:

http://pah.cert.ucr.edu/vistas/

http://pah.cert.ucr.edu/vistas/vistas2/

In addition, during the project, VISTAS is provided updates by e-mail or telephone.

Document control is the system that ensures that only the latest revisions of the defined documents are used by the Modeling Team personnel engaging in project activities. 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, 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, meteorology and air quality modeling is performed on computer equipment located at either the ENVIRON, Alpine 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 a Linux Cluster 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. All staff also have their own state-of-the-art PCs and have 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 Alpine Geophysics Modeling Center Hardware

Alpine Geophysics' computing facilities consist of SUN Microsystems SPARCstation computers and a very powerful array 10 multiprocessor Linux-based workstations. The aggregate network has over 7.3 Gbytes of memory and 2500 Gbytes of aggregate disk space with over 2000 Gbytes of SCSI and IDE Raid-5 protected space. All client data is stored on at least one RAID-5 protected disk array. To further protect client data, two of our main servers backup their disk drives on a weekly basis to a second server that is physically disconnected from the power supply when not doing an active transfer. This way a catastrophic power failure will not compromise the ability for Alpine Geophysics to deliver.

To efficiently share network resources, 100-BaseT fast ethernet switches interconnect the computers within each office. Additionally, the Arvada based computers have both the Parallel Virtual Machine (PVM) software package for computation on multiple nodes on the network and Open MP capabilities for shared memory multiprocessing within each computer. For the majority of model simulations, using a job level parallelization, where individual periods of a simulation are put onto each computational node, maximizes network throughput. However, the computational network also has the ability to share the multi-Gbyte memory and 20 processors on a single MM5 model simulation.

A key feature of the AG computer network is the ability for AG to add computational resources quickly and cost effectively. Alpine scientists have been using Linux and Unix for meteorological and air quality modeling for over 16 years. This knowledge base, along with existing relationships with hardware vendors, software vendors, and system specialists, enable AG to meet the computational requirements of the VISTAS modeling study.

4.1.3 UCR Modeling Center Hardware

The UCR computer laboratory is designed to process large data sets for air quality modeling. It includes 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.

4.1.4 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 (over 23 TB) 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 back up of critical project data. Back-ups 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 VISTAS modeling is 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 VISTAS Emissions and Air Quality Modeling are provided by other VISTAS contractors with the data subjected to quality assurance and quality control (QA/QC) prior to delivery to the Modeling team. In addition the Modeling Team have formed data "Gatekeeper" functions to further QA/QC provided to the Modeling Team prior to its use. Below we discuss the data used in the modeling and the function of the Gatekeeper roles, which are described in detail in Section 2.2.2.1:

Air Quality Gatekeeper: The Air Quality Gatekeeper downloads air quality data from the VIEWS, SEARCH and AIRS websites and subjects it to QA/QC. The data are reformatted and processed for use in the modeling.

Meteorological Gatekeeper: The Meteorological Gatekeeper evaluates the MM5 data provided by the VISTAS Meteorological Modeling Contractor (BAMS), subjects it to QA/QC and processes it for input to the CMAQ/CAMx air quality models.

Emissions Gatekeeper: The Emissions Gatekeeper receives emissions data from the VISTAS Emissions Contractor (MACTEC), subjects them to a comprehensive QA/QC and rejects 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 maintains the project website, keeps back ups of data, responds to data requests and updates reports and files on the website.

5.0 EMISSIONS MODELING

The project objective is to integrate mezoscale 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 and Section 6.0 addresses meteorological modeling as they are applied to this project.

The VISTAS Modeling Team uses the Sparse Matrix Operator Kernel Emissions (SMOKE) emissions model to model 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 Phase II Modeling Protocol (ENVIRON, 2004a) and is summarized in this section.

The purpose of SMOKE is to convert the resolution of the 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 shows an example of how the matrix approach organizes 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 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 it’s 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.

