# Appendix A:
# Early Action Compact Modeling Analysis for the State of Tennessee

## Draft Technical Protocol (30 May 2003)

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# 1. Introduction and Study Design

This protocol document outlines the methods and procedures to be followed in conducting an Early Action Compact (EAC) 8-hour ozone attainment modeling analysis for the States of Arkansas, Tennessee, and Mississippi. The EAC modeling exercise will leverage off the accomplishments of the Arkansas-Tennessee-Mississippi Ozone Study (ATMOS) modeling analysis, which was originally designed to provide technical information relevant to attainment of an 8-hour National Ambient Air Quality Standard (NAAQS) for ozone primarily in the Memphis, Nashville, and Knoxville areas. In addition, the ATMOS analysis was also to provide information for addressing the emerging 8-hour ozone issues in the Hamilton County (Chattanooga), Tennessee; Lee County (Tupelo), Mississippi; and Little Rock, Arkansas areas.

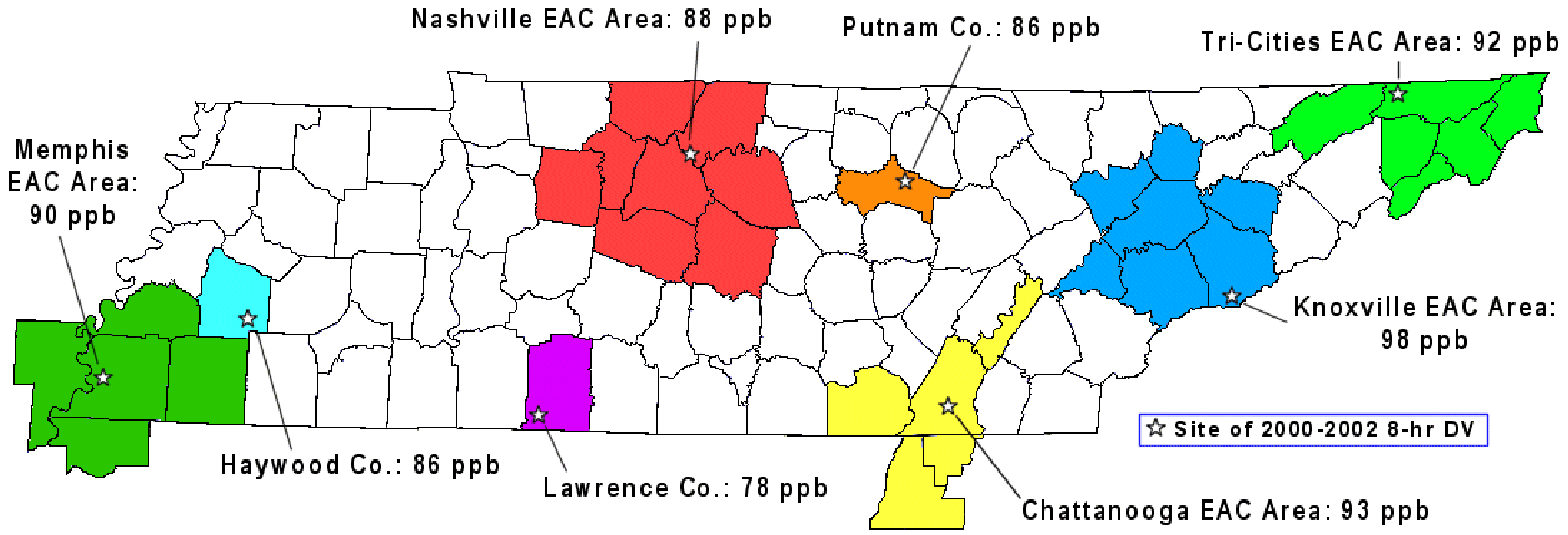
On December 31, 2002, the State of Tennessee entered into Early Action Compact agreements with EPA for eight areas within the state. The EAC areas include 30 counties within Tennessee, 2 adjacent counties in Georgia, and 1 adjacent county each in Arkansas and Mississippi, as well as 7 municipalities. Representatives from each of these jurisdictions signed the EAC. The EAC areas include the following:

- **Nashville EAC Area**: Davidson, Rutherford, Sumner, Williamson, Wilson, Cheatham, Dickson, and Robertson counties.
- **Knoxville EAC Area**: Anderson, Blount, Knox, Loudon, Sevier, Union, and Jefferson counties
- **Chattanooga EAC Area**: Hamilton, Marion and Meigs, counties (Tennessee), and Walker and Catoosa counties, (Georgia)
- **Memphis EAC Area**: Shelby, Tipton, and Fayette counties (Tennessee); Crittenden County, (Arkansas); De Soto County, (Mississippi).
- **Tri-Cities EAC Area**: Carter, Hawkins, Johnson, Sullivan, Unicoi, and Washington counties.
- **Haywood County**
- **Lawrence County (Florence, AL MSA)**
- **Putnam County**

A map of the EAC areas, including the 2000-2002 design values for each area, is provided in Figure 1-1.

The existing committee structure and framework established for the ATMOS modeling analysis will be utilized to conduct the EAC modeling, and this protocol will serve as the overall protocol for the modeling to be conducted for each of the EAC areas. Information regarding the organizational structure of ATMOS/EAC, study participants, communication structures, and the resolution of technical difficulties is presented in this section. The goals, objectives, and technical components of the EAC modeling/analysis study are briefly described. Issues related to the study protocol are discussed and a schedule for the study is provided.

**Figure 1-1. Tennessee EAC areas with 2000-2002 8-hour design values.**



## Committee Composition and Responsibilities

Three committees direct the ATMOS/EAC work. The Policy Committee is composed of upper management persons from the state and municipal organizations funding the project. The Operations Committee is composed of persons from the Technical Committee representing the principal states and organizations funding the project. The Technical Committee is composed of persons with technical expertise from the participating entities. In addition, persons representing themselves or organizations not participating in the funding of this study may be members of the Technical Committee. A Memorandum of Understanding (MOU) has been executed among the principal funding entities to effect a common agreement of the scope of work to be completed in ATMOS.

The Policy Committee secures funding for the project, enlists new members from entities wanting to participate in the funding, and makes final judgments on matters that cannot be resolved within the technical committee. The policy committee is made up of representatives from the states of Arkansas, Tennessee, and Mississippi as well as representatives from the Chattanooga, Knoxville, Memphis, and Nashville air programs.

The Operations Committee directs the work of the contractor. The Operations Committee is a subset of the Technical Committee and is composed of a member from each of the policy committee states and organizations drawn from the Technical Committee (including the Chairs) and the project manager (from SESARM) who will collectively approve the work products from the consultant for payment and make final decisions on the work products discussed among the full Technical Committee.

The Technical Committee is a broad-based committee of stakeholders with technical expertise that meets regularly to discuss and takes action on specific tasks to be completed by the contractor. These tasks include, but are not limited to, procedures used to select episodes for modeling, development of appropriate emissions inventories, development of meteorological fields associated with the selected episodes, sensitivity runs of the photochemical grid model, control strategy runs for the photochemical grid model, and presentation of results.

## Study Participants and Their Roles

The principal participants in the study are those states and organizations that are funding the study. These include the states of Arkansas, Tennessee, and Mississippi and the cities of Memphis, Nashville, Knoxville, and Chattanooga. In addition, the U.S. Environmental Protection Agency (Regions IV and VI), and other stakeholders (e.g., TVA, Entergy, etc.) also participate.

The role of all the principal participants is somewhat greater than that of the other participants. The principal participants are funding the study and play a more direct role in the day-to-day operations and contact with the contractor. Final decisions on tasks and project management are made by the principal participants through the Operations Committee. The involvement of others is through their active participation on the Technical Committee.

Systems Applications International, Incorporated (SAI), will conduct the ATMOS EAC modeling and analysis tasks under a contract with the Southeast States Air Resource Managers, Inc. (SESARM), which is under the direction of Mr. John Hornback. Jay Haney and Sharon Douglas will serve as co-project managers for SAI.

## Communications Structures

Communication among the participants occurs during scheduled face-to-face meetings of the Technical Committee, teleconferences of the Operations Committee, and continuous (as necessary) e-mail and telephone. A Web site set up by the consultant contains information and results generated in the study (see http://atmos.saintl.com).

Communication between the contractor and the participants will be through the contractor’s participation in the face-to-face and teleconference meetings, and by an e-mail distribution list. Outside of these meetings, communication between the contractor and the participants will be from the members of the Operations Committee.

SAI will report directly to SESARM and the ATMOS Operations Committee.

## Resolution of Technical Difficulties

Technical difficulties encountered by SAI will be brought to the attention of the Operations Committee, either verbally or through written correspondence. SAI will also offer suggestions or recommendations on how to resolve such difficulties. All major issues or difficulties (whether or not they are fully or satisfactorily resolved during the course of the study) will be documented, in either a technical memorandum or the modeling/analysis report.

## Goals and Objectives of the Study

The ATMOS/EAC modeling/analysis is designed to provide technical information related to 8-hour ozone issues in the EAC areas located primarily in the State of Tennessee. The EAC modeling provides an opportunity for these areas to conduct photochemical modeling to support decisions regarding control measures that could be adopted earlier than would be required by EPA, once the areas are formally designated nonattainment in 2004 under the new 8-hour National Ambient Air Quality Standard (NAAQS) for ozone. Based on data for 1997-2002, the calculated design values for the areas listed above are given in Table 1-1.

**Table 1-1. 1997-2002 Maximum 8-Hour Ozone "Design Values" for the ATMOS EAC Areas of Interest.**

| | Maximum 8-hour Ozone Design Values (ppb) | | | |
|---|---|---|---|---|
| | 1997–1999 | 1998–2000 | 1999–2001 | 2000–2002 |
| Nashville EAC Area | 102 | 100 | 93 | 88 |
| Knoxville EAC Area | 104 | 104 | 98[1] | 98 |
| Chattanooga EAC Area | 94 | 97 | 92 | 93 |
| Memphis EAC Area | 95 | 97 | 93 | 94 |
| Tri-Cities EAC Area | 91 | 94 | 90 | 92 |
| Haywood County | 98 | 93[2] | 89 | 86 |
| Lawrence County | 88 | 89 | 83 | 78 |
| Putnam County | 88 | 91 | 87 | 86 |

The primary objective of this study is to provide the modeling/analysis results needed to support an attainment demonstration for each of these areas. As such, the study has been designed in accordance with draft EPA guidance (EPA, 1999) for using modeling and other analyses for 8-hour ozone attainment demonstration purposes. Note the while the guidance is currently in draft form, the final version is not expected to be substantively different from the draft (EPA, personal communication).

The results of this study will be presented in a single report, with separate sections for the presentation of results for each area of interest. The analytical results will also be presented in electronic/database format such that each of the areas can be examined separately. In this manner, the study results will be easily referenced or directly incorporated into State Implementation Plan (SIP) documentation prepared by the state or local agencies.

## Modeling/Analysis Study Components

The ATMOS EAC modeling analysis components include a comprehensive episode selection analysis (identifying suitable periods for modeling), application and evaluation of a photochemical modeling system for two simulation periods, projection of emissions and ozone concentrations for two future years, and evaluation of ozone attainment strategies. All technical tasks will be conducted in accordance with draft EPA guidance regarding the use of modeling and other analyses for 8-hour ozone attainment demonstration (EPA, 1999). The documentation prepared as part of this study will be appropriate for inclusion as part of a SIP technical support document for each of the areas of interest.

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[1] Look Rock (470090101-2) operated for 1999 only. Based on one year of data, design value would be 104 ppb.

[2] Site 4707500021 closed in 1999. Based on one year of data, the design value would be 98 ppb.

## Protocol Objectives, Contents, and Amendment Procedures

This protocol document should be viewed as a set of general guidelines and is intended to provide focus, consistency, and a basis for consensus for all parties involved in the study.

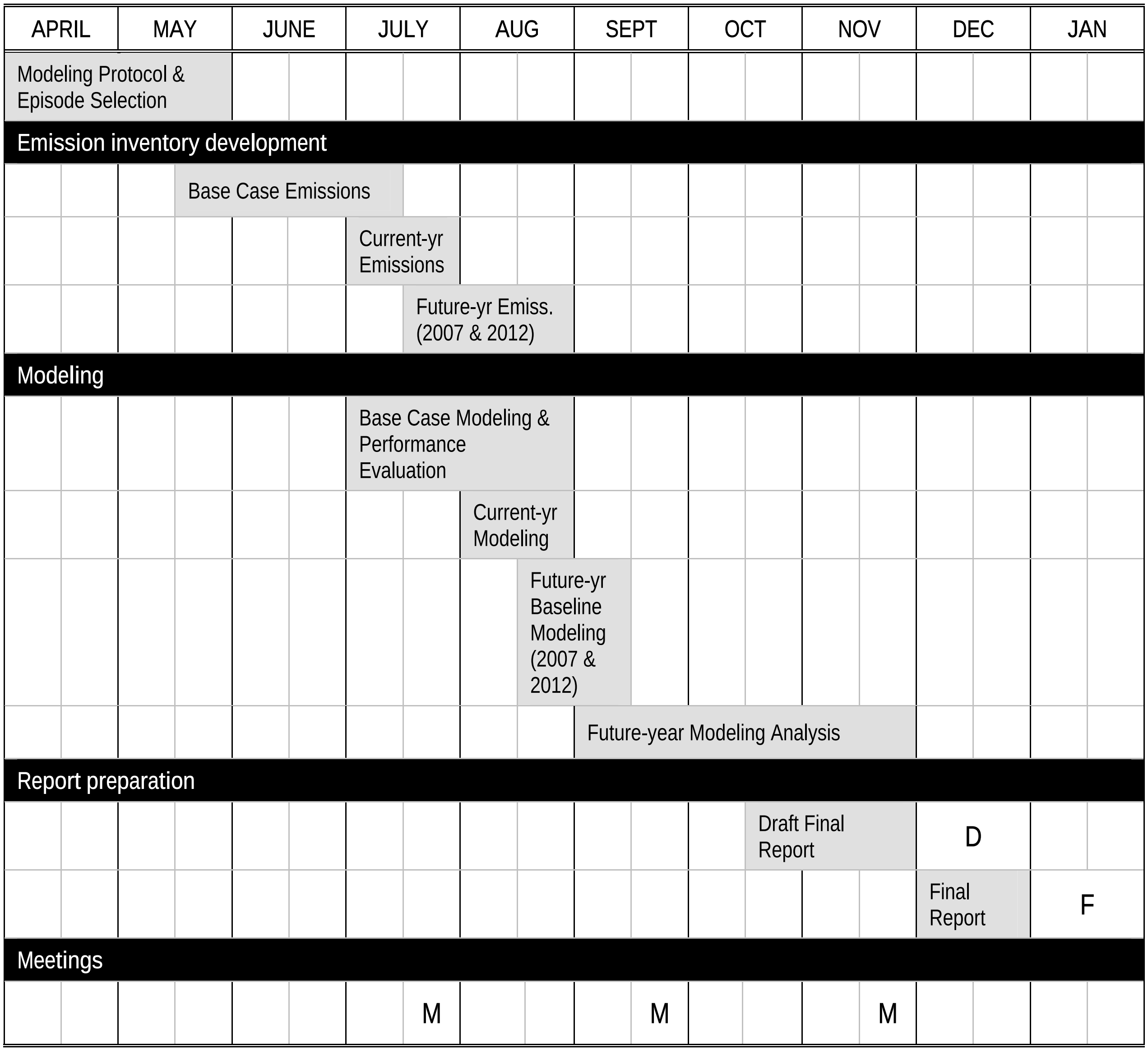
The primary purpose of the protocol document is to outline the methodologies to be followed throughout the study. At this time some of the methodologies to be used in the modeling/analysis study have not been finalized. It will be necessary for the study participants to make decisions regarding these issues as the study progresses. Amendment of the protocol document will occur only upon the direction of the ATMOS Operations Committee. Each time the protocol document is amended, a revised version of the entire document will be made available in electronic format on the ATMOS web site.

The remainder of this document provides detailed information on each element of the modeling/analysis. Selection of the primary modeling tools is summarized in Section 2 and a brief overview of each is provided. The methods and results of the episode selection analysis are provided in Section 3. The modeling domain is presented in Section 4. Model input preparation procedures are described in Section 5. Model performance evaluation is discussed in Section 6. The use of diagnostic and sensitivity analysis is outlined in Section 7. Future-year modeling is discussed in Section 8. A description of the attainment demonstration procedures is given in Section 9. Documentation procedures are detailed in Section 10. The deliverables and schedule for the project are summarized in Section 11. Archival and data acquisition procedures are outlined in Section 12.

## Schedule

A schedule for the ATMOS/EAC modeling analysis is provided in Figure 1-2.

**Figure 1-2. Proposed timeline for completion of the ATMOS/EAC photochemical modeling analysis.**



| APRIL | MAY | JUNE | JULY | AUG | SEPT | OCT | NOV | DEC | JAN |
|---|---|---|---|---|---|---|---|---|---|
| Modeling Protocol & Episode Selection | | | | | | | | | |
| **Emission inventory development** | | | | | | | | | |
| | Base Case Emissions | | | | | | | | |
| | | | Current-yr Emissions | | | | | | |
| | | | Future-yr Emiss. (2007 & 2012) | | | | | | |
| **Modeling** | | | | | | | | | |
| | | | Base Case Modeling & Performance Evaluation | | | | | | |
| | | | | Current-yr Modeling | | | | | |
| | | | | Future-yr Baseline Modeling (2007 & 2012) | | | | | |
| | | | | | Future-year Modeling Analysis | | | | |
| **Report preparation** | | | | | | | | | |
| | | | | | | Draft Final Report | | D | |
| | | | | | | | | Final Report | F |
| **Meetings** | | | | | | | | | |
| | | | M | | M | | M | | |

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# 2. Model Selection

The selection of modeling tools for this study considered (1) technical formulation, capabilities, and features, (2) comprehensiveness of testing, and (3) demonstrated successful use in previous applications (similar in scope to the ATMOS analysis). The primary modeling tools selected for use in this study include: the variable-grid Urban Airshed Model (UAM-V), a regional- and urban-scale, nested-grid photochemical model; the Emissions Preprocessing System (EPS2.5), for preparation of model ready emission inventories; the Biogenic Emission Inventory System (BEIS), for estimating biogenic emissions; the MOBILE model, for estimating motor-vehicle emissions; and the Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Model, Version 5 (MM5), for preparation of the meteorological inputs. The rationale for selecting each of these modeling tools (in keeping with EPA guidance) is discussed in this section; an overview of each modeling tool is also provided.

## Selection and Overview of the Photochemical Model

The UAM-V modeling system (Version 1.5) was selected for use in this study. The UAM-V is a state-of-the-science photochemical modeling system that incorporates the latest version of the Carbon-Bond chemical mechanism (Carbon Bond 5 (CB-V)), incorporating the most current updates to the mechanism (SAI, 2002). It is designed for the regional- and urban-scale simulation of the physical and chemical processes that determine the spatial and temporal distribution of ozone and precursor pollutants within the atmospheric boundary layer. It is typically applied for multi-day simulation (or episode) periods. Key features of the UAM-V modeling system that are relevant to its use in this study include multiple nested-grid capabilities, ability to explicitly incorporate output from a dynamic meteorological model, a detailed plume-in-grid (P-i-G) treatment for emissions from elevated point sources, and the accommodation of process-level analysis of the simulation results. The UAM-V modeling system is currently the most widely used and comprehensively tested photochemical modeling system in the world and its utility for both regional- and urban-scale analysis has been successfully demonstrated in dozens of applications (e.g., regional-scale modeling of the eastern U.S. as part of the Ozone Transport Assessment Group (OTAG) modeling study, SIP modeling of the Atlanta ozone nonattainment area by the Georgia Department of Natural Resources, and 8-hour regional modeling as part of the Gulf Coast Ozone Study (GCOS)).

EPA (1999) lists five factors to be considered in selecting a model for use in an 8-hour ozone attainment demonstration. These are listed (in bold) and discussed in the following text.

- **Nature of the air quality problem leading to nonattainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem**. Based on an analysis of the observed data (included as part of the episode selection analysis), the potential ozone nonattainment problem for the areas of interest appears to have both regional and local components. The data also indicate that high ozone concentrations are not confined to the urban areas and that the higher concentrations are often downwind of the urban areas and/or at higher elevation sites. Thus, terrain and meteorological influences are likely important. The UAM-V modeling system is well suited for this application in that it is a regional- and urban-scale model (with nested-grid capabilities) and accommodates the use of detailed meteorological inputs from a dynamic meteorological model. The nested-grid feature will enable the use of a large domain so that any influence from surrounding areas can be directly simulated, yet will accommodate high resolution over the areas of interest.

The use of detailed meteorological inputs will enable representation of the important mesoscale meteorological features such as the regional- and local transport patterns, terrain-induced airflow patterns, and vertical mixing patterns. The process-analysis feature of the UAM-V modeling system will enable an assessment of model performance at the process level and thus a comparison of the simulation results relative to available conceptual models of ozone formation (e.g. from intensive measurement studies for Nashville).

- **Availability, documentation, and past performance should be satisfactory.** The UAM-V modeling system is available at no cost, is fully documented, and has been demonstrated to perform satisfactorily in more than ten recent applications. Several references are provided later in this section. More are available upon request.
- **Relevant experience of available staff and contractors should be consistent with choice of a model.** The modeling tasks will be performed by SAI staff who are knowledgeable and experienced in the application of the UAM-V modeling system.
- **Time and resource constraints may be considered.** Use of the UAM-V modeling system is consistent with the time and resource constraints of the ATMOS modeling study.
- **Consistency of the model with what was used in adjacent regional applications should be considered.** The UAM-V modeling system was used for the OTAG regional-scale modeling effort and is currently being used for regional- and urban-scale modeling of Baton Rouge, Lake Charles, Shreveport, the Gulf Coast area, and areas within the State of South Carolina. It is currently being used for EAC modeling of South Carolina and Shreveport, Louisiana. It has been used by the Texas Commission on Environmental Quality and the Tennessee Valley Authority for regional or subregional modeling of their respective areas. It was also used by the Minerals Management Service (MMS) for modeling of the effects of emissions from offshore oil and gas production on the Gulf Coast area (Haney et al., 1995), a study explicitly called for in the Clean Air Act Amendments of 1990.

## *Overview of the UAM-V Modeling System*

The variable-grid Urban Airshed Model (UAM-V) is a three-dimensional photochemical grid model that calculates concentrations of pollutants by simulating the physical and chemical processes in the atmosphere. The basis for the UAM-V is the atmospheric diffusion or species continuity equation. This equation represents a mass balance that includes all of the relevant emissions, transport, diffusion, chemical reactions, and removal processes in mathematical terms.

The major factors that affect photochemical air quality include:

- the pattern of emissions of $NO_x$ and volatile organic compounds (VOC), both natural and anthropogenic
- composition of the emitted VOC and $NO_x$
- spatial and temporal variations in the wind fields
- dynamics of the boundary layer, including stability and the level of mixing
- chemical reactions involving VOC, $NO_x$, and other important species
- diurnal variations of solar insolation and temperature

- loss of ozone and ozone precursors by dry and wet deposition
- ambient background of VOC, $NO_x$, and other species in, immediately upwind of, and above the study region.

The UAM-V simulates all of these processes. The species continuity equation is solved using the following fractional steps: emissions are injected; horizontal advection/diffusion are solved; vertical advection/diffusion and deposition are solved; and chemical transformations are performed for reactive pollutants. The UAM-V performs these four calculations during each time step. The maximum time step is a function of the grid size, maximum wind velocity, and diffusion coefficient. The typical time step is 10–15 minutes for coarse (10–20 km) grids and a few minutes for fine (1–2 km) grids.

Because it accounts for spatial and temporal variations as well as differences in the reactivity of emissions, the UAM-V is ideal for evaluating the air-quality effects of emission control scenarios. This is achieved by first replicating a historical ozone episode to establish a base-case simulation. Model inputs are prepared from observed meteorological, emissions, and air quality data for the episode days using prognostic meteorological modeling and/or diagnostic and interpolative modeling techniques. The model is then applied with these inputs, and the results are evaluated to determine model performance. Once the model results have been evaluated and determined to perform within prescribed levels, the same base-case meteorological inputs are combined with *modified* or *projected* emission inventories to simulate possible alternative/future emission scenarios.

The UAM-V modeling system incorporates the Carbon-Bond IV chemical mechanism with enhanced isoprene chemistry. It represents an extension of the UAM (also referred to as UAM-IV). Features of the UAM-V modeling system include:

1. *Variable vertical grid structure:* The structure of vertical layers can be arbitrarily defined. This allows for higher resolution near the surface and facilitates matching with output from prognostic meteorological models.
2. *Three-dimensional meteorological inputs:* The meteorological inputs for UAM-V vary spatially and temporally. These are usually calculated using a prognostic meteorological model.
3. *Variable grid resolution for chemical kinetic calculations:* A chemical aggregation scheme can be employed, allowing chemistry calculations to be performed on a variable grid while advection/diffusion and emissions injections are performed on a fixed grid.
4. *Two-way nested grid:* Finer grids can be imbedded in coarser grids for more detailed representation of advection/diffusion, chemistry, and emissions. Several levels of nesting can be accommodated.
5. *Updated chemical mechanism:* The original carbon bond chemical mechanism has been updated with the inclusion of Carbon Bond 5, (CB-V), which has included enhancements to some of the chemical reactions in the CB-IV version of the mechanism.
6. *Dry deposition algorithm:* The dry deposition algorithm is similar to that used by the Regional Acid Deposition Model (RADM).
7. *True mass balance:* Concentrations are advected and diffused in the model using units of mass per unit volume rather than parts per million. This maintains true mass balance in the advection and diffusion calculations.

8. *Plume-in-grid treatment:* Emissions from point sources can be treated by a subgrid-scale Lagrangian photochemical plume model. Pollutant mass is released from the subgrid-scale model to the grid model when the plume size is commensurate with grid cell size.
9. *Plume rise algorithm:* The plume rise algorithm is based on the plume rise treatment for a Gaussian dispersion model.
10. *Oxidant tagging capabilities:* Provides ozone contribution analysis information (Ozone Precursor Tagging Methodology (OPTM)) by precursor (NOx and VOC), source category, or geographic region, which is useful in designing and testing effective emission reduction strategies.

## *Acceptability Relative to the EPA "Alternative Model" Requirements*

In accordance with draft EPA guidance (EPA, 1999), use of the UAM-V modeling system for this study represents the use of an "alternative model" for 8-hour ozone attainment demonstration purposes. It is available to the public at no cost and is not proprietary. Use of the UAM-V modeling system further satisfies the third condition offered by EPA in the guidance document, which requires that the alternative model "is more appropriate than the preferred model for a given application or there is no preferred model." In this case, there is no "preferred" model (EPA, 1999). In the draft guidance document, EPA provides six criteria for a model to qualify as a candidate for use in an attainment demonstration. These are listed (in bold) and compliance with each is established in the following text.

- **The model has received a scientific peer review.** A formal scientific peer review of the UAM-V modeling system was conducted by ENSR (1993). Since that time, hundreds of scientists and modelers have reviewed the modeling system code as a routine part of their work with the modeling system.
- **The model can be demonstrated applicable to the problem on a theoretical basis.** As noted in the previous section, the UAM-V modeling system represents (either explicitly or implicitly) the physical and chemical processes that are currently known to influence the formation and transport of ozone as well as the emission, chemical transformation, and dispersion of ozone precursor pollutants. The features and capabilities of the modeling system are consistent with the application on both regional and urban scales, as required for this study.
- **Databases needed to perform the analysis are available and adequate.** The UAM-V modeling system requires several different types of input data files. These will be prepared using available data and EPA-recommended techniques. Their adequacy for use with the modeling system will be assessed as part of the modeling study.
- **Available past appropriate performance evaluations have shown the model is not biased toward underestimates.** Past applications of the UAM-V modeling system do not indicate a bias toward underestimation. Some examples of recent applications include OTAG, 1997; BAAQMD, 1998; and Douglas et al., 1998 as well as the GCOS modeling analysis (SAI, 2001). Each of these applications includes several days and day-to-day variations in model performance, but a consistent bias toward underestimation is not indicated.
- **A protocol on methods and procedures to be followed has been established.** The protocol is outlined in this document. The modeling will be conducted in a manner that is

consistent with established practice and EPA guidelines regarding air quality modeling related to the 8-hour ozone standard.

- **The developer of the model must be willing to make the model available to users for free or for a reasonable cost, and the model cannot be proprietary.** The version of the UAM-V to be used for this study is available from SAI (the developer of UAM-V) at no cost. The UAM-V is not a proprietary model and as such complies with each element of the definition put forth recently by the North American Research Study of Tropospheric Ozone (NARSTO).

## Selection and Overview of the Emissions Modeling and Processing Tools

The EPS2.5, BEIS, and MOBILE emissions processing/modeling tools were selected for use in this study. EPS2.5 is an extended version of EPS (EPA, 1992a) that has been enhanced to facilitate the preparation of regional-scale emission inventories. BEIS-2 is the latest available version of the EPA biogenic emission estimation model. Note that the UAM-V modeling system includes a representation of isoprene chemistry that is consistent with the use of BEIS-2. MOBILE6 is the current version of the EPA tool for calculation of on-road motor vehicle emissions.

EPA (1999) lists five factors to be considered in selecting a model for use in an 8-hour ozone attainment demonstration. These are listed (in bold) and discussed in the following text.

- **Nature of the air quality problem leading to nonattainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.** Use of EPS2.5 facilitates the preparation of a regional-scale emission inventory, as needed for this study. BEIS is currently the recommended tool for estimation of biogenic emissions, which are likely to play an important role in ozone formation within the Tennessee Valley area. The latest available version of BEIS will be used. As noted earlier, MOBILE is the model developed and recommended by EPA for calculating emissions from on-road mobile sources. Use of this tool facilitates the use of the county- and parish-specific estimates of vehicle miles traveled (VMT) and detailed temperature information available for this study. The latest available version of MOBILE will be used for this study.
- **Availability, documentation, and past performance should be satisfactory.** EPS2.5, BEIS, and MOBILE are available for free and are fully documented. These tools have been used successfully in more than five recent applications including OTAG (1997) and sub-regional modeling of the southeastern U.S. (Douglas et al., 1998). Additional references are available upon request.
- **Relevant experience of available staff and contractors should be consistent with choice of a model.** The modeling tasks will be performed by SAI staff who are knowledgeable and experienced in the application of EPS2.5, BEIS-2, and MOBILE6.
- **Time and resource constraints may be considered.** Use of EPS2.5, BEIS, and MOBILE is consistent with the time and resource constraints of the ATMOS/EAC modeling study.
- **Consistency of the model with what was used in adjacent regional applications should be considered.** EPS2.5, BEIS-2, and MOBILE6 are currently being used for

regional- and urban-scale modeling of the Baton Rouge, Gulf Coast, and South Carolina areas. EPS2.5 was also used by the Minerals Management Service (MMS) for modeling of the effects of emissions from offshore oil and gas production on the Gulf Coast area. BEIS-2 was used for the OTAG regional-scale modeling effort.

### *Overview of the EPS2.5*

EPS2.5 is a series of FORTRAN modules that perform the intensive data manipulations required to incorporate spatial, temporal, and chemical resolution into an emission inventory used for photochemical modeling. It enables the user to conform to EPA emission inventory requirements, and evaluate proposed control measures for meeting required emission reductions. EPS2.5 provides emission inputs to the UAM-V; specific features and capabilities related to the UAM-V application are described in Section 5 of this protocol document.

### *Overview of BEIS-2*

BEIS-2 is a computer algorithm used to generate biogenic emissions for air quality simulation models, such as UAM-V. Emission sources that are modeled include volatile organic compound (VOC) emissions from vegetation and nitric oxide (NO) emissions from soils. BEIS-2 includes an up-to-date, county-level biomass database and emission factors for a variety of plant species. It accommodates the use of solar-radiation information in calculating emission rates.

### *Overview of MOBILE6*

The EPA's highway vehicle emission factor model, MOBILE6, is a FORTRAN program that provides average in-use fleet emission factors for volatile organic compounds (VOC), oxides of nitrogen ($NO_X$) and carbon monoxide (CO) for eight categories of vehicles, for any calendar year between 1970 and 2020 and under various conditions affecting in-use emission levels (e.g., ambient temperatures, average traffic speeds, gasoline volatility) as specified by the model user. It has been used in evaluating control strategies for highway mobile sources, by States (except California) and other local and regional planning agencies in the development of emission inventories and control strategies for SIPs, for conformity issues related to Transportation Improvement Plans (TIPs), and in the development of environmental impact statements (EIS). This version of the model was released by EPA in Spring 2002.

## Selection and Overview of the Meteorological Model

The MM5 meteorological modeling system was selected for use in this study. MM5 is a state-of-the-science dynamic meteorological modeling system that has been used in several previous air quality modeling applications. Key features of the MM5 modeling system that are relevant to its use in this study include multiple nested-grid capabilities, incorporation of observed meteorological data using a four-dimensional data-assimilation technique, detailed treatment of the planetary boundary layer, and the ability to accurately simulate features with non-negligible vertical velocity components, such as the gulf breeze (a non-hydrostatic option). The MM5 modeling system is widely used and is currently supported by NCAR. Its use in conjunction with the UAM-V modeling system has been successfully demonstrated as part of a regional- and urban-scale modeling application for the southeastern U.S. (Douglas et al., 1998).

EPA (1999) lists five factors to be considered in selecting a model for use in an 8-hour ozone attainment demonstration. These are listed (in bold) and discussed in the following text.

- **Nature of the air quality problem leading to nonattainment of the ozone NAAQS should first be assessed, and the selected model should have the attributes and capabilities consistent with the perceived nature of the problem.** The MM5 modeling system should enable a physically realistic simulation of the meteorological features that characterize the study area and episode period, including terrain-induced airflows and summertime vertical mixing/inversion features. The nested-grid feature will support the preparation of inputs for a regional- and urban-scale application of UAM-V.
- **Availability, documentation, and past performance should be satisfactory.** The MM5 modeling system is free and documentation is available. It has been used in conjunction with UAM-V to support regional- and urban-scale modeling of the southeastern U.S. and has been used for several other air quality modeling studies (e.g., for California’s San Joaquin Valley and the eastern Gulf Coast area). Versions of the modeling system have been used for the past two decades to support research in the area of mesoscale meteorology.
- **Relevant experience of available staff and contractors should be consistent with choice of a model.** The modeling tasks will be performed by SAI staff who are knowledgeable and experienced in the application of the MM5 modeling system.
- **Time and resource constraints may be considered.** Use of the MM5 modeling system is consistent with the time and resource constraints of the ATMOS modeling study.
- **Consistency of the model with what was used in adjacent regional applications should be considered.** MM5 was recently used for regional- and urban-scale modeling of the southeastern U.S., with emphasis on Atlanta, Birmingham, and the eastern Gulf Coast.

## *Overview of MM5*

A general description of this three-dimensional, prognostic meteorological model is found in Anthes and Warner (1978). The governing equations include the equations of motion, the continuity equations for mass and water vapor, and the thermodynamic equation. Those features relevant to this application are briefly described in this section.

The current version of MM5 can be applied in a non-hydrostatic mode for the improved simulation of small-scale vertical motions (such as those associated with the sea breeze and terrain effects). Use of this optional feature can be important to the accurate simulation of the airflow and other features at high horizontal resolution and will be utilized for this study.