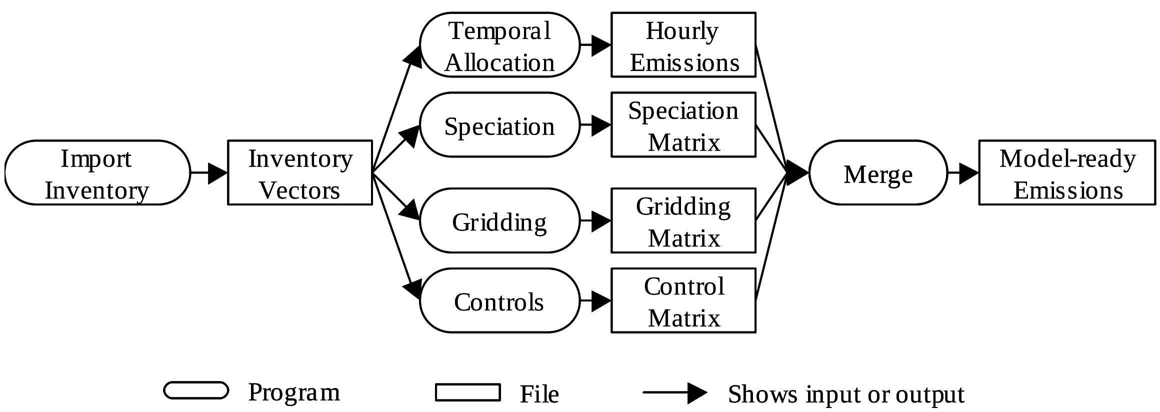

Figure 5-1. Flow Diagram of Major SMOKE Processing Steps.

5.1 Quality Assurance Components of Emissions Modeling

The quality assurance (QA) 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 VISTAS 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 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 will include 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 VISTAS 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 2.2.2.5 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 will ensure 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 meteorology 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 gate keeping 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 VISTAS work, the Project Manager is the liaison between the emissions modeling team and the VISTAS TAWG and in this role communicates any issues raised during the emissions QA process.

Figure 5-2 presents the QA framework developed by the VISTAS Modeling Team for SMOKE modeling. Identifying the specific participants in the VISTAS 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.