The MM5 model employs the sigma vertical coordinate: $\sigma = (p - p_t)/(p_s - p_t)$, where $p$ is pressure, $p_t$ is the constant pressure specified as the top of the modeling domain, and $p_s$ is the surface pressure. The sigma-coordinate surfaces follow the variable terrain. The governing equations are integrated over a grid that is staggered in the horizontal and vertical (Messinger and Arakawa, 1976). In the horizontal, the u and v wind components are calculated at points that are staggered with respect to those for all other variables. In the vertical, vertical velocity is defined at the sigma levels while all other variables are defined at intermediate sigma levels.

The MM5 modeling system also supports the use of multiple nested grids. This feature is designed to enable the simulation of any important synoptic scale features at coarser resolution, while incorporating a high-resolution grid over the primary area(s) of interest. In this manner, the computational requirements associated with use of a high-resolution grid over a large domain are avoided. A one-way nesting procedure in which information from the simulation of each outer grid is used to provide boundary conditions for the inner grids is generally recommended and will be used for this application.

To facilitate the realistic simulation of processes within the atmospheric boundary layer, variable surface parameters (including albedo, roughness length, and moisture availability) and a high-resolution planetary boundary layer (PBL) parameterization may be specified. The PBL parameterization also requires use of a multi-layer soil temperature model (an otherwise optional feature of MM5). For the coarse grids, several cumulus parameterization schemes are available to parameterize the effects of convection on the simulated environment. Several explicit moisture schemes are available for high-resolution grids.

The MM5 model supports four-dimensional data assimilation (FDDA), a procedure by which observed data are incorporated into the simulation. FDDA option include (1) “analysis nudging” in which the simulation variables are relaxed or “nudged” toward an objective analysis that incorporates the observed data and (2) “obs nudging” in which the variables are nudged toward individual observations.

The MM5 modeling system has been modified to include the output of the internally calculated vertical exchange coefficients ($K_v$) for use with UAM-V.

# 3. Episode Selection

Episode selection for the ATMOS modeling/analysis was based on a review of historical meteorological and air quality data, and application of an objective procedure for optimizing representation of typical ozone exceedance events across the areas of interest. The episode selection analysis was focused on Memphis, Nashville, and Knoxville. The applicability of the episodes selected for these areas for modeling of Chattanooga, Tupelo, and Little Rock was also examined. The original episode selection exercise conducted in 2000 examined data through 1999, and resulted in the selection of the original ATMOS episode (29 August—9 September 1999). As part of the EAC modeling, the episode selection analysis was re-done using data through the year 2002 to select an additional episode to complement the 1999 episode.

The primary objective of the episode selection analysis was to identify suitable periods for analysis and modeling related to the 8-hour ozone NAAQS for the Memphis, Nashville, and Knoxville areas. Important considerations include (1) representing the range of meteorological conditions that accompany ozone exceedances, (2) representing the ozone concentration levels that characterize the nonattainment problem (and result in the designation of nonattainment), and (3) accounting for the frequency of occurrence of the relevant meteorological/air quality events (to avoid using results from infrequent or extreme events to guide the decision making process).

The approach to episode selection is consistent with current (draft) EPA guidance (EPA, 1999) on episode selection for 8-hour ozone attainment demonstration modeling. In this guidance, EPA lists the following as the most important criteria for choosing episodes:

- Monitored ozone concentrations comparable to the severity as implied by the form of the NAAQS
- Representation of a variety of meteorological conditions observed to correspond to monitored ozone concentrations of the severity implied by the form of the NAAQS
- Data availability
- Selection of a sufficient number of days so that the modeled attainment test is based on several days

EPA also provides several additional (secondary) criteria for episode selection:

- Episodes used in previous modeling exercises
- Episodes drawn from the period on which the current design value is based
- Observed concentrations are “close” to the design value for as many sites as possible
- Episodes are appropriate for as many of the nonattainment areas as possible (when several areas are being modeled simultaneously)
- Episodes include weekend days

## Methodology

The methodology used for the episode selection analysis was based on that developed for a similar study by Deuel and Douglas (1998) and used for the several other modeling studies including GCOS (Douglas et al. 1999). A detailed description of the methods and results is presented by Douglas et al. (2000). For the original episode selection of Memphis, Nashville, and Knoxville, days within the period 1990 to 1999 were classified according to meteorological and air quality parameters using the Classification and Regression Tree (CART) analysis technique.

The frequency of occurrence of ozone exceedances for each classification type was then determined for each area of interest. Days with maximum ozone concentrations within approximately 10 ppb of the respective design value were also identified. Design values were calculated for each area on a site-specific basis. For each area, the “regional” design value was then specified to be the maximum value among all sites in the area. For 8-hour ozone, the design value is the average of the fourth highest daily maximum concentration for each of the three years of the calculation period.

Next, an optimization procedure was applied to the selection of multi-day episodes for maximum achievement of the specified episode selection criteria (as outlined above). A combined optimization was performed for the three primary areas of interest.

Finally, a more detailed analysis of the episode days with respect to the location and number of exceedance sites as well as local meteorological conditions was conducted. The suitability of the episodes for modeling of Chattanooga, Tupelo, and Little Rock was also examined. Among these three areas, meteorological representativeness was only examined for Chattanooga (using CART results from a previous study).

In selecting a new episode for the EAC modeling, data for the years 2000, 2001, and 2002 were added to the CART database and the algorithm was re-run.

## Results—Original ATMOS Episode

In accordance with EPA guidance, the primary objectives of the episode selection analysis were to identify days that (1) represent the types of meteorological conditions that are most frequently associated with ozone exceedances and (2) have ozone concentrations that are representative of the design value. The guidance quantifies the latter with a range of 10 ppb.

In addition, several other considerations were used to guide the selection of multiple episode periods for modeling.

- It is important that the candidate modeling episode days encompass the range of meteorological conditions that accompany ozone exceedances (i.e., that all key meteorological regimes, or as many as feasible, are included).
- EPA guidance suggests that a modeling attainment test should include several days. For this analysis, this is assumed to be the number of days with maximum 8-hour ozone within 10 ppb of the design value for each area.
- Since the response of the modeling system to emission reductions can vary according to concentration level, some consideration was given to ensuring that the values within 10 ppb of the design were distributed about the design value and that several exceedance days were included for each area.

The episode selection algorithm was applied to the identification of candidate 8-hour ozone modeling episodes for the three areas of interest. As noted earlier, the objective was to identify episodes that are characterized by typical (frequently occurring) meteorological conditions, and maximum ozone concentrations that are close to the regional design values for the 1997-1999 period. In preparing this protocol document, we have also considered the design value for the 1998-2000 period. Each area was considered separately and as part of an integrated analysis. The integrated analysis was designed such that the selected episode days are representative of not just one, but two or more of the regions included in the analysis.

Following application of the objective episode selection procedures, a final set of episode days was selected such that (1) the best candidate modeling episodes (i.e., those best meeting the representativeness criteria given above) were included, (2) the significant meteorological regimes were represented, and (3) only episodes that occurred during 1997-1999 were included in the final list of candidate episodes. This was done for each ozone metric separately and for the integrated analysis.

In comparing the individual-area results with the integrated results, we found that some days that are good modeling candidates for one area are not good for another area and the best episodes for modeling all three areas may not represent the first choice for each area individually. Considering the criteria given above, the best overall candidate episode originally selected for the ATMOS modeling is 29 August—9 September 1999. This rather long simulation period includes multiple days of interest for all three areas. The meteorological and air quality characteristics of the this set of days are summarized in Table 3-1 for Memphis, Nashville, and Knoxville.

**Table 3-1a. SUMMARY of Maximum 8-Hour Ozone Concentration and Meteorological Regime for the 29 August–9 September 1999 Episode Days for Memphis.**

*Exceedances and key meteorological regimes (CART bins) are highlighted in bold.*

| Year | Month | Day | Maximum 8-Hour Ozone (ppb) | CART Bin[3] |
|---|---|---|---|---|
| 1999 | 8 | 29 | 79 | 22 |
| 1999 | 8 | 30 | 71 | 20 |
| 1999 | 8 | 31 | 96 | 15 |
| 1999 | 9 | 1 | 87 | 21 |
| 1999 | 9 | 2 | 95 | 34 |
| 1999 | 9 | 3 | 97 | 18 |
| 1999 | 9 | 4 | 106 | 29 |
| 1999 | 9 | 5 | 64 | 35 |
| 1999 | 9 | 6 | 80 | 2 |
| 1999 | 9 | 7 | 87 | 26 |
| 1999 | 9 | 8 | 55 | 25 |
| 1999 | 9 | 9 | 49 | 4 |

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[3] Key exceedance bins for Memphis are 21, 18, and 34. Other potentially important bins are 15 and 26.

### Table 3-1b. SUMMARY of Maximum 8-Hour Ozone Concentration and Meteorological Regime for the 29 August–9 September 1999 Episode Days for Nashville.

*Exceedances and key meteorological regimes (CART bins) are highlighted in bold.*

| Year | Month | Day | Maximum 8-Hour Ozone (ppb) | CART Bin[4] |
|---|---|---|---|---|
| 1999 | 8 | 29 | 74 | 30 |
| 1999 | 8 | 30 | 65 | 10 |
| 1999 | 8 | 31 | 92 | 4 |
| 1999 | 9 | 1 | 100 | 11 |
| 1999 | 9 | 2 | 91 | 12 |
| 1999 | 9 | 3 | 91 | 25 |
| 1999 | 9 | 4 | 110 | 26 |
| 1999 | 9 | 5 | 109 | 26 |
| 1999 | 9 | 6 | 96 | 11 |
| 1999 | 9 | 7 | 79 | 13 |
| 1999 | 9 | 8 | 89 | 25 |
| 1999 | 9 | 9 | 60 | 30 |

### Table 3-1c. Summary of Maximum 8-Hour Ozone and Meteorological Regime for the 29 August–9 September 1999 Episode Days for Knoxville.

*Exceedances and key meteorological regimes (CART bins) are highlighted in bold.*

| Year | Month | Day | Maximum 8-Hour Ozone (ppb) | CART Bin5 |
|---|---|---|---|---|
| 1999 | 8 | 29 | 84 | 36 |
| 1999 | 8 | 30 | 82 | 20 |
| 1999 | 8 | 31 | 90 | 22 |
| 1999 | 9 | 1 | 105 | 32 |
| 1999 | 9 | 2 | 104 | 32 |
| 1999 | 9 | 3 | 101 | 33 |
| 1999 | 9 | 4 | 107 | 32 |
| 1999 | 9 | 5 | 90 | 35 |
| 1999 | 9 | 6 | 86 | 32 |
| 1999 | 9 | 7 | 102 | 21 |
| 1999 | 9 | 8 | 98 | 32 |
| 1999 | 9 | 9 | 86 | 28 |

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[4] Key exceedance bins for Nashville are 11, 26, 16, and 28. Other potentially important bins are 23, 19, and 22.

[5] Key exceedance bins for Knoxville are 32, 21, and 15. Other potentially important bins include 37, 27, 36, 19, and 33.

The representativeness of these days for each of the three primary areas of interest is summarized in Table 3-2—first with respect to the 1997-1999 design values (Table 3-2a) and then with respect to the 1998-2000 design values (Table 3-2b). Days with maximum concentrations within 10 ppb of the design value are marked with a single asterisk. Of these days, those within a key meteorological regime are given a second asterisk.

**Table 3-2a. Summary of Representativeness of Recommended Simulation Periods 8-Hour Ozone for Memphis, Nashville, and Knoxville.**

*Concentrations within approximately 10 ppb of the regional design values was based on the 1997-1999 design values of 95, 102 and 105 ppb for Memphis, Nashville, and Knoxville, respectively.*

| Year | Month | Day | Memphis | Nashville | Knoxville |
|---|---|---|---|---|---|
| 1999 | 8 | 29 | | | |
| 1999 | 8 | 30 | | | |
| 1999 | 8 | 31 | * | * | |
| 1999 | 9 | 1 | ** | ** | ** |
| 1999 | 9 | 2 | ** | * | ** |
| 1999 | 9 | 3 | ** | * | * |
| 1999 | 9 | 4 | * | ** | ** |
| 1999 | 9 | 5 | | ** | |
| 1999 | 9 | 6 | | ** | |
| 1999 | 9 | 7 | * | | ** |
| 1999 | 9 | 8 | | | ** |
| 1999 | 9 | 9 | | | |

**Table 3-2b. Summary of Representativeness of Recommended Simulation Periods 8-Hour Ozone for Memphis, Nashville, and Knoxville.**

*Concentrations within 10 ppb of the regional design values was based on the 1998-2000 design values of 97, 102, and 102 ppb for Memphis, Nashville, and Knoxville, respectively.*

| Year | Month | Day | Memphis | Nashville | Knoxville |
|---|---|---|---|---|---|
| 1999 | 8 | 29 | | | |
| 1999 | 8 | 30 | | | |
| 1999 | 8 | 31 | * | * | |
| 1999 | 9 | 1 | ** | ** | ** |
| 1999 | 9 | 2 | ** | * | ** |
| 1999 | 9 | 3 | ** | * | * |
| 1999 | 9 | 4 | * | ** | ** |
| 1999 | 9 | 5 | | ** | |
| 1999 | 9 | 6 | | ** | |
| 1999 | 9 | 7 | * | | ** |
| 1999 | 9 | 8 | | | ** |
| 1999 | 9 | 9 | | | |

The 29 August–9 September 1999 includes:

- six 8-hour exceedance days, six days within approximately 10 ppb of the 1997-1999 design value, six days within 10 ppb of the 1998-2000 design value, and three of three key meteorological regimes (plus two other regimes) for Memphis
- eight 8-hour exceedance days, seven days within approximately 10 ppb of the 1997-1999 design value, seven days within 10 ppb of the 1998-2000 design value, and two of four key regimes (plus three other regimes) for Nashville
- ten 8-hour exceedance days, six days within approximately 10 ppb of the 1997-1999 design value, six days within 10 ppb of the 1998-2000 design value, and two of three key regimes (plus four other regimes) for Knoxville

## Results—Additional ATMOS/EAC Episode

This section summarizes the results for selecting a modeling episode period to complement the original ATMOS episode and to support Early Action Compact (EAC) modeling for several areas within Tennessee and adjacent areas in Arkansas and Mississippi. The methodology used to identify new candidate episodes is the same as that used for the original ATMOS episode selection discussed above. It includes the use of Classification and Regression Tree (CART) analysis to classify days according to meteorological and air quality conditions, and the use of an objective optimization scheme (EPISODES) for selecting periods to represent key meteorological conditions and 8-hour ozone design values for multiple geographic areas. In applying CART, we used meteorological and ozone data for the period 1996 through 2003. Our analysis focused on the Memphis, Nashville, Knoxville, and Chattanooga areas. As a second step in the analysis we added Little Rock and Tupelo to the selection process. As a final step we reviewed the ozone concentrations for each candidate episode for Haywood, Lawrence, Meigs, Putnam, and the Tri-Cities counties in Tennessee. All candidate episodes were reviewed with respect to how well they complement the current ATMOS 1999 simulation period in achieving the episode selection objectives.

### *Primary Candidate Episodes*

Of the candidates chosen by the EPISODES algorithm, the following episodes were favored for representing additional key meteorological regimes for the areas of interest, months different than those in the original 1999 episode, and more recent years: July 23 - 30, 2000, June 16 - 22, 2001, and July 5 - 10, 2002. Start-up and clean-out days are listed, but not considered in the analysis. Characteristics of the episodes are summarized in Table 3-3 below.

First we present the 1999 episode, and then each of the candidate episodes combined with the 1999 episode. “Key bins represented” refers to frequently occurring meteorological conditions or regimes that result in ozone exceedances. This is followed by a summary of ozone concentrations in the other areas of interest throughout Tennessee and a discussion of the attributes and limitations of the three candidate episode periods.

**Table 3-3a. Original ATMOS Episode, August 29–September 9, 1999.**

| Metric | Memphis | Nashville | Knoxville | Chattanooga | Tupelo | Little Rock |
|---|---|---|---|---|---|---|
| 2000–2002 DV | 94 | 88 | 98 | 93 | 81 | 86 |
| Mean exceedance val. | 95.0 | 100.7 | 95.7 | 95.8 | 94.1 | NA |
| Range of exceedances | 86–106 ppb | 90–110 ppb | 86–104 ppb | 88–107 ppb | 85–98 ppb | NA |
| Exceedance days | 6 | 8 | 8 | 6 | 4 | 0[6] |
| Days with 50% sites within 10ppb of DV | 4 | 6 | 4 | 7 | 4 | 2 |
| Key bins represented: | 2 / 3 | 2 /5 | 3 / 5 | 2 / 3 | 1 / 2 | 0 / 3 |

**Table 3-3b. July 23–30, 2000 Combined with August 29–September 9, 1999.**

| Metric | Memphis | Nashville | Knoxville | Chattanooga | Tupelo | Little Rock |
|---|---|---|---|---|---|---|
| 2000–2002 DV | 94 | 88 | 98 | 93 | 81 | 86 |
| Mean exceedance val. | 95.3 | 97.8 | 97.3 | 94.3 | 94.1 | 105 |
| Range of exceedances | 86–106 ppb | 87–110 ppb | 86–104 ppb | 85–107 ppb | 85–98 ppb | 105 ppb |
| Exceedance days | 9 | 11 | 11 | 7 | 4 | 1 |
| Days with 50% sites within 10 ppb of DV | 7 | 10 | 4 | 9 | 7 | 5 |
| Key bins represented: | 2 / 3 | 3 / 5 | 4 / 5 | 2 / 3 | 1/2 | 0 / 3 |

**Table 3-3c. June 16–22, 2001 Combined with August 29–September 9, 1999.**

| Metric | Memphis | Nashville | Knoxville | Chattanooga | Tupelo | Little Rock |
|---|---|---|---|---|---|---|
| 2000–2002 DV | 94 | 88 | 98 | 93 | 81 | 86 |
| Mean exceedance val. | 94.4 | 99.9 | 97.6 | 95.4 | 94.1 | 86.7 |
| Range of exceedances | 86–106 ppb | 90–110 ppb | 86–104 ppb | 88–107 ppb | 85–98 ppb | 86–87 ppb |
| Exceedance days | 8 | 10 | 12 | 8 | 4 | 2 |
| Days with 50% sites within 10 ppb of DV | 7 | 8 | 8 | 10 | 6 | 5 |
| Key bins represented: | 2 /3 | 3 / 5 | 4 / 5 | 2 / 3 | 1 / 2 | 2 / 3 |

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[6] Note that the 1999 episode includes one exceedance day for Little Rock, but this is a start-up day.

**Table 3-3d. July 5–10, 2002 Combined with August 29–September 9, 1999.**

| Metric | Memphis | Nashville | Knoxville | Chattanooga | Tupelo | Little Rock |
|---|---|---|---|---|---|---|
| 2000–2002 DV | 94 | 88 | 98 | 93 | 81 | 86 |
| Mean exceedance val. | 94.8 | 99.8 | 95.5 | 93.9 | 94.1 | 89.6 |
| Range of exceedances | 86–106 ppb | 90–110 ppb | 86–104 ppb | 85–107 ppb | 85–98 ppb | 86–91 ppb |
| Exceedance days | 8 | 9 | 11 | 8 | 4 | 3 |
| Days with 50% sites within 10 ppb of DV | 7 | 7 | 6 | 9 | 5 | 5 |
| Key bins represented: | 2 / 3 | 3 / 5 | 3 / 5 | 2 / 3 | 1 / 2 | 2 / 3 |

**Table 3-3e. Occurrence of Exceedances in Other Areas of Interest within Tennessee for Each Candidate Episode.**[7]

| Episode | Days with exceedances for at least 2 other TN areas | Days with at least 3 other TN areas within 10 ppb of DV | # of areas with at least one (near) exceedance day |
|---|---|---|---|
| July 23–30, 2000 | 0 | 1 | 1 |
| June 16–22, 2001 | 2 | 2 | 2 |
| July 5–10, 2002 | 2 | 2 | 4 |

## July 23–30, 2000

This episode adds exceedances days for the Tennessee areas and important key bins for Nashville and Knoxville. However, the episode's ability to represent the Knoxville area is called into question by the fact that no days have at least half the sites near design value. A closer look at the original site data reveals that the Knoxville area maximums on these days are driven by high ozone at only one or two of the seven Knoxville sites. While this episode does a little bit better at representing Tupelo (there is a near-exceedance day that represents an additional key bin), it does not appear to be good for representing Little Rock. These days are also not characterized by high ozone within many of the other Tennessee areas of interest.

## June 16–22, 2001

This candidate episode does fairly well at representing all areas of interest. Nashville and Knoxville each obtain a new key bin, and Little Rock gains two. Although no new key bins are added for Memphis or Chattanooga, for these areas the episode provides more days from key bins already included in the 1999 episode. Of the primary candidates, this episode provides the most new key bins. In general, the episode is characterized by exceedances in all ATMOS areas except Tupelo, and in two of the non-ATMOS (other Tennessee) areas, as well as

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[7] The "other TN areas" considered in here are Haywood County, Lawrence County, Meigs County, Putnam, and the Tri-Cities area. The July 2000 episode seems only to reach Meigs County. The June 2001 ozone episode affects Meigs County and the Tri-Cities area. The July 2002 dates seem to capture a widespread ozone episode, with exceedances in Haywood, Meigs County, Putnam, and the Tri-Cities area. No exceedance days are found in Lawrence County during these episodes, although all three episodes have days where the Lawrence County site is within 10 ppb of its design value.

multiple sites near the design value for all ATMOS areas and sites near design value for three non-ATMOS areas.

### July 5–10, 2002

This candidate stands out as being the best episode for Little Rock, with all three of its days in new key Little Rock bins and with both Little Rock sites within 10 ppb of their design value for each of these days. The episode is also characterized by widespread exceedances in non-ATMOS areas of Tennessee. However, for the four principal ATMOS/Tennessee areas of interest, it adds only one new key bin (for Nashville). In terms of achieving days with multiple sites near the site-specific design value, this episode is somewhat weaker than the June 2001 episode in representing Nashville, Knoxville, Chattanooga, and Tupelo.

## *Other Episodes*

The episode selection algorithm also selected an August 2000 and an August 2002 episode, both of which are worth some consideration. The information tabulated for the June and July episodes above is done so for the August episodes in Table 3-4 below.

These episodes are good to excellent by some measures, for some areas, but in other ways comparable to or not as good as the June 2001 episode. The June and July episodes have the advantage of adding greater variety in terms of time of year.

**Table 3-4a. August 12–18, 2000 with August 29–September 9, 1999**

| Metric | Memphis | Nashville | Knoxville | Chattanooga | Tupelo | Little Rock |
|---|---|---|---|---|---|---|
| 2000–2002 DV | 94 | 88 | 98 | 93 | 81 | 86 |
| Mean exceedance val. | 95.1 | 98.8 | 97.8 | 97.3 | 93.5 | 90.7 |
| Range of exceedances | 86–107 ppb | 89–110 ppb | 86–104 ppb | 88–107 ppb | 85–98 ppb | 89–91 ppb |
| Exceedance days | 9 | 11 | 11 | 8 | 5 | 2 |
| Days with 50% sites within 10 ppb of DV | 7 | 9 | 6 | 8 | 7 | 5 |
| Key bins represented: | 2 / 3 | 2 / 5 | 4 / 5 | 2 / 3 | 1 / 2 | 0 / 3 |

**Table 3-4b. August 6–14, 2002 with August 29–September 9, 1999**

| Metric | Memphis | Nashville | Knoxville | Chattanooga | Tupelo | Little Rock |
|---|---|---|---|---|---|---|
| 2000–2002 DV | 94 | 88 | 98 | 93 | 81 | 86 |
| Mean exceedance val. | 93.9 | 98.8 | 98.9 | 93.7 | 94.1 | 86.8 |
| Range of exceedances | 86–107 ppb | 85–110 ppb | 83–109 ppb | 85–112 ppb | 85–98 ppb | 86 ppb |
| Exceedance days | 8 | 12 | 14 | 11 | 4 | 1 |
| Days with 50% sites within 10 ppb of DV | 4 | 9 | 10 | 12 | 5 | 4 |
| Key bins represented: | 2 /3 | 4 / 5 | 4 / 5 | 3 / 3 | 1 / 2 | 1 / 3 |

**Table 3-4b. Occurrence of Exceedances in Other Areas of Interest within Tennessee, for Above Episodes.**

| Episode | Days with exceedances for at least 2 other TN areas[8] | Days with at least 3 other TN areas within 10 ppb of DV | # of areas with at least one (near) exceedance day |
|---|---|---|---|
| August 12–18, 2000 | 2 | 2 | 3 |
| August 6–14, 2002 | 6 | 6 | 4 |

### August 12–18, 2000

This candidate episode adds one or more exceedance days for all of the primary areas of interest, with the exception of Tupelo. Additional key meteorological regimes are added for the Knoxville area.

### August 6–14, 2002

This candidate episode does fairly well at representing all areas of interest. Key bins are added for Nashville, Knoxville, Chattanooga, and Little Rock. Some additional bins are also added for Memphis, although these are not among the most frequently occurring exceedance regimes. Overall, the episode provides the most new key bins. In general, the episode is characterized by exceedances in all ATMOS areas except Tupelo, and in four of the non-ATMOS (other Tennessee) areas. The values for Meigs, Putnam, Blount, and Kings Counties are high relative to the design values for these areas.

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[8] “Other TN areas” defined in Table 3-3e above.

## *Final Episode Selection*

The following tables summarize the candidate episodes in terms of the number of exceedance days and representation of additional (to the 1999 episode) key meteorological regimes.

**Table 3-5. Number of 8-Hour Ozone Exceedance Days for Each Candidate Episode Period.**

| Episode | Memphis | Nashville | Knoxville | Chattanooga | Tupelo | Little Rock |
|---|---|---|---|---|---|---|
| August/September 1999 | 6 | 8 | 8 | 6 | 4 | 0 |
| July 2000 | 3 | 3 | 3 | 1 | 0 | 1 |
| August 2000 | 3 | 3 | 3 | 2 | 1 | 2 |
| June 2001 | 2 | 2 | 4 | 2 | 0 | 2 |
| July 2002 | 2 | 1 | 3 | 2 | 0 | 3 |
| August 2002 | 2 | 4 | 6 | 5 | 0 | 1 |

**Table 3-6. Original Count and Number of Additional, Distinct Key Meteorological Bins (Regimes) for Exceedance (or Near-Exceedance) Days for Each Candidate Episode Period.**

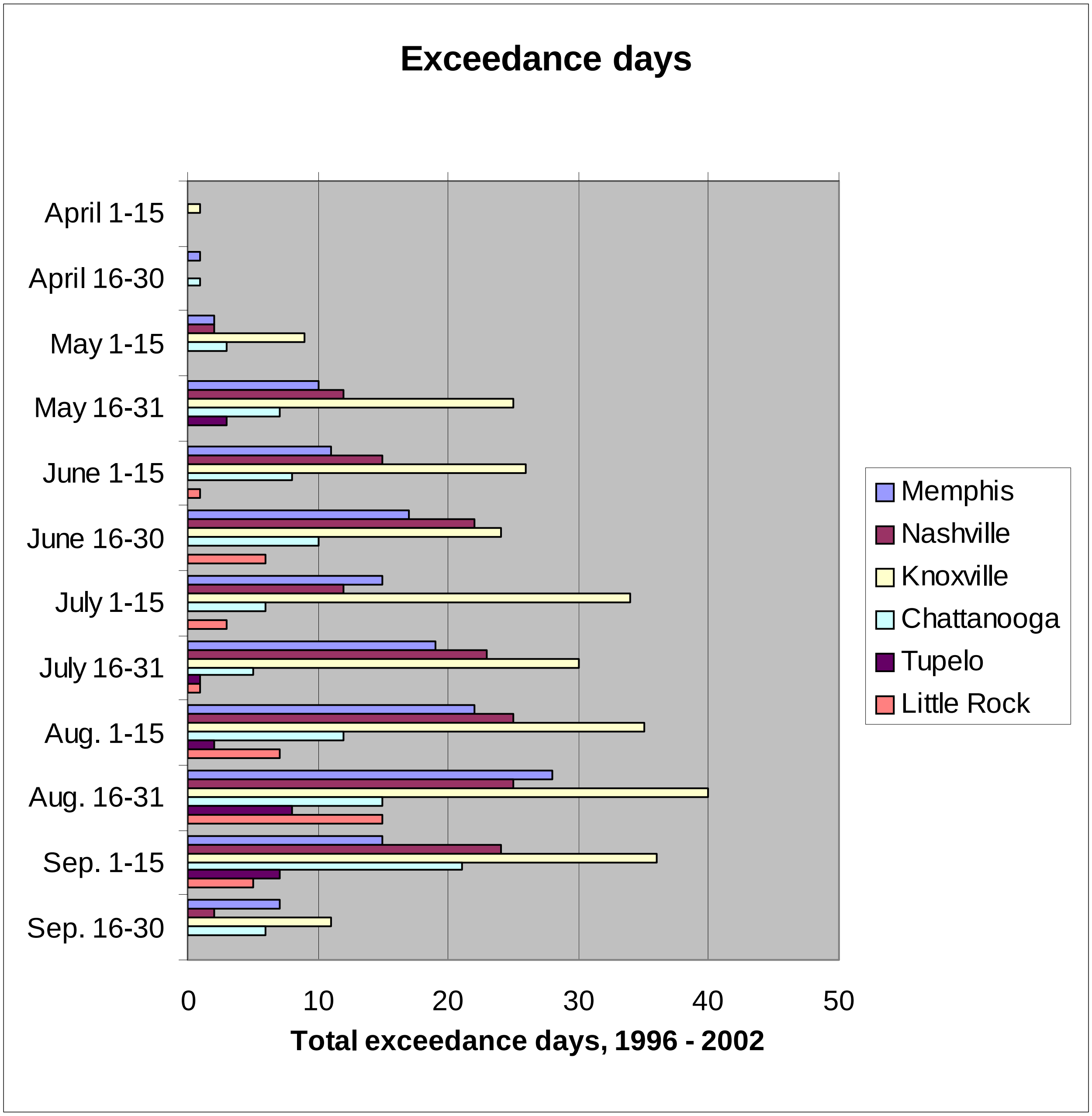
| Episode | Memphis | Nashville | Knoxville | Chattanooga | Tupelo | Little Rock |
|---|---|---|---|---|---|---|
| August/September 1999 | 2/3 | 2/5 | 3/5 | 2/3 | 1/2 | 0/3 |
| July 2000 | 0 | 1 | 1 | 0 | 0 | 0 |
| August 2000 | 0 | 0 | 1 | 0 | 0 | 0 |
| June 2001 | 0 | 1 | 1 | 0 | 0 | 2 |
| July 2002 | 0 | 1 | 0 | 0 | 0 | 2 |
| August 2002 | 0 | 2 | 1 | 1 | 0 | 1 |

Based on a discussion with the ATMOS Operations Committee, the episode selected for the EAC modeling is June 16-22, 2001. When combined with the August/September 1999 simulation period, this episode provides 8 to 12 exceedance days for the four key Tennessee areas of interest, two exceedance days for Little Rock, and four exceedance days for Tupelo. The two episodes combined also provide between two and eight exceedance days for the other Tennessee areas of interest.

The June 2001 episode provides for representation of an important key bin (meteorological regime) for Nashville that is not accounted for in the original ATMOS episode, as well as for further representation of a key bin already represented by the 1999 ATMOS episode. For Knoxville, the June 2001 exceedance days represent one new key bin, two already represented key bins, and one additional bin. For Memphis, the June 2001 exceedance days represent one already represented key bin (the largest bin), and one additional bin that is a neighbor to the key bin that is not represented and is thus likely similar in its features. For Chattanooga, the June 2001 exceedance days represent the key bin for that area. Finally, two of the three key bins for Little Rock are represented by exceedance days.

The June 2001 episode is more seasonally different from the August/September 1999 episode, although both episodes represent key periods during which ozone exceedances tend to occur, as illustrated in Figure 3-1 below.

**Figure 3-1. Distribution of Exceedance Days, 1995–2002.**



# 4. Photochemical and Meteorological Modeling Domain Specification

The modeling domain for application of the UAM-V was designed to accommodate both regional and subregional influences as well as to provide a detailed representation of the emissions, meteorological fields, and ozone (and precursor) concentration patterns over the area of interest. The modeling domain to be used in the EAC modeling analysis is the same as what has been used for the ATMOS modeling. The UAM-V modeling domain is presented in Figure 4-1 and includes a 36-km resolution outer grid encompassing the southeastern U.S; a 12-km resolution intermediate grid; and a 4-km resolution inner grid encompassing Tennessee and portions of Mississippi, Arkansas, and other neighboring states.

The regional extent of the modeling domain is intended to provide realistic boundary conditions for the primary areas of interest and thus avoid some of the uncertainty introduced in the modeling results through the incomplete and sometimes arbitrary specification of boundary conditions. The use of 4-km grid resolution over the primary area of interest is consistent with an urban-scale analysis of each of the areas of interest.

The UAM-V domain is further defined by eleven vertical layers with layer interfaces at 50, 100, 200, 350, 500, 750, 1000, 1250, 1750, 2500, and 3500 meters (m) above ground level (agl). Further testing of the appropriateness of the vertical grid structure may be performed as part of the diagnostic testing, as described in Section 7 of this protocol document.

The modeling domain for application of MM5 is shown in Figure 4-2. This domain is much larger than that for UAM-V, in order to enable the simulation of any important synoptic scale features and their influence on the regional meteorology. The modeling domain consists of an extended outer grid with approximately 108-km horizontal resolution and four inner (nested) grids with approximately 36, 12, and 4-km resolution. The horizontal resolution was specified to match that for UAM-V. A one-way nesting procedure and 22 vertical levels will be employed. The vertical grid is defined using the MM5 sigma-based vertical coordinate system. The layer thickness increases with height such that high resolution is achieved within the planetary boundary layer. The vertical layer heights for application of MM5 are listed in Table 4-1.