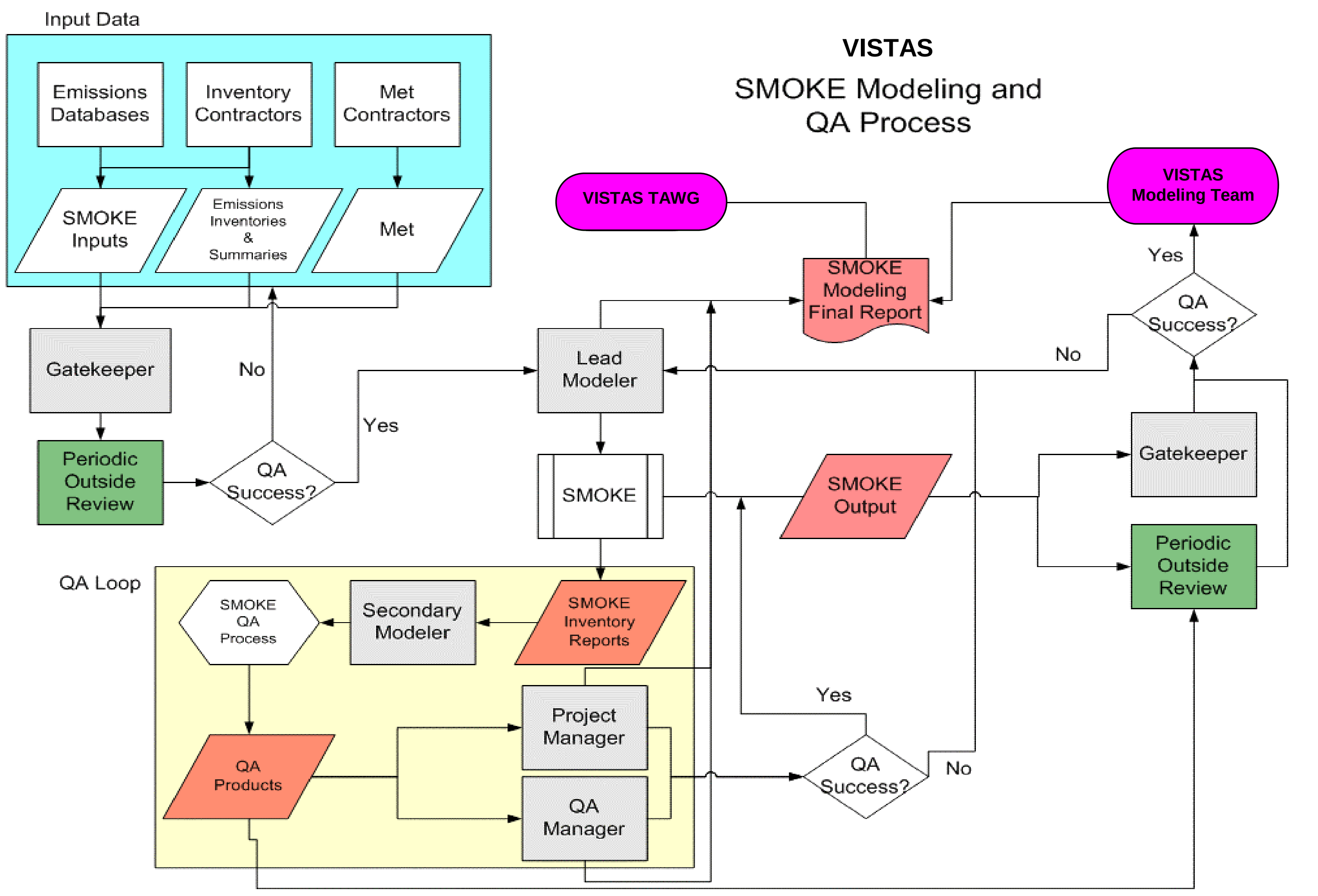

Figure 5-2. Diagram of VISTAS Modeling Team Approach to SMOKE Modeling.

6.0 METEOROLOGICAL MODELING

The EPA Models-3/CMAQ system is the primary regional ozone and particulate matter (PM) air quality model being used in VISTAS modeling. Meteorological inputs for CMAQ are being generated by the VISTAS Meteorological Modeling Contractor using the MM5 meteorological model. The model will be applied for the entire year of 2002 on two grids: a continental scale domain with 36 km grid spacing and a regional-scale domain with 12 km grid spacing covering the eastern United States. The CMAQ model requires inputs of three-dimensional gridded wind, temperature, humidity, cloud/precipitation, and boundary layer parameters. The current version of CMAQ can only utilize output fields from the Fifth Generation Mesoscale Model (MM5), developed and maintained by the Pennsylvania State University and National Center for Atmospheric Research (PSU/NCAR). MM5 is being used to develop hourly meteorological fields on the 36 km and 12 km grids.

A detailed protocol for utilizing MM5 as part of VISTAS has been prepared. The procedures used for applying MM5 for VISTAS are based on an extensive evaluation of MM5 and a series of sensitivity tests. The MM5 protocol contains a detailed description of MM5, the VISTAS modeling domain, the MM5 physical configuration, and a model application approach. The protocol also presents a plan for evaluating the performance of the model in replicating the evolution of observed winds, temperature, humidity, and boundary layer morphology to the extent that resources and data availability allow; this will serve as the primary approach to assess the reliability of the meteorological fields to adequately characterize the state of the atmosphere for input to CMAQ. Details on the VISTAS MM5 modeling can be found on the VISTS Meteorological Modeling website:

http://www.baronams.com/projects/VISTAS/

MM5 is an atmosphere model that 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.

7.0 CMAQ MODELING SYSTEM

EPA’s Models-3 CMAQ modeling system is the primary air quality modeling system used in the VISTAS Emissions and Air Quality Modeling activities.

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 October 2004 and is the version that will be used in the VISTAS Phase II Revised 2002 Base Case modeling (Although the Phase I modeling runs used CMAQ version 4.3).

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

A description of the newest features implemented in CMAQ ver 4.4 (released October 2004) is available on the CMAS 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. For the VISTAS Phase I modeling and the Phase II Initial 2002 CMAQ run version 4.3 (released August 2003) was used, whereas for the Phase II Task 7 CB4/SAPRC sensitivity tests and Phase II Revised 2002 CMAQ runs Version 4.4beta (released March 2004) and 4.4, respectively, were used.