**Table 4-1. MM5 vertical levels for the ATMOS application.**

| Level | Sigma | Average Height[9] (m) |
|---|---|---|
| 1 | 0.996 | 30 |
| 2 | 0.988 | 80 |
| 3 | 0.982 | 125 |
| 4 | 0.972 | 215 |
| 5 | 0.960 | 305 |
| 6 | 0.944 | 430 |
| 7 | 0.928 | 560 |
| 8 | 0.910 | 700 |
| 9 | 0.890 | 865 |
| 10 | 0.860 | 1115 |
| 11 | 0.830 | 1370 |
| 12 | 0.790 | 1720 |
| 13 | 0.745 | 2130 |
| 14 | 0.690 | 2660 |
| 15 | 0.620 | 3375 |
| 16 | 0.540 | 4260 |
| 17 | 0.460 | 5240 |
| 18 | 0.380 | 6225 |
| 19 | 0.300 | 7585 |
| 20 | 0.220 | 9035 |
| 21 | 0.140 | 10790 |
| 22 | 0.050 | 13355 |

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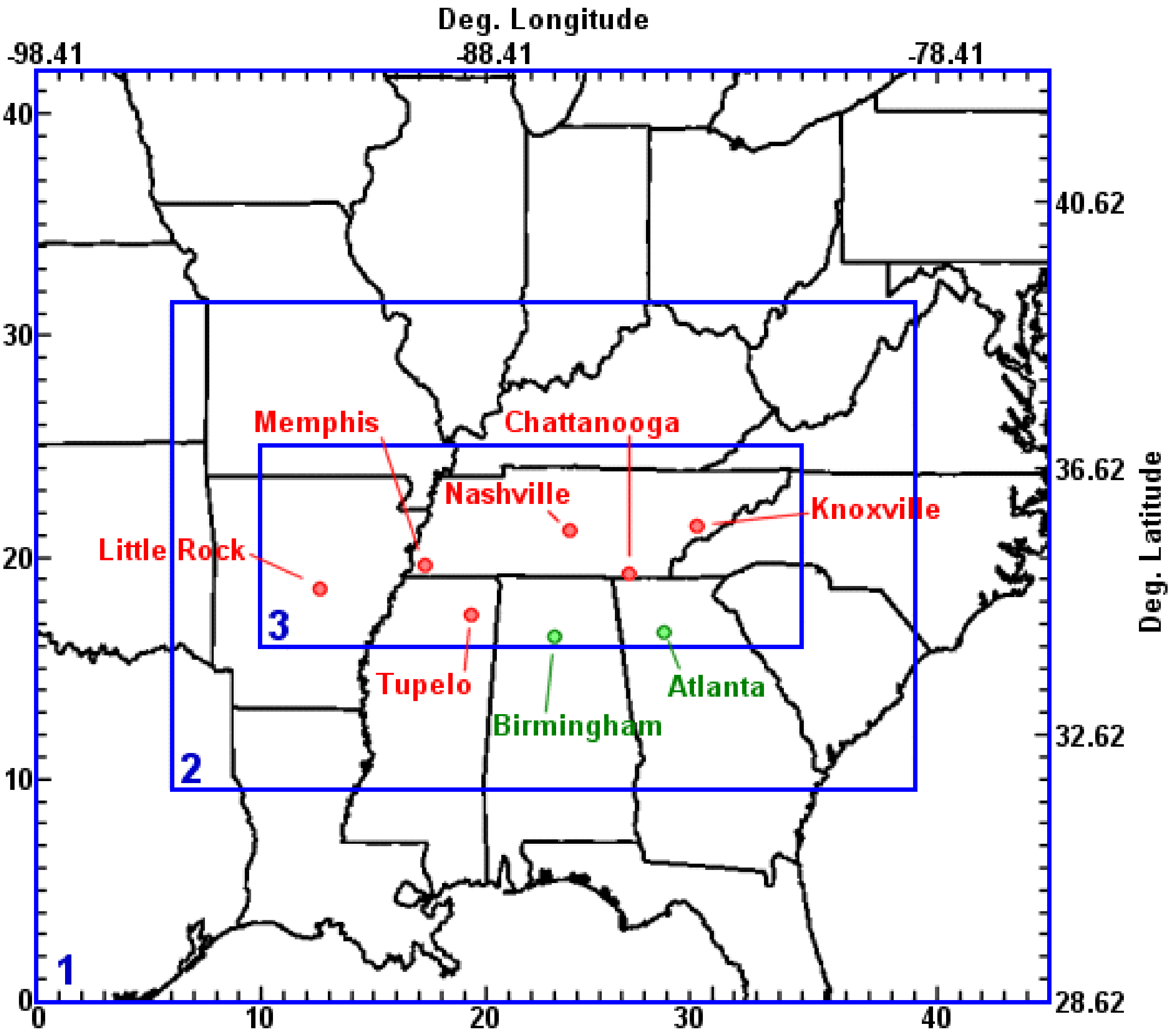
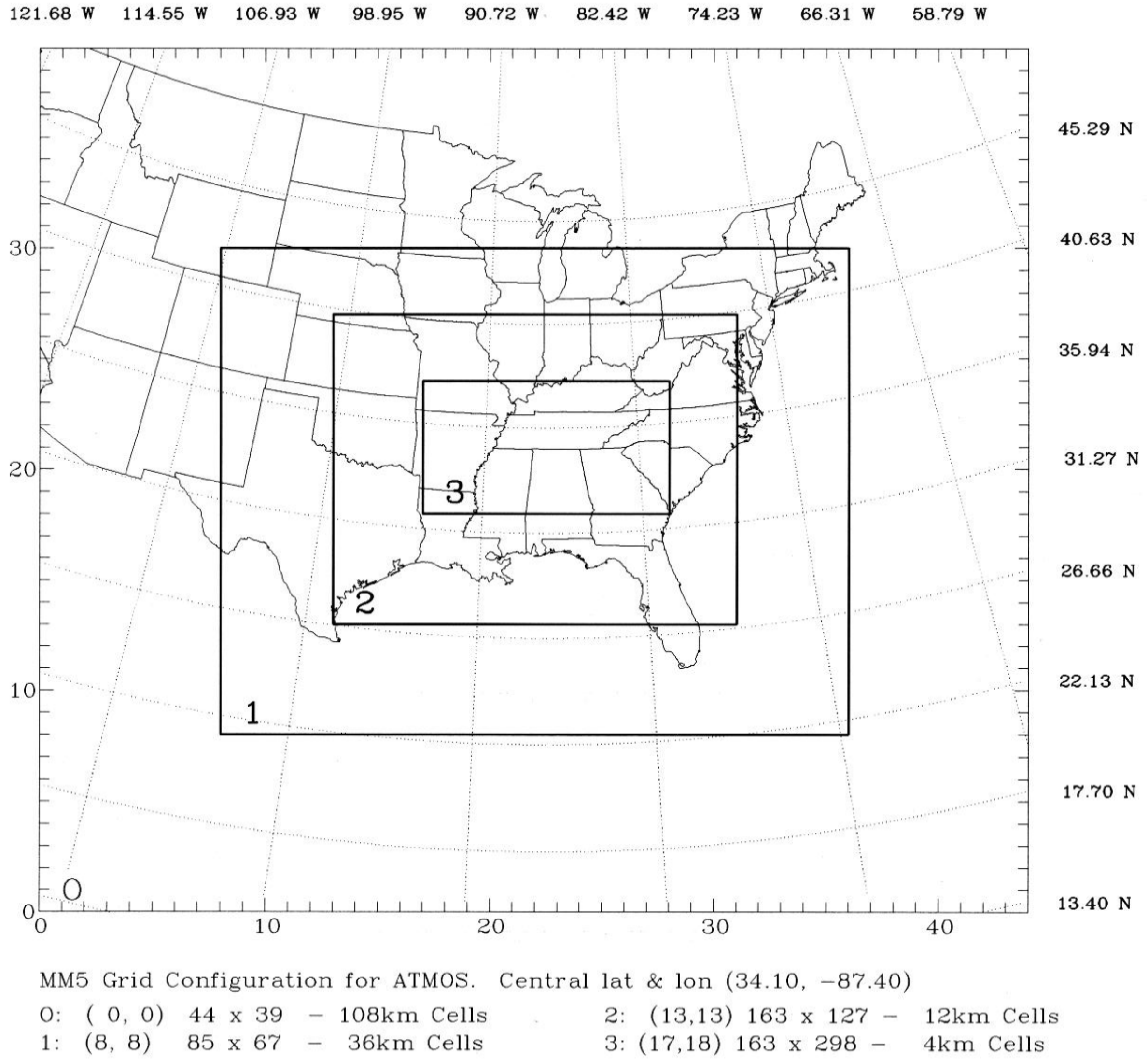
[9] Approximate heights—to be updated following initial application of MM5.

Figure 4-1. UAM-V modeling domain for the ATMOS study.



Grid 1: (-98.41,28.62)—45x42—36-km Cells
Grid 2: (-95.41,31.79)—99X66—12-Km Cells
Grid 3: (-93.41,33.96)—215x81—4-km Cells

Figure 4-2. MM5 modeling domain for the ATMOS application.



MM5 Grid Configuration for ATMOS. Central lat & lon (34.10, −87.40)

0: ( 0, 0) 44 x 39 − 108km Cells
1: (8, 8) 85 x 67 − 36km Cells
2: (13,13) 163 x 127 − 12km Cells
3: (17,18) 163 x 298 − 4km Cells

# 5. Input Preparation

Version 1.5 of the UAM-V modeling system will be used for the ATMOS modeling analysis. This latest version of the model includes the Carbon Bond 5 chemical mechanism, accommodates the use of a variety of horizontal coordinate systems, and provides for the use of either the standard or enhanced (“fast”) chemistry solver. It also includes process analysis and oxidant tagging capabilities.

The UAM-V modeling system requires a variety of input files that contain information pertaining to the modeling domain and simulation period. These include gridded, day-specific emissions estimates and meteorological fields; initial and boundary conditions; land-use information; and chemistry parameters. The methods and data to be used in preparing the UAM-V inputs for the ATMOS/EAC base-case modeling exercises are described in this section of the protocol document.

## Base-Year Emission Inventory Preparation

The UAM-V requires specification of gridded low-level emissions for the full domain and each subdomain. Elevated point source emissions for all sources within the domain are contained in a single input file. The preparation of these input files is described in this section.

### *Emission Inventory Requirements for Modeling*

In order for photochemical simulation models to adequately simulate temporal and spatial variations in ozone concentrations, the emission inventories input to these models must contain considerably more detail than an inventory generated to meet periodic emission inventory reporting requirements. The primary additional requirements of the photochemical modeling inventory are summarized below. This information is primarily derived from the EPA guidance document entitled *Procedures for the Preparation of Emission Inventories for Carbon Monoxide and Precursors of Ozone, Volume II: Emission Inventory Requirements for Photochemical Air Quality Simulation Models*, prepared by SAI (EPA, 1992b).

Spatial Allocation: Emission estimates of precursor pollutants must be provided for each individual cell of a grid system within the modeling domain instead of at a county or regional level.

Temporal Allocation: Emissions must be specified as hourly rather than annual or daily rates. Additionally, annual or seasonal average rates should be adjusted to reflect episodic or day-specific conditions as accurately as possible.

Chemical Speciation: Total reactive VOC and $NO_x$ emissions estimates must be disaggregated into several classes of VOC and NO and $NO_2$, respectively; spatially and temporally resolved emission estimates of CO may also be required (EPA requires that CO emissions be input to the UAM-V in ozone attainment demonstrations).

Stack Parameters: For models such as the UAM-V that provide for vertical resolution of pollutants, stack and exhaust gas parameters must be provided for each large point source.

Each of these is discussed further below.

## Spatial Allocation of Emissions

*Point Sources.* Point source locations are typically reported to within a fraction of a kilometer; hence, assigning emissions from these sources to the appropriate grid cell is simple.

*Area Sources.* By contrast, spatial resolution of area source emissions requires substantially more effort. Two basic methods can be used to apportion area source emissions to grid cells. The most accurate (and resource-intensive) approach is to obtain area source activity level information directly for each grid cell. The alternative approach, more commonly employed, is to apportion the county-level emissions from the existing annual inventory to grid cells using representative apportioning factors for each source type.

This latter approach requires the determination of apportioning factors based on the distribution of some spatial surrogate indicator of emission levels or activity (e.g., population, census tract data, or type of land use) for each grid cell. These factors are then applied to the county- or parish-level emissions to yield estimates of emissions from that source category by grid cell. The major assumption underlying this method is that emissions from each area source category behave spatially in the same manner as the spatial surrogate indicator. In most large urban areas, local planning agencies can provide detailed land use, population, or in some cases, employment statistics at the sub-county level. These data can be used to spatially apportion most of the area source emissions in the modeling inventory.

A spatial surrogate indicator is a parameter with a known distribution at a sub-county level and a behavior that is similar to the activity levels of interest. Commonly used spatial surrogate indicators include land-use parameters, employment in various industrial and commercial sectors, population, and dwelling units. Different surrogate indicators can be used to apportion emissions for the various area source categories, of course, depending on which of the available indicators best describes the spatial distribution of the emissions.

*Mobile Sources.* Planning, land-use, and transportation models are already in use in many urban areas, and can provide much of the data necessary to allocate mobile source emissions and develop emission estimates by link for highway motor vehicles. Such models are also generally capable of developing forecasts for future years which can be utilized in the development of projection inventories.

Mobile sources differ from stationary source categories in that their spatial variation is more accurately described using a link-based rather than a surrogate-based gridding procedure. In a link-based spatial allocation approach, emissions are distributed only to those grid cells that contain transportation pathways (e.g., roadways, railways, airports, shipping channels, etc.). This approach is usually used in conjunction with a surrogate-based procedure to complete the spatial resolution of the mobile source inventory.

Emissions from on-road vehicles on limited access roadways (interstates and expressways), railroad locomotives, aircraft, and vessels are often spatially allocated with a link-based procedure, since the transport routes used by these vehicles are both easily identifiable and readily modeled as a series of lines or links. This results in more accurate allocation of emissions from these sources than could be achieved using surrogates such as population or land use.

Non-link surrogates are commonly used to spatially allocate mobile emissions in the following situations:

- Links are too numerous to define and process, as is typically the case for on-road rural and urban vehicles and for off-road vehicles.
- Emission totals are too insignificant when compared with emissions from other sources in the modeling domain to warrant the development of link data.
- Use of gridded spatial surrogates based on land-use or population data provides a more accurate allocation of vehicle emissions. For example, recreational boating activities may be distributed approximately equally over the surface of a large lake.

In most modeling applications, a combination of link and land-use surrogates is used for the spatial allocation of mobile source emissions.

### Temporal Resolution of Emissions

In order to simulate hourly concentrations of ozone and other pollutants, photochemical models require hour-by-hour estimates of emissions at the grid cell level. Several approaches can be used to provide the temporal detail needed in the modeling inventory. The most accurate and exacting approach is to determine the emissions (or activity levels) for specific sources for each hour of a typical day in the time period being modeled.

As an alternative, typical hourly patterns of activity levels can be developed for each source category. These are then applied to the annual or seasonally adjusted emissions to estimate hourly emissions. This approach is commonly employed for area sources, including highway motor vehicles, and is usually used for all but the largest point sources.

Usually, the photochemical air quality model is applied for an episode in the season of the year in which meteorological conditions are most conducive to ozone formation; for most locations, this means the summer months (i.e., May through September). Consequently, emissions must be adjusted to reflect typical levels for the appropriate season.

Similarly, emissions must also be adjusted to reflect whether the simulation day is a weekday or a weekend day. For simulation periods that include both weekday and weekend days, temporal pattern information pertaining to both weekday and weekend days is required.

*Point Sources.* The modeling inventory should represent as accurately as possible day-specific emission estimates for each hour of the modeling episode. By contrast, the existing point source inventory will more likely contain annual or typical ozone season day estimates of emissions and a general description of the operating schedule (seasonal fractions of annual throughput, and operating schedule in terms of weeks/year, days/week, and hours/day in operation).

Ideally, each facility would be contacted to obtain hourly operating records for the modeling episode, or, if this information is unavailable, representative operating schedules for a typical ozone season day. Certain local agencies may also have this type of temporal information. Some sources for which this type of data may be available include the following: power plants (which generally keep detailed, hourly records of fuel firing rates and power output for each day of operation), major industrial facilities such as automotive assembly plants and refineries, and tank farms.

For many smaller point sources, reasonable temporal resolution can be obtained from the operating data that are typically collected for each point source.

*Area Sources.* Since the basic area source inventory usually contains estimates of annual (or sometimes seasonally adjusted) emissions, the emissions modeler must expend additional effort to estimate hour-by-hour emission rates for the episode days. Several approaches can be employed to develop hourly emissions resolution; all involve the use of assumed diurnal patterns of activity. In addition to hourly patterns, estimates of seasonal fractions of annual activity will be needed if the county-level inventory is not seasonally adjusted. Activity profiles by day of week will also be required.

*Mobile Sources.* Temporal adjustment of the mobile source inventory into monthly, daily, and hourly specific totals is not significantly different than the treatment of other area source categories. If hourly vehicular speeds and VMT distributions are available from the local Metropolitan Planning Organizations (MPOs), these can be utilized in estimating hourly mobile source emissions.

## Chemical Resolution of Emissions

Because photochemical models like the UAM-V are intended to simulate photochemistry, they require specific information as to the proportions of the various types of VOC emissions present in the inventory. For this reason, VOC emission totals must be disaggregated into subtotals for various chemical classes. $NO_x$ emissions also have to be distributed as NO and $NO_2$. Literally thousands of individual chemical compounds typically compose the total VOC emissions in an urban area. No photochemical model considers each organic compound individually; instead, VOC emissions are distributed into chemical classes which behave similarly in photochemical reactions. The UAM-V employs a carbon-bond classification scheme based on the presence of certain types of carbon bonds in each VOC molecule. The latest version of this mechanism is CB-V.

Two basic approaches can be followed for determining split factors. Ideally, VOC split factors should be source-specific, reflecting the actual composition of VOC emissions from each individual source.

In some instances, source-specific VOC species data may be available for certain individual facilities (perhaps through source tests or material composition considerations). Generally, however, most industries cannot provide reliable VOC or $NO_x$ species data or accurately apportion their emissions into appropriate classes, in which case generalized VOC and $NO_x$ distributions must be assumed for various source categories.

Because of resource limitations and unavailability of solvent composition data, however, collecting source-specific speciation data is generally impractical for all but a very few large point or area source emitters. An alternative method employs generalized VOC speciation data from the literature to develop VOC split factors by source type.

## Elevated Point Source Requirements

The emission inventory must include stack information (e.g., physical stack height and diameter, stack gas velocity, and temperature) for the major point sources in the area. All point sources with an effective stack height (i.e., the sum of the physical height of the stack and any plume rise) greater than 25 meters is considered to be an elevated point source. The emissions from elevated point sources are assigned to the grid cells based on location of the stack and effective plume rise.

## Emissions Data

The ATMOS EAC modeling inventory will be based primarily on the Version 2 of EPA's 1999 National Emissions Inventory (NEI-99), and will follow procedures similar those followed in preparing emissions for the original ATMOS episode. To ensure the most accurate estimation of base-year ozone precursor emissions for the AR-TN-MS area possible, we will also obtain the latest information available for each of these states and incorporate these data into the modeling inventory as permitted by schedule and resource limitations. Specifically, the following information will be solicited from each of these states:

- Area source data (county/parish level emission estimates, population, and activity information)
- Point source data (stack parameters, emission rates, etc.)
- Mobile source data (VMT, speeds, fleet mix, fuel characteristics, program characteristics, etc.)

An updated mobile source inventory for the State of Tennessee, prepared by the University of Tennessee's Center for Transportation Research, will be used.

### Episode-Specific Information

To further refine the base-year inventories, it is desirable to refine the annual inventory to incorporate known differences for the specific episode being simulated. For example, if a particular large point source was not operating during the episode, this information should be incorporated in the episode-specific inventory. Emission estimates should also be adjusted to reflect seasonal conditions. We will thus obtain any available episode-specific and/or seasonal information that would affect any portions of the inventory for the episode.

For each episode to be modeled, the types of information needed include the following:

- Daily (or preferably hourly, if available) emissions data for major point sources for each of the episode days. If significant differences in associated stack parameters such as temperature, flow rate, and velocity are documented, these data can be used as well.
- List of sources not in operation for each episode day.

## Emissions Processing Tools and Procedures

To facilitate development of the detailed emission inventories required for photochemical modeling for this analysis, a version of the EPA UAM Emissions Preprocessor System (EPS 2.5) will be used. This system, developed by SAI under the sponsorship of the EPA's Office of Air Quality Planning and Standards, consists of a series of computer programs designed to perform the intensive data manipulations necessary to adapt a county-level annual or seasonal emission inventory for modeling use. EPS 2.5 provides the capabilities to support the CAAA requirements, to conform to EPA emission inventory requirements, and to allow the evaluation of proposed control measures for meeting Reasonable Further Progress (RFP) regulations and special study concerns.

In addition, the latest available version of EPA's Biogenic Emissions Inventory System (BEIS) will be used to estimate day-specific biogenic emissions for the modeling analysis. Currently, this is BEIS-2, but BEIS-3 will be used if it is available in version that can be used in this modeling analysis. County-level biomass estimates are provided as part of the BEIS input data package. Temperature and solar radiation estimates will be extracted from the output of the MM5 meteorological model.

EPA's MOBILE model will be used to provide estimates of motor vehicle emissions. The current operational version of this model is MOBILE6.2. The MOBILE model will be applied at the county level, using county level estimates of vehicle miles traveled (VMT). The VMT will be distributed temporally using a weekly profile as presented in Table 5-1. These values are based on more recent national average traffic count information (collected in the 1990s).

**Table 5-1. Proposed Weekly Profile for On-Road Motor Vehicles.**

| Day of Week | Fraction of Average Daily Emissions |
|---|---|
| Sunday | 0.84 |
| Monday | 1.01 |
| Tuesday | 1.03 |
| Wednesday | 1.02 |
| Thursday | 1.04 |
| Friday | 1.11 |
| Saturday | 0.96 |

In addition to the temporal adjustment, MOBILE will be used along with the MM5-derived gridded surface temperature fields to adjust the emission estimates to reflect ambient conditions for each hour of the simulation.

The latest version of EPA's NONROAD model (NONROAD 2002) will also be used to estimate nonroad emissions throughout the domain.

The core EPS 2.5 system consists of a series of FORTRAN modules that incorporate spatial, temporal, and chemical resolution into an emissions inventory used for photochemical modeling. EPS 2.5 system input files which must be created specific to each modeling region include: (1) projection factors used to forecast or back-cast emission rates from the year of input emissions to the episode modeling year, (2) gridded area, population, and land use surrogates used to spatially allocate area source emissions, and (3) digitized link data used to spatially allocate selected source categories (routinely mobile sources). Point, area, and mobile source emission data are usually processed separately through the EPS 2.5 system to facilitate both data tracking for quality control and the use of the data in evaluating the effects of alternative proposed control strategies on predicted air pollutant concentrations.

Point source data are initially processed by the PREPNT module, which performs an initial screening of the data to determine whether each source will be treated as low-level or elevated. PREPNT also converts the input data to the EPS 2.5 internal Emission Model Binary Record

(EMBR) format. The point source inventory is then ready for projection to future year levels, temporal allocation, and chemical speciation.

County-level (or other aggregated) area and mobile source emissions data enter the EPS 2.5 system through the PREAM module, which separates the area and on-road motor vehicle emissions data into two files. (If data for calculating link-based mobile source emissions are available, the LBASE module serves as the entry point for these data.) The emissions files created by PREAM are in the EMBR format. The PREAM module also disaggregates total motor vehicle emissions, which are usually reported in the input data by road type (limited access, urban, suburban, and rural) and vehicle class (light-duty gasoline vehicles, light-duty gasoline trucks, heavy-duty gasoline vehicle, and heavy-duty diesel vehicle), into the four emission component categories employed by EPA's MOBILE models (versions 4.0 and higher): exhaust, evaporative, refueling losses, and running losses. The on-road motor vehicle emissions are then adjusted to reflect episodic and scenario-specific conditions, such as existing or proposed Inspection and Maintenance (I/M) programs, Stage II vapor recovery controls, and ambient temperatures.

Each of the inventory components (e.g., point sources, area sources, on-road motor vehicles) are then processed separately through the remaining modules of EPS 2.5 to facilitate quality control tracking and control strategy analysis. After projection to the year to be modeled (performed by the CNTLEM module), each file is chemically speciated and temporally allocated by the CHMSPL and TMPRL modules, respectively. For area sources, non-road mobile sources, and on-road motor vehicles, county-level emission totals by source category are spatially allocated to individual grid cells in the UAM-V modeling domain by the GRDEM module; point source emissions are allocated to grid cells based on source location. The GRDEM module has a user option specifying the desired format of the output emissions file, either gridded EMBR format or UAM-V low-level emissions file format. The gridded anthropogenic emissions files are then merged with the biogenic emissions file into a single low-level emissions file, as the final step prior to input to the UAM-V.

## *Selection of Sources for P-i-G Treatment*

Point sources for plume-in-grid (P-i-G) treatment will be selected according to $NO_x$ emission rate as follows:

- For Grid 3 (4 km high-resolution grid) - Impose P-i-G on all sources with facility totals > 5 tpd NOx, except for those individual sources within the facility that are < 1 tpd
- For Grids 1 and 2 (36 and 12-km resolution grids, respectively) - Impose P-i-G on all sources with facility totals > 10 tpd NOx, except for those individual sources within the facility that are < 2 tpd.

### Quality Assurance of the Emissions Inputs

Obviously, the accuracy and representativeness of any UAM-V modeling inventory will be limited by the quality of the input emissions data. Although the EPS 2.5 modules do perform some basic validity checks upon data input to each module, verifying the accuracy of the original emissions data is not a function of the EPS 2.5 system. Consequently, appropriate quality assurance procedures must be performed on the input emissions data prior to processing through EPS 2.5. Our proposed approach to quality assurance of the emissions inventory, which addresses both of these concerns, accordingly distinguishes between two basic levels of quality assurance. The first regards the inherent quality of the data input to EPS 2.5; the second pertains to tracking the data through each step of processing.

We will review the base year inventory database used to develop the UAM-V modeling inventories, along with any available documentation, and assess the methodologies, assumptions, emission factors, and other parameters used to estimate emissions to the extent that this information is available from existing documentation or internally documented within the inventory database. The quality review process will follow the guidance set forth in *Quality Review Guidelines for 1990 Base Year Emission Inventories* (EPA-454/R-92-007, EPA, 1992c). This document describes a two-tiered approach to quality review; SAI will employ a similar procedure in reviewing the base year inventory for the ATMOS modeling domain. The first phase of this review will consist of an overall assessment of the inventory to ensure that the minimum data requirements and quality standards set forth in *Emission Inventory Requirements for Ozone State Implementation Plans* (EPA-450/4-91-010, March 1991) are met. The types of issues that will be addressed include the following:

- inclusion of all required components (i.e., point, area, on-road motor vehicles, biogenics)
- geographical coverage of the inventory (emission estimates should be provided for all counties in the modeling domain, not just the counties located in the actual nonattainment area)
- assessment of completeness of database (identification of default or missing values for inventory parameters such as source location, stack parameters, operating schedules, etc.)
- inclusion of existing regulatory requirements, including rule effectiveness and rule penetration factors for applicable sources and source categories.

The quality review process described above addresses the inherent quality of the data input to the EPS 2.5 system. The second phase of this effort will address the processing of the input inventory data to generate the base year UAM-V modeling inventory. To conduct this review, SAI will track the emissions data set through each stage of EPS 2.5 processing. SAI will verify that the specified input and output files for each processing step contain the appropriate information required to process the emissions data in the expected manner. Temporal profile assignments for each source category, including seasonal, weekly, and diurnal variations will be reviewed. The spatial allocation surrogate data and surrogate assignments for each source category will also be examined. SAI will ascertain that all required processing steps have been completed in an appropriate order and will track input and output emissions totals for each processing step to identify any gross errors in processing. For the future year modeling inventory, the review will focus on the control assumptions and projection factors used to estimate future year emission rates.

Each of the EPS 2.5 core modules and utilities produces a message output file containing summary information on the processed files, as well as errors or warning conditions encountered during execution. These messages can be broadly categorized into three types: (1) messages pertaining to unsuccessful input/output (I/O) operations (i.e., opening, reading, and writing data files), (2) messages notifying the user that internal EPS 2.5 maximum parameters (which are used to dimension internal data arrays) have been exceeded, and (3) messages indicating invalid or questionable input data. SAI will examine the message files produced at each stage of processing to identify any warning or error conditions and reprocess data as needed to alleviate these conditions.

SAI will also make use of the quality control and reporting modules provided with EPS 2.5 as well as in-house quality assurance tools (e.g., plotting programs for examining temporal variations and spatial distribution of gridded emissions) to further examine the modeling inventory.

Upon completion of the quality review, SAI will prepare a technical memorandum summarizing the data included in the base year inventory, focusing on sources of VOC and $NO_x$ emissions.

To facilitate the quality assurance and review of the emissions inputs, the following tabular and graphical summaries will be prepared and examined:

- Plots illustrating the magnitude and spatial distribution of low-level emissions of VOC, $NO_x$, and CO (by component, total anthropogenic, and total anthropogenic and biogenic)
- Plots illustrating the magnitude and spatial distribution of elevated point-source emissions of VOC, $NO_x$, and CO
- Plots illustrating the temporal distribution of low-level emissions of VOC, $NO_x$, and CO (by component, total anthropogenic, and total anthropogenic and biogenic)
- Plots illustrating the temporal distribution of elevated point-source emissions of VOC, $NO_x$, and CO
- Tables summarizing emissions totals for VOC, $NO_x$, and CO (by component, total anthropogenic, and total anthropogenic and biogenic) for each UAM-V grid
- Tables summarizing emissions totals for VOC, $NO_x$, and CO (by component, total anthropogenic, and total anthropogenic and biogenic) for the potential nonattainment counties in the area of interest.

## Meteorological Input Preparation

### *Meteorological Input Requirements*

The UAM-V requires hourly, gridded inputs of wind, temperature, water-vapor concentration, pressure, vertical exchange coefficients ($K_v$), cloud-cover, and rainfall-rate. Meteorological inputs for this UAM-V application were prepared using the MM5 meteorological model. All meteorological inputs will be directly specified for UAM-V Grids 1, 2, and 3 (refer to Figure 4-1 for the grid definitions). This section summarizes the preparation of meteorological inputs using the MM5 modeling system.

### *Meteorological Data*

Meteorological data for the application of MM5 will be obtain from NCAR and will include the National Center for Environmental Prediction (NCEP) global analysis and surface and upper air wind, temperature, moisture, and pressure data for all routine monitoring sites within the domain. These include National Weather Service (NWS) sites, buoys, and a few international monitoring sites. Sea-surface temperature data will also be obtained from NCAR. These data comprise the standard data set for application of the MM5 modeling system and will be used for data assimilation as well as for the evaluation of the modeling results. In addition to these data, surface and upper-air data for a small number of additional monitoring sites within the domain (representing special study or facility-specific monitoring sites) will also be obtained and used for model performance evaluation as well as in the diagnosis of model performance problems.

## Meteorological Modeling Tools and Procedures

A general description of the MM5 meteorological model is found in Anthes and Warner (1978). The governing equations include the equations of motion, the continuity equations for mass and water vapor, and the thermodynamic equation. Those features relevant to this application are briefly described in this section.

The current version of MM5 can be applied in a non-hydrostatic mode for the improved simulation of small-scale vertical motions (such as those associated with the sea breeze and terrain effects). Use of this optional feature can be important to the accurate simulation of the airflow and other features at high horizontal resolution and will be utilized for this study.

The MM5 model employs the sigma vertical coordinate: $\sigma = (p - p_t)/(p_s - p_t)$, where $p$ is pressure, $p_t$ is the constant pressure specified as the top of the modeling domain, and $p_s$ is the surface pressure. The sigma-coordinate surfaces follow the variable terrain. Twenty vertical levels will be employed for this application such that the greatest vertical resolution is obtained within the boundary layer. Information on the vertical structure of the MM5 modeling domain is given in Table 4-1.

The governing equations are integrated over a grid that is staggered in the horizontal and vertical (Messinger and Arakawa, 1976). In the horizontal, the u and v wind components are calculated at points that are staggered with respect to those for all other variables. In the vertical, vertical velocity is defined at the sigma levels while all other variables are defined at intermediate sigma levels.

The MM5 modeling system also supports the use of multiple nested grids. This feature is designed to enable the simulation of any important synoptic scale features at courser resolution, while incorporating a high-resolution grid over the primary area(s) of interest. In this manner, the computational requirements associated with use of a high-resolution grid over a large domain are avoided. For this study, the MM5 modeling system will be applied for a much larger area than that used for the UAM-V modeling. The modeling domain was presented in Figure 4-2 and consists of an extended outer grid with approximately 108 km horizontal resolution and four inner (nested) grids with approximately 36, 12, and 4 km resolution, respectively. A Lambert Conformal map projection will be used for the application, to minimize the distortion of the grids within the area of interest. A one-way nesting procedure in which information from the simulation of each outer grid is used to provide boundary conditions for the inner grids will be employed.

To facilitate the realistic simulation of processes within the atmospheric boundary layer, variable surface parameters (including albedo, roughness length, and moisture availability) and a high-resolution planetary boundary layer (PBL) parameterization will be used for the simulations. The PBL parameterization also requires use of a multi-layer soil temperature model (an otherwise optional feature of MM5).

For the coarse grids, the Kain-Fritsch cumulus parameterization scheme (Kain and Fritsch, 1990) will be used to parameterize the effects of convection on the simulated environment. This feature will not be employed for the high resolution grids (AB and C) where an explicit moisture scheme (stable precipitation) will be used.

The MM5 model supports four-dimensional data assimilation (FDDA), a procedure by which observed data are incorporated into the simulation. FDDA option include (1) “analysis nudging” in which the simulation variables are relaxed or “nudged” toward an objective analysis that incorporates the observed data and (2) “obs nudging” in which the variables are nudged toward individual observations. These two approaches to FDDA are described in some detail by Stauffer and Seaman (1990) and Stauffer et al. (1991). For this study, analysis nudging will be used for all variables.

The data for preparation of the terrain, initial and boundary condition, and FDDA input files for this application will be obtained from NCAR. The MM5 input files will be prepared using the preprocessor programs that are part of the MM5 modeling system (Gill, 1992).

The MM5 modeling system was recently modified to include the output of the internally calculated vertical exchange coefficients ($K_v$). The $K_v$ values are intended to represent non-local or multi-scale diffusion coefficients (rather than local diffusion coefficients) as described by (Hong and Pan, 1995). This information will be used to specify the vertical exchange coefficients required by the UAM-V modeling system.

For each simulation period, the model will be initialized at 0000 GMT on the first day of the period. Thus, the MM5 simulation period will include a five-hour initialization period, before the output will be used to prepare inputs for the UAM-V model. For the three outer grids, the MM5 will be run continuously for the nine-day simulation period. For the higher-resolution grid, the model will be reinitialized after each three days of simulation. Each re-initialization will also include an additional 5-hour initialization period. Re-initialization times may vary based on a review of the simulation results. The input fields from each simulation will be inspected to ensure that piecing together the simulations does not create discontinuities in the meteorological inputs (the use of FDDA will alleviate this possibility).

The time step used for the simulations will range from several minutes for the outermost (approximately 108 km) grid to approximately 12 seconds for the innermost (approximately 4 km) grid.

The MM5 output will be postprocessed to correspond to the UAM-V modeling domain and the units and formats required by the modeling system using the MM52UAMV postprocessing software. Wind, temperature, water-vapor concentration, pressure, vertical exchange coefficient, cloud-cover, and rainfall-rate input files containing hourly, gridded estimates of these variables will be derived from the MM5 output. Surface temperature and solar radiation will be postprocessed for use in preparing the mobile-source and biogenic emissions estimates.

## *Quality Assurance of the Meteorological Inputs*

The MM5 simulation results will be evaluated using graphical and statistical analysis. A list of graphical and statistical products is included at the end of this section. The overall evaluation of the MM5 results will include the following elements. For the outer grids, examination of the MM5 output will focus on representation of the regional-scale meteorological features and airflow patterns and will include a comparison with weather maps as well as the items listed below. A more detailed evaluation of the results for the inner (high-resolution) grid will emphasize representation of the observed data, terrain-induced and other local meteorological features, and vertical mixing parameters. To the extent possible, the modeling results will be compared with observed data. In the absence of data, they will be examined for physical reasonableness as well as spatial and temporal consistency. Since data assimilation will be used, a comparison with the observed data primarily serves as a check on the data assimilation but can also reveal potential bias in the meteorological inputs. The ability of the MM5 model to reproduce observed precipitation patterns will be qualitatively assessed by comparing the simulated and observed rainfall patterns (based on NWS data). A detailed analysis of the timing and amount of the precipitation will not be performed.

The UAM-V ready meteorological inputs will also be plotted and examined to ensure that the characteristics and features present in the MM5 output are retained following the postprocessing step.

The following graphical summaries will be prepared to facilitate the review/evaluation of the meteorological inputs:

- 3-dimensional visualizations of the MM5 output using the WXPortal software (an enhanced version of VIS-5D)
- x-y cross-section plots of the MM5 wind fields for several levels and times with observations overplotted for MM5 Grids 1, 2, and 3
- x-y cross-section plots of the UAM-V ready wind, temperature, water-vapor concentration, vertical exchange coefficient, cloud-cover, and rainfall-rate fields for several times and levels (as appropriate).