7.2 CMAQ Configuration for Phase II Modeling

One of the principal accomplishments in the Phase I modeling was the identification and justification of the CMAQ science options recommended for Phase II modeling. We summarized the Phase I findings briefly in the introduction. In this section we briefly identify the main science options we recommend for annual PM modeling with CMAQ, more details ate provided in the Modeling Protocols (ENVIRON, 2003a; 2004a). The model would be set up and exercised on the same nested 36/12 km grid domain used in Phase I, employing one-way grid nesting. That is, boundary conditions for the 12 km grid simulation are extracted from the 36 km run using the CMAQ BCON processor. A total of 19 vertical layers would be implemented, extending up to a region top of 100 mb (approximately 15 km AGL).

The PPM advection solver would be used along with the spatially varying (Smagorinsky) horizontal diffusion approach and K-theory for vertical diffusion. MM5 meteorological output based on the Pleim-Xiu Land-Surface Model (LSM) and the ACM planetary boundary layer (PBL) scheme will be used and the latest CMAQ Meteorological-Chemistry Interface Processor (MCIP2.2 for Phase I and MCIP2.3 for Phase II) would 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 initial CMAQ 2002 modeling. Treatment of reversible secondary organic aerosols would be simulated by the SORGAM implementation in CMAQ (ver 4.3). Under the Phase I modeling, VISTAS evaluated three photochemical mechanisms: CB4, CB4-2002 and SAPRC99. CB4-2002 produced nearly identical results as CB4 but took much longer to run since it is only implemented in the slower SMVGEAR chemistry solver, compared to CB4 that is also implemented in the faster EBI chemistry solver. Thus, CB4-2002 was dropped from consideration in Phase II. The Phase I comparisons of CB4 and SAPRC99 found they produced mostly similar but different model performance. However, one mechanism was not performing better than the other across all species, sites and periods. The Phase I testing only evaluated the mechanism’s base case performance, not their response to emission reductions. Given that CB4 runs twice as fast as SAPRC99, for Phase II it was decided to perform initial 2002 CMAQ modeling using CB4 and evaluate CB4 and SAPRC99 responses to emission reductions using the Phase I episodes.

7.3 Alternative Models

EPA’s guidance on model selection for PM2.5 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 PM2.5 SIPS or RH reasonable progress requirements should meet the requirements for alternative models. The CMAQ, CMAQ-AIM and CAMx modeling systems all meet these requirements.

We believe that there is potentially significant value in including an alternative regional modeling system or multiple systems as an adjunct to the SMOKE/MM5/CMAQ system proposed as the mainstay of the Phase II analyses. Our testing of the CAMx model in Phase I and other recent PM2.5/regional haze applications demonstrates that the model is capable of producing results of comparable accuracy and reliability as CMAQ, given similar effort in preparing model inputs, diagnosing and improving model performance and in conducting weight-of-evidence investigations. The Phase I testing of CMAQ-AIM model raised questions on whether it was performing correctly; the differences with CMAQ could not be explained based on their differences in formulation with CMAQ-AIM performing poorer than CMAQ. Accordingly, at this time we cannot recommend adopting CMAQ-AIM in Phase II and recommend VISTAS consider the parallel use of CAMx in the Phase II program for seven specific purposes:

- **Diagnosis:** To serve as an efficient diagnostic tool addressing model performance issues that may arise in the establishment of the CMAQ annual 2002 and episodic base cases. CAMx's suite of diagnostic probing tools plus it's flexi-nesting algorithms make it an attractive tool for assisting in the diagnosis of CMAQ performance should this unexpected situation arise.

- **Model Evaluation Corroboration:** To provide corroboration of the base case model performance evaluation exercises to be performed with CMAQ and help identify any compensatory errors in the MM5/SMOKE/CMAQ modeling system.

- **Emissions Control Response Corroboration:** To provide corroboration of the response of the CMAQ 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 model performance in the annual and episodic base case simulations, and in the estimate of PM2.5 and visibility reductions associated with future emissions change scenarios.

- **Alternative Science:** CAMx contains alternative science algorithms that may elucidate model performance issues with CMAQ or provide an alternative approach for simulating aerosols.

- **Consistency with Other RPOs:** The Midwest RPO (MWRPO) may end up using CAMx for their regional haze modeling. As sources in the MWRPO likely influence visibility at Class I areas in VISTAS and vice versa, having results from a common model would be useful for reconciling any differences.