If the plots or statistics suggest that certain of the features or components of the meteorology are not well represented by MM5, the MM5 application and postprocessing procedures will be reexamined, and additional modeling or processing may be conducted to improve this representation.

Evaluation of the meteorological inputs will continue as the diagnostic analysis and model performance evaluation proceeds. The process analysis feature of UAM-V will also be used to further examine the role of the meteorological inputs in determining the simulated concentration patterns and levels (and their contribution to good or poor model performance). If the UAM-V results suggest that certain of the features or components of the meteorology are not well represented by MM5, the MM5 application and postprocessing procedures will be reexamined, and additional modeling or processing may be conducted to improve this representation.

There are no specific criteria as to what constitutes an acceptable set of meteorological inputs. Similarly, there is no guarantee that the MM5 results will provide the basis for a successful modeling exercise. Problems that can be identified and corrected within the resource and time constraints of this study will be addressed. Others will be documented and recommendations for future applications will be developed.

## Air Quality Input Preparation

### *Air Quality Input Requirements*

There are three UAM-V air quality input files that define pollutant concentrations for each of the UAM-V state species (1) throughout the three-dimensional grid at the initial simulation time (coarse-grid only), (2) along the lateral boundaries of the modeling domain for each hour of the simulation period, and (3) along the top of the modeling domain for the entire simulation period.

## Air Quality Data

For each simulation period, pollutant concentration data for all monitoring sites located within the modeling domain will be obtained from the EPA Aerometric Information Retrieval System (AIRS) and will be supplemented with data from the CASTNET and SCION data collection programs. Species will include ozone, NO, $NO_2$, CO, and hydrocarbons, as available. It is expected that there will be fewer measurements of the precursors species, compared to ozone. Estimates of background concentrations of the various pollutants will be obtained from EPA (1991b).

## Air Quality Tools and Procedures

Preparation of the initial and boundary condition input files will entail the application of the air quality preprocessor programs included as part of the UAM-V modeling system. The model will be initialized at 0000 EST on the first day of each simulation period. Initial conditions will be obtained through the interpolation of observed data. Note that the degree to which the observations can represent the initial concentration fields will depend upon data availability. To avoid the unrealistic interpolation of the observed data to unmonitored areas, a homology mapping technique in which data from actual sites are assigned to the centroids of unmonitored counties will first be employed. Development and preliminary evaluation of this technique is described by Iwamiya and Douglas (1999). This will provide more complete geographical coverage for the interpolation; the resulting dataset used in the interpolation will consist of both actual and homologue monitors. This will provide more complete geographical coverage for the interpolation; the resulting dataset used in the interpolation will consist of both actual and homologue monitors. Initial conditions aloft will be set equal to EPA default values for each pollutant species.

The primary reason for using a nested-grid, regional-scale modeling configuration is to reduce the uncertainty in the boundary conditions for the area of interest. In this case, lateral boundary conditions need only be specified for the outermost (coarse-grid) domain. Top boundary conditions are specified for all domains in a single file. For this study, the lateral and top boundary concentrations for all pollutants will initially be set equal to continental background values. Recommended concentrations include 40 ppb for ozone, 1 ppb for $NO_x$ (0 ppb for NO; 1 ppb for $NO_2$), 25 ppb of hydrocarbons (divided among the lumped hydrocarbon species according to the default CB-V speciation profile), and 200 ppb of CO. All other species will be set equal to the EPA default concentrations given by EPA (1991b). The boundary condition value for ozone will be updated for each simulation day using a “self-generating” boundary condition estimation technique. Using this technique, an average ozone concentration from the upper layer of the modeling domain is calculated for the last hour of each day and is used to specify the ozone boundary value (along the lateral and top boundaries) for each subsequent day. In this manner, regional-scale build up of ozone can be represented in the simulation.

The lack of pollutant concentration data (especially aloft) as well as the length of the simulation periods precludes a more detailed specification of the boundary conditions. However, given the geographical extent of the modeling domain beyond the primary area of interest, the coarse-grid boundary conditions are not expected to significantly influence the simulation results within the area of interest. As noted in a subsequent section of the protocol document on diagnostic and sensitivity testing, this assumption will be tested as part of the modeling analysis.

### Quality Assurance of the Air Quality Inputs

Tabular summaries of the initial and boundary values for ozone, NO, $NO_2$, CO, and selected hydrocarbon species will be prepared. Stepwise quality assurance of the air quality input preparation procedures will also be conducted.

## Land-Use Input Preparation

### Land-Use Input Requirements

A gridded land-use file is required for the full domain and each subdomain.

### Land-Use Data

The surface characteristics file will be prepared using the latest available 200-m resolution land-use data obtained from the U.S. Geological Survey (USGS). Each of the categories in the USGS land-use database will be assigned to one of the 11 UAM-V categories. These include urban, agricultural, range, deciduous forest, coniferous forest (including wetlands), mixed forest, water, barren land, non-forest wetlands, mixed agricultural and range, and rocky (low shrubs). These data will be supplemented, to the extent possible, with more refined local data, if available.

### Land-Use Tools and Procedures

Preparation of the land-use input files (for the full domain and each subdomain) will entail the application of the land-use preprocessor program included as part of the UAM-V modeling system. The 200-m resolution data are aggregated to the grid cells and the percent distribution among the categories is calculated. The resulting distribution for grid cells along the Gulf Coast will be carefully examined and refined, as needed, to better reflect the high-resolution data along the land-water boundary.

### Quality Assurance of the Land-Use Inputs

Plots of the percentage distribution of land-use for each of the 11 land-use categories will be prepared and examined. Stepwise quality assurance of the land-use input preparation procedures will also be conducted.

## Chemistry Input Preparation

### Chemistry Input Requirements

Application of the UAM-V modeling system requires preparation of several additional input files that contain information on albedo, ozone column, photolysis rates, and chemical reaction rates. This information is required for the full domain and each subdomain.

## Ozone Column Data

For each simulation period, day-specific ozone column data will be obtained from the National Aeronautics and Space Administration (NASA).

## Chemistry Related Input Tools and Procedures

Preparation of the chemistry related input files will entail the application of the standard preprocessor programs included as part of the UAM-V modeling system. The range of ozone column values for the entire domain for each simulation period will be calculated for use in the photolysis rates preprocessor program. The haze parameter for UAM-V (aerosol optical depth) will be set to 0.094 (a value typical of rural conditions) for the entire modeling domain. Albedo will be specified according to land-use type (based on information contained in the surface file) by the albedo/haze/ozone column processor.

Chemical reaction rates, activation energies, and maximum/minimum species concentrations, as used in the validation of the CB-V chemical mechanism against smog chamber data, will be utilized along with appropriate updates for the enhanced treatment of radical-radical termination reactions and isoprene chemistry.

Photolysis rates will be calculated using JCALC preprocessor program, utilizing the values of albedo, haze, and total ozone column information discussed above.

## Quality Assurance of the Chemistry Related Inputs

The ozone column values and photolysis rates will be tabulated and examined. Stepwise quality assurance of the chemistry related input preparation procedures will also be conducted.

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# 6. Model Performance Evaluation

A typical application of the UAM-V modeling system for ozone air quality assessment purposes consists of several simulations, including an initial simulation and a series of diagnostic and sensitivity simulations (designed to examine the effects of uncertainties in the inputs on the simulation results, identify deficiencies in the inputs, and investigate the sensitivity of the modeling system to changes in the inputs). For each simulation, model performance is primarily assessed through graphical and statistical comparison of the simulated pollutant concentrations with observed data. The results of this comparison are used to guide the modeling analysis (through the determination of additional diagnostic and sensitivity simulations) and to assess whether the model is able to adequately replicate the air quality characteristics of the simulation period. Model performance evaluation tests and procedures are described in this section. Diagnostic and sensitivity analyses that may be performed to understand and improve model performance are discussed in Section 7.

EPA guidance (EPA, 1999) stresses the need to evaluate the model relative to how it will be used in the attainment demonstration; that is in simulating the response to changes in emissions. Various aspects of the model performance evaluation, such as assessment of the ability of the model to simulate weekday-weekend differences in concentration levels and patterns, detailed evaluation of the changes in process-level contributions, and comparison with air quality and emissions trends will be used to evaluate the reliability of the modeled response.

Once acceptable model performance is achieved (based on the results of the graphical, statistical, and sensitivity analysis), the simulation is subsequently referred to as the base-case simulation. The establishment of a base-case simulation is integral to the reliable use of the modeling system to assess the effects of changes in emissions on future air quality.

This section of the protocol document describes the procedures to be used to evaluate model performance.

## Model Performance Data

Data from all air quality monitoring sites within the ATMOS modeling domain will be used in the evaluation of model performance. For the most part, these include measurements of ozone, NO, $NO_2$, $NO_x$, and CO for routine monitoring sites (including photochemical assessment monitoring sites, PAMS) located throughout the region (and primarily in the urban/nonattainment areas). These data will be obtained from AIRS. We will supplement this database with data from the CASTNET and SCION monitoring program. Several CASTNET and SCION monitors are located throughout the Southeast. Data from these sites will typically include higher resolution $NO_x$ measurements (compared to the routine monitoring sites) and may also include measurements of hydrocarbon species. Data from special studies commensurate with the simulation periods will also be solicited and incorporated as time and resources permit. Note that the analysis and use of special-study data can sometimes be very resource intensive.

## Model Performance Objectives

As noted earlier, the overall objective of a model performance evaluation is to establish that the modeling system can be used reliably to predict the effects of changes in emission reductions on future-year ozone air quality and to evaluate the effectiveness of possible attainment demonstration strategies. Specific objectives for the ATMOS study include: (1) ensuring that the regional-scale modeling results provide appropriate boundary conditions for the primary area of interest (Grid 3), (2) ensuring that the ozone concentration patterns and levels and the day-to-day variations in these are well represented, and (3) ensuring that the modeling system exhibits a reasonable response to changes in the inputs (and that the inputs do not contain significant biases or compensating errors).

## Model Performance Evaluation Procedures

The evaluation of model performance will follow the general procedures outlined in this section. Variations to these may be proposed and incorporated during the course of the study to address specific issues that arise. All additions/changes will be discussed with the ATMOS Technical Committee.

### *Model Performance Evaluation Components*

The evaluation of model performance will include both qualitative and quantitative components. For each simulation conducted as part of the base-case modeling analysis, a variety of graphical and statistical analysis products will be prepared. These are listed and described in the remainder of this section and will provide the basis for the model performance evaluation. The analysis and integration of these results, relative to the objectives (as given earlier in this section), will complete the evaluation of model performance.

### *Geographical Considerations*

The simulation results for the full domain and each subdomain will be examined using a variety of graphics, metrics, and statistics (these are summarized later in this section). Analysis of results for the coarse-grid (36 and 12-km resolution) domains will emphasize representation of the regional-scale concentration levels and patterns, as well as day-to-day variations in regional-scale air quality. Statistics will be calculated for the coarser grids, but are not expected to be very meaningful for the scale represented by these grids (due to the fact that the data are representative of a much smaller scale). A more detailed analysis of the results will be performed for the high-resolution (4-km) grid and subregions thereof. This will include the analysis of the magnitude and timing of site-specific concentrations (1-hour and 8-hour), a more rigorous statistical evaluation (compared to the coarser grids), and the use of process analysis (for selected simulations for all or portions of Grid 3).

### *Temporal Considerations*

The ability of the modeling system to depict the day-to-day differences in ozone concentration, as indicted by the observations, will be examined for each domain and episode period. Diurnal variations in ozone for the coarser grids will be examined relative to the boundary condition estimates for the finer grids. Site-specific, hourly variations for ozone and precursor species will be examined (using time-series plots and statistical measures) for sites within the high-resolution domains.

The analysis of model performance will focus on 1-hour concentrations of ozone and other species, since the data are typically reported as hourly values. However, the ability of the model to represent maximum 8-hour ozone concentration is related to its ability to represent the hourly values that comprise the 8-hour maximum. Thus, a comparison of maximum 8-hour average ozone concentration will also be performed for the high resolution grids.

As the modeling study progresses, variations in model performance among the simulation periods will also be examined. Specifically, differences in model performance among the simulation periods will be documented and reasons for the differences will be examined.

## *Species*

All relevant species represented by the observed data within the high-resolution domains will be included in the model performance evaluation. We will also consider the calculation of ratios or other derived parameters. The use and interpretation of ratios will be based on discussions with the ATMOS Technical Committee.

## *Summary of Graphical Displays, Metrics, and Statistical Parameters*

Graphical displays and statistical/tabular summaries of the UAM-V simulation results will provide the basis for model performance evaluation and will be used to guide the interpretation and use of the UAM-V simulation results. For each simulation performed as part of the base-case modeling analysis, the graphical displays and tabular summaries will include:

- Isopleth plots of daily maximum simulated ozone concentration (1-hour and 8-hour), with observed values overplotted for all UAM-V grids
- Time-series plots (with range shading) of hourly ozone, NO, $NO_2$, $NO_x$, VOC, and CO concentrations for each monitoring site (and possibly other unmonitored locations) within Grid 3
- Scatter plots of hourly ozone (and possibly NO, $NO_2$, $NO_x$, VOC, and CO concentrations and selected indicator species) for monitoring sites within Grids 1, 2, and 3
- Scatter plots of 8-hour maximum ozone concentration for each monitoring site within Grids 1, 2, and 3
- Scatter plots comparing the time of the simulated and observed 8-hour maximum ozone concentrations for each monitoring site within Grids 1, 2, and 3
- Standard SAI list of 20 metrics and performance statistics for 1-hour ozone (as listed in Table 6-1, these include various max, min, mean, accuracy, bias, error, residual, and ratio-based parameters) for Grids 1, 2, and 3
- EPA recommended average accuracy statistics for 8-hour ozone
- Time-series plots and bar charts of selected metrics and statistics for ozone for Grids 1, 2, and 3
- Animations of simulated ozone concentrations for selected grids/levels (and selected simulations).

These plots and tabular summaries will be used to display/convey the results of a single simulation or to compare two different simulations, as appropriate. In the latter case, the plots and animations may be presented as concentration differences.

If the UAM-V process-analysis technique is employed for a given simulation, the process-analysis results (for ozone, $NO_x$, and VOC) will be displayed using SAI's standard 3-panel plots which show the hourly contribution (separately and cumulatively) and the daily net contribution for each simulation process. These will be used to display the results of a single simulation or to compare two different simulations, as appropriate.

## Determination of Acceptable Model Performance

An integrated assessment of the above information (obtained as part of the base-case modeling analysis) will be used to document and qualitatively and quantitatively assess whether an acceptable base-case simulation has been achieved. Certain of the statistical measures will be compared to the EPA recommended ranges for acceptable model performance for urban-scale photochemical model applications. EPA has provided ranges for three key statistical measures for 1-hour ozone. The measures and recommended ranges are as follows: unpaired accuracy of the peak concentration (± 20 percent), normalized bias (± 15 percent), and normalized gross error (35 percent). We will also examine the average accuracy of the peak concentration and compare this with the range for the unpaired accuracy. These criteria are most applicable for the assessment of model performance for the high-resolution grid and/or selected urban-scale subregions thereof. However, they will also be used to guide the assessment of model performance for the regional-scale domains (Grids 1 and 2). The additional statistical measures recommended by EPA in the draft guidance for 8-hour ozone modeling will also be calculated and compared with the recommended ranges. These include the domain-wide average accuracy of the 8-hour ozone peak and the site-specific average accuracy of the peak over all simulation days. The recommended range for both of these measures is ± 20 percent. The 8-hour statistics will be calculated for the high-resolution grid and selected subregions only.

## Use of Model Performance Results to Guide the Interpretation and Use of Modeling Results in the Attainment Demonstration

Information obtained as part of the model performance evaluation will be carried through the analysis and used to guide the interpretation and use of the results in the attainment demonstration. A simple example of such use is the case where ozone concentrations are overestimated for one or more sites in the base-case simulation. It is possible that the overestimation could affect the response of the modeling system to emissions changes. If the site(s) for which ozone is overestimated show a different result in the attainment demonstration than most other sites, and there are no other apparent reasons for these differences, the overestimation might explain the different response. This would be further examined and possibly offered as “weight of evidence”. As a second example, differences in model performance among days or episodes might cause a different weighting of the results in the attainment demonstration analysis.

**Table 6-1. Standard List of UAM-V Simulation Metrics and Performance Statistics.**

| |
|---|
| Number of data pairs |
| Maximum domain-wide simulated value |
| Max. station-wide sim. value |
| Maximum observed value |
| Domain-wide unpaired accuracy |
| Station-wide unpaired accuracy |
| Average accuracy of peak |
| Normalized bias |
| Normalized gross error |
| Fractional bias |
| Fractional gross error |
| Ratio of bias to mean observation |
| Ratio gross error to mean observation |
| Maximum residual |
| Minimum residual |
| Mean unsigned error |
| Mean residual |
| Mean simulated value |
| Mean observation |
| Root mean square error |
| Standard deviation of fractional bias |

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# 7. Diagnostic and Sensitivity Analysis

In accordance with EPA guidance, diagnostic and sensitivity analysis will be used in this study to:

- better understand the simulation results
- obtain information that will help to prioritize efforts to improve/refine model inputs
- obtain insights in the effectiveness of various control strategies
- assess the "robustness" of a control strategy.

The first two bullet items pertain to the base-case modeling analysis and are addressed in this section of the protocol document. The latter two items pertain to the future-year analysis and are addressed in Sections 8 and 9, respectively.

The number and nature of the diagnostic and sensitivity simulations performed as part of the base-case modeling effort will likely vary by episode, based on the inputs and/or assumptions used in preparing the inputs and the simulation results (for the initial and diagnostic/sensitivity simulations). They will include simulations incorporating modification or refinement of the inputs as well as a detailed analysis of the simulation processes (using the process analysis feature of UAM-V).