- **Backup Contingency:** To provide a 'backstop' model to CMAQ in the event that unforeseen difficulties with the primary model make it necessary to switch to an alternative 'One-Atmosphere' model at some point during Phase II.

The benefits of employing a pair of complimentary state-of-science air quality models are thus quite significant and well worth considering. Especially considering that the same MM5 output (through MM5CAMx) and SMOKE output and CMAQ IC/BC files (through CMAQ-to-CAMx emissions and IC/BC converters) can be used to operate CAMx without performing any additional meteorological or emissions modeling. Accordingly, below we provide an overview of the CAMx regional photochemical/PM modeling system and the science options recommended for use in Phase II.

7.3.1 CAMx Overview

The Comprehensive Model with Extensions (CAMx) modeling system is a publicly available (www.camx.com) three-dimensional multi-scale photochemical/aerosol grid modeling system that is developed and maintained by ENVIRON International Corporation. CAMx was developed with all new code during the late 1990s using modern and modular coding practices. This has made the model an ideal platform for the extension to treat a variety of air quality issues including ozone, particulate matter (PM), visibility, acid deposition, and air toxics. The flexible CAMx framework has also made it a convenient and robust host model for the implementation of a variety of mass balance and sensitivity analysis techniques including Process Analysis (IRR and IPR), Decoupled Direct Method (DDM), and the Ozone Source Apportionment Technology (OSAT). Designed originally to address multiscale ozone issues from the urban- to regional-scale, CAMx has been widely used in recent years by a variety regulatory agencies for 1-hr and 8-hr ozone 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 NOx point source plumes.
- Ability to interface with a variety of meteorological models including the MM5 and RAMS prognostic hydrostatic meteorological models and the CALMET diagnostic meteorological model (others also compatible).

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

- The 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 4.3+) code was released in the autumn of 2003 as a truly "One-Atmosphere' models that rigorously integrates the gas-phase ozone chemistry with the simulation of primary and secondary fine and course particulate aerosols. This extension of CAMx to treat PM involved the addition of several science modules to represent important physical processes for aerosols. Noteworthy among these are:

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

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

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

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

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

CAMx (ver 4.3+) 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 episode) may be addressed using the version that treats N-size sections (N is typically 10) and the rigorous, but computationally-extensive CMU multi-section aqueous-phase chemistry module.

7.3.2 CAMx Configuration for Phase II Modeling

We recommend exercising CAMx (ver 4.10s) as a companion model to CMAQ using as many similar science options and input data sets as possible. 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. At this time VISTAS has not budgeted any resources in Phase II for CAMx modeling, however it remains an option if desired at a later date.

The latest version of CAMx (ver 4.10s) will be employed and the model will be set up and exercised on the same 36/12 km grid as CMAQ. However, CAMx would be run using two-way grid nesting. The base configuration of CAMx would use 19 vertical layers that exactly match those used by CMAQ. The PPM advection solver would be used along with the spatially varying (Smagorinsky) horizontal diffusion approach. Vertical diffusion in CAMx would be modeled by K-theory. The MM5 simulation using the Pleim-Xiu Land-Surface Model (LSM) and the ACM Planetary Boundary Layer (PBL) scheme would be used in the CAMx base configuration using the MM5CAMx processor that is similar to the CMAQ MCIP2.2 “pass through” option of the MM5 data invoked. CAMx would be exercised with the CB4 gas-phase, RADM aqueous-phase, and CMU/ISORROPIA aerosol chemistry schemes. The SOAP secondary organic aerosol scheme would be used for the base configuration in CAMx.

Note that it may be desirable to exercise CAMx using its “full-science” configuration for selected periods to investigative scientific issues that may be of interest that can not 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 VISTAS domain, especially when looking at clean days or natural background; and

- The full sectional aqueous-phase chemistry module may be important for sulfate formation.

8.0 ASSESSMENTS AND OVERSIGHT

8.1 Assessment Responsibilities

The primary point of contact for VISTAS Modeling project assessment is that of the Project Manager (PM). This PM is available to the VISTAS Contracting Officer, Technical Contact, TAWG, external reviewers, and internal staff by direct contact through e-mail and phone and is linked to each of the four VISTAS listservs (see Table 3-2). 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, legally defensible. 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 quality control 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 VISTAS TAWG 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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