## Determination of Appropriate Diagnostic/Sensitivity Simulations

The exact simulations to be performed for each simulation period will be determined based on a review of the initial (and subsequent diagnostic/sensitivity) simulations results or knowledge of sources of uncertainty in the inputs. Up to four diagnostic/sensitivity simulations (not including the future-year emission sensitivity simulations described in Section 8 of the protocol document) will be performed for each simulation period. At least one simulation will investigate the use of "clean" values (as defined in Section 5) for the coarse-grid boundary conditions. Design of the simulations will consider the eventual use of the modeling results in the relative sense (in the attainment demonstration). Specification of the diagnostic and sensitivity simulations will be made in conjunction with the ATMOS Technical Committee.

## Diagnostic/Sensitivity Analysis Procedures

All diagnostic and sensitivity simulations will be conducted using the general procedures outlined in Section 5 and 6 of the protocol document. Per EPA guidance, adjustment to the inputs to improve model performance will be within reasonable bounds. Review of the results will consider the possible effects of any modifications on the calculation of relative reduction factors in the attainment demonstration.

## Use of the Diagnostic/Sensitivity Analysis Results

The results of the diagnostic and sensitivity analyses may be used to (1) modify or enhance inputs, (2) improve model performance, and (3) guide the interpretation and use of the modeling results in the attainment demonstration. Errors in the inputs that are uncovered as part of the diagnostic/sensitivity analysis will be documented and corrected. Adjustment to the inputs to accommodate uncertainty will be within reasonable bounds and will not be commensurate with poorer model performance (EPA, 1999). For example, as noted in Section 5, the UAM-V results may indicate that additional review of the meteorological inputs, re-application of the MM5, or re-postprocessing of the MM5 output is required. All such modifications/adjustments to the inputs will be technically justifiable, and will be documented. Finally, information obtained as part of the diagnostic/sensitivity analysis will be carried through the analysis and used to guide the interpretation and use of the results in the attainment demonstration. For example, if we find as part of the diagnostic analysis (using process analysis) that high simulated ozone concentrations in a given portion of the domain are due to advection of precursors into the area, we would design the control strategy to include emission reductions in the upwind area. Process analysis could then be used to assess whether the reductions were sufficient/beneficial for 8-hour ozone attainment.

# 8. Future-Year Modeling

Once an acceptable base case has been achieved, the UAM-V can be used to predict future-year air quality and to evaluate the effectiveness of attainment strategies. In this section, we summarize the procedures to be followed in conducting future-year modeling to support an attainment demonstration for the ATMOS areas of interest.

## Selection of a Future Year

The ATMOS EAC attainment demonstration will be performed for the year 2007, and a maintenance simulation will be performed for 2012 to assess the effects of growth. This is consistent with EPA guidance regarding 8-hour attainment demonstrations for traditional nonattainment areas.

## Future-Year Emission Inventory Preparation

The future-year modeling for the ATMOS EAC modeling will focus primarily on the year 2007. Prior to preparing the 2007 inventory, a “current” year inventory for 2001 will be prepared for the 1999 episode. This will put both episodes on the same current year and will allow for the calculation of the future-year design value using a consistent base-year design value. To prepare the future baseline inventory for 2007, we will apply growth and control factors to the 2001 base-year emission inventory. To the extent that such data are available, growth and control factors will be obtained from the states of Arkansas, Tennessee, and Mississippi. In the absence of state-specific data, default growth projections prepared by the Bureau of Economic Analysis (BEA) or the Economic Growth Analysis System (EGAS) will be applied based on 2-digit SIC code for point sources and on the EPS 2.5 default projection factor assignments by source category code for area and mobile sources. The control factors to be applied will represent reductions in emissions that should occur as a result of existing control regulations. For mobile sources, VMT estimates provided by EPA for each of the states for 2007 will be used along with the MOBILE model to estimate mobile emissions. Again, state-specific or local data will be used to the extent available.

The future-year baseline emissions inventory will be prepared in accordance with EPA guidance, *Emissions Inventory Guidance for Implementation of Ozone and Particulate Matter National Ambient Air Quality Standards (NAAQS) and Regional Haze Regulations* (EPA-454/R-99-006, April 1999), and will incorporate emission reductions associated with the $NO_x$ SIP Call and the Tier II low-sulfur fuels and vehicle standards program.

## Specification of Other Inputs for Future-Year Simulations

With the exception of the emission inventories (and the boundary conditions which are “self-generating”), all inputs for the future-year simulations will be identical to those for the corresponding base-case simulation.

## Future-Year Modeling

The objective of the future-year modeling exercises is to evaluate the likelihood of future-year compliance with the 8-hour ozone NAAQS and, as necessary, assess the effectiveness of various control strategies to improve ozone air quality in the Nashville, Knoxville, Chattanooga, Memphis, and Tri-Cities EAC areas, and Putnam, Haywood, and Lawrence county EAC areas. The future-year modeling analysis will include a future-year baseline simulation, a series of "across-the-board" emission sensitivity simulations, and specific control- or attainment-strategy simulations. The present modeling analysis includes the establishment of a 2007 baseline simulation, a series of approximately XX across-the-board emission sensitivity simulations and approximately XX control-strategy simulations.

## *Future-Year Baseline Simulation*

The future-year baseline simulation incorporates the effects of population and industry growth (or, in some cases, decline) as well as national or statewide control measures or programs that are expected to be in place by the attainment date. The future-year baseline emissions inventory is based on typical summer day emissions, with adjustments for source-specific and episode-specific information. The baseline simulation results provide the starting point for assessment of the effects of further emission reductions on future ozone air quality.

## *Emissions-Based Sensitivity Simulations*

One of the objectives of the future-year modeling exercises is to evaluate the likelihood of future-year compliance with the 8-hour ozone NAAQS and, as necessary, assess the effectiveness of various effective control strategies to improve ozone air quality in the ATMOS area, in general, and in each of the EAC areas, in particular. This will be accomplished by first conducting a series of emission reduction sensitivity simulations. As part of the ATMOS analysis of the 1999 episode, a series of emission reductions simulations have been conducted for a future- baseline year of 2010. Much of what has been learned in these sensitivity simulations for the 1999 episode will be utilized in designing sensitivity simulations for the second ATMOS episode (June 2001).

The sensitivity analysis will involve an initial set of simulations reflecting simple, across-the-board emission reductions from the established 2007 baseline inventory. The modeling effort may include a number of across-the-board emission sensitivity simulations involving varying reductions in VOC and $NO_x$ emissions. An example set of sensitivity simulations is as follows:

- 15 percent reduction in anthropogenic VOC emissions
- 15 percent reduction in anthropogenic $NO_x$ emissions
- 35 percent reduction in anthropogenic VOC emissions
- 35 percent reduction in anthropogenic $NO_x$ emissions
- 15 percent reduction in anthropogenic VOC emissions and 35 percent reduction in anthropogenic $NO_x$ emissions
- 35 percent reduction in anthropogenic VOC emissions and 15 percent reduction in anthropogenic $NO_x$ emissions
- 35 percent reduction in anthropogenic VOC and $NO_x$ emissions.

The final set and number of simulations to be performed will be determined in consultation with the ATMOS Operations Committee. The results of the emission sensitivity simulations will be compared with the 2007 baseline simulation results using difference plots and through comparison of the metrics to determine the relative effectiveness of the different types and amounts of emission reductions, as well as any synergistic effects (i.e., the decrease in maximum 8-hour ozone concentration obtained from the combined VOC and $NO_x$ reductions may be greater than the sum of the decreases when the emission reductions are applied separately). Approximately 12 emission sensitivity simulations (of varying complexity) will be conducted.

### *Control-Strategy Simulations*

On the basis of the results of the emission reduction sensitivity modeling, control strategy options will be identified, simulated, and evaluated in this task. Draft guidance for demonstrating attainment of the 8-hour NAAQS has been developed by EPA. This guidance will provide the methodologies to be followed in conducting a modeling attainment demonstration, as described in more detail in Section 9 of the protocol document.

The control scenarios to be simulated will likely involve a combination of reductions from all source sectors including mobile, area, and point sources. The various options can be evaluated in terms of the cost effectiveness of reducing future-year ozone concentrations. The simulation results will be presented with the graphical and statistical tools used for the sensitivity modeling analysis. Special products will be prepared, if necessary, to meet the reporting requirements for the attainment demonstration exercise as outlined in the EPA guidance document. Up to six control strategy simulations (of varying complexity) will be performed.

## Display and Presentation of Future-Year Simulation Results

Graphical displays and statistical/tabular summaries of the UAM-V simulation results will be used to assess the future-year simulation results (and to compare the base- and future-year ozone concentrations). The graphical displays and tabular summaries will include:

- Isopleth and isopleth difference (2007 minus 1999) plots of daily maximum simulated 1-hour and 8-hour ozone concentration
- Animations of simulated ozone concentrations and concentration differences for selected simulations
- Interactive ACCESS™ database (referred to as ACCESS™ Database for Visualizing and Investigating Strategies for Ozone Reduction or ADVISOR) containing information for review, comparison, and assessment of the simulation results by all study participants. The database will contain both emissions and simulated ozone concentrations (as represented by several different metrics) for all grids and selected subregions of the domain. Users will be able to view (and extract) the data in spreadsheet format and to create plots, the contents of which will reflect various user-specified options.

  Metrics will include:

  - maximum 1-hour ozone concentration (ppb)
  - maximum 8-hour ozone concentration (ppb)
  - number of grid cell · hours with maximum 8-hour ozone concentrations ≥ 85 ppb

- number of grids cells with daily maximum 8-hour ozone concentrations ≥ 85 ppb
- total ozone exposure (ppb · grid cell · hour)
- exceedance ozone exposure (ppb · grid cell · hour) for concentrations ≥ 85 ppb
- population exposure (to concentrations ≥ 85 ppb)
- total emissions ($NO_x$, VOC)

Options for displaying the metrics will include:

- value
- difference (relative to a selected base simulation)
- effectiveness (change in ozone metric relative to the change in emissions, again relative to a selected base simulation)

Geographies will include:

- Grid 1: Outer 36 km X 36 km grid
- Grid 2: Intermediate 12 km X 12 km grid
- Grid 3: Inner 4 km x 4 km inner grid
- Sumner, Davidson, Wilson, & Rutherford Counties, TN (Nashville)
- Knox, Anderson, Jefferson, Sevier, and Blount Counties, TN (Knoxville)
- Shelby, DeSoto, and Crittenden Counties (Memphis)
- Shelby County, TN
- DeSoto County, MS
- Crittenden County, AR
- Lee County, MS (Tupelo)
- Pulaski County, AR (Little Rock)
- Hamilton County, TN; Walker and Catoosa Counties, GA (Chattanooga)
- Nashville EAC Area: (Davidson, Rutherford, Sumner, Williamson, Wilson, Cheatham, Dickson, and Robertson counties)
- Knoxville EAC Area: (Anderson, Blount, Know, Loudon, Sevier, Union, and Jefferson counties)
- Chattanooga EAC Area: (Hamilton, Marion and Meigs, counties (Tennessee), and Walker and Catoosa counties, (Georgia))
- Memphis EAC Area: Shelby, Tipton, and Fayette counties (Tennessee); Crittenden County, (Arkansas); De Soto County, (Mississippi)
- Tri-Cities EAC Area: (Carter, Hawkins, Johnson, Sullivan, Unicoi, and Washington counties)
- Haywood County
- Lawrence County
- Putnam County

In addition to these specific areas, the ozone monitoring sites in the ATMOS Grid 3 will also be included in the ADVISOR database.

The future-year modeling results will also be reviewed using the procedures outlined in the EPA guidance document on the use of models and other analyses in attainment demonstrations for the 8-hour ozone NAAQS.

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# 9. Attainment Demonstration

The procedures to be followed in conducting the attainment demonstration analysis are outlined in this section of the protocol document. The attainment demonstration analysis for the ATMOS EAC study will include application of the new modeled attainment test (EPA, 1999) as well as other corroborative analyses. As this 8-hour modeling guidance is still in draft form, we will adapt the final attainment demonstration procedures to reflect any changes to the draft guidance that might be issued by EPA in time for use in this study. Given that the results of the modeling analysis are unknown at this time, the details of the corroborative analyses cannot be specified. However, the general approach to identifying and conducting such analyses is presented. The present modeling analysis includes the preparation of the ADVISOR database to support the application of the attainment demonstration procedures.

## Geographical Considerations

The ATMOS ADVISOR database and associated analysis procedures outlined in this and the previous section are designed to support a separate 8-hour attainment demonstration analysis for each of the areas of interest (as required by the pending nonattainment designations). The current list of areas includes the Nashville, Knoxville, Chattanooga, Memphis, and Tri-Cities EAC areas, and Putnam, Haywood, and Lawrence county EAC areas. For each area of interest, the analysis will include the modeled attainment test, any requisite screening tests, and additional corroborative analysis.

## Modeled Attainment Test

The modeled attainment test as described in the draft EPA guidance on 8-hour ozone attainment demonstrations (EPA, 1999) will be included along with all base- and future-year simulation results in the ATMOS ADVISOR database. Key implementation issues are presented and discussed in this section.

An important component of the attainment test is the calculation of a relative reduction factors (RRF) for each site and each simulation day, for each relevant (attainment demonstration) simulation. The RRF represents the ratio of the future-year daily maximum 8-hour ozone concentration to the corresponding base-year value. It is calculated for each site using simulated ozone concentrations within the “vicinity” of the site. For the 4-km ATMOS subdomain, “vicinity” will be defined as within one grid cell of the grid cell in which the monitoring site is located. That is, the nine grid cells surrounding a monitoring site will be included. For the 4-km grid this results in a radius of influence of approximately 4 km.

This radius of influence is smaller than that suggested in the EPA guidance document; however, there are good technical reasons to refine the default definitions given the EPA guidance document. Use of a 15-km radius of influence, as recommended by EPA, would mean that the influence zone for a number of sites would encompass (or nearly encompass) other nearby sites. This would occur in all three primary areas of interest, and for sites that exhibit very different concentration characteristics during the episode period. For example, several of the Knoxville area monitoring sites are located with 15 km of one another but at very different elevations. As a result they frequently experience very different ozone peaks. The use of a more limited (4 km) radius of influence, in this case, would accommodate the geographic and meteorological variability and the observed concentration gradients.

Use of a smaller value than the EPA default will ensure that the sites are considered independently from one another, and will preserve the site-specific nature of the attainment-demonstration exercise. This is important in the context of an attainment demonstration that is based on site-specific design values. In using the simulation results to adjust site-specific design values, it is important that the simulation results reflect the concentration characteristics of specific sites (not other nearby sites, as would be the case with the larger radius of influence).

The RRF for a given monitor will be calculated using the grid-cell level simulated maximum 8-hour ozone concentration in the vicinity of the monitor, as defined above. The grid cell containing this value may be different for the base year and the future year, since changes in emissions can alter the timing of the chemistry and the location of the maximum value. This approach is also consistent with the use of a high-resolution grid, since relocation of the maximum to a different grid cell in the vicinity of a monitoring site will not represent a large spatial shift.

The RRF can be calculated for a single day or as an average over multiple days. The ADVISOR database is designed to allow the user to specify which simulation days will be included in the calculation of the RRF. The user may select the day(s) directly or use one of three “automated” day selection options. These include (1) for each simulation day for which the simulated maximum 8-hour ozone value is greater than a user-specified value (including the EPA recommended default of 70 ppb), (2) for all observed 8-hour ozone exceedance days, and (3) for all days for which the base-case simulation results are within a user-specified range of model performance.

The estimated design value (EDV) for each site is then calculated by multiplying the RRF by the site-specific design value. In the ADVISOR database, the user will be able to select any of the design values from the period 1997 through 2002, or the maximum of these. The predicted future design value for each area will then be the maximum of the values for the monitoring sites within the area. If this value is less than 85 ppb, the test is passed.

Use of the 2000-2002 design value is consistent with date of the new June 2001 episode and the use of the 1999 episode with a “current year” 2001 inventory.

## Screening Test

For unmonitored areas within the modeling domain that consistently exhibit simulated exceedances of the 8-hour NAAQS, the EPA recommended screening test will be applied. To apply the screening test to the regional-scale ATMOS domain, we will first define subregions within the domain (encompassing each EAC areas). Within these subregions, we will then adopt the EPA definition of “consistently”[10] to identify locations for application of the screening test. The screening test will be applied using the mean design value for the subregion in which the unmonitored-area exceedance is consistently simulated. The predicted future design value for each area will then be the maximum of the values for all monitored and unmonitored “sites” within the subregion or area. If this value is less than 85 ppb, the test is passed.

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[10] Daily maximum 8-hour daily ozone at the location in question is more than five percent higher than near any monitored location on 50 percent or more of the modeled days.

## Other Components of the Weight of Evidence Determination

If the modeled attainment and screening tests are passed or nearly passed, states may opt to include additional analyses as part of a "weight of evidence" determination. Current EPA guidance does not encourage a weight of evidence determination if the predicted design value for a given area is greater than or equal to 90 ppb. The specific analyses to be performed for each area will be determined based on the findings and results of the modeling analysis as well as a review of available data and information. EPA (1999) suggests some core analyses. However, the currently available air quality data do not support the reliable use of observation-based models.

Per EPA guidance, the weight of evidence analysis will include additional analysis of the model output for each nonattainment area including (1) relative change in grid-cell-hours with maximum 1-hour ozone concentrations greater than or equal to 85 ppb, (2) relative change in the number of grid cells with 8-hour ozone concentrations greater than or equal to 85 ppb, and (3) relative change in the amount by which the 8-hour NAAQS is exceeded by 1-hour simulated concentrations. Note that each of these will be included in the ADVISOR databases described in Section 8. A large reduction in these metrics would support a weight of evidence argument. In all cases, EPA guidance suggests that a value of 80 percent should be considered to be a large reduction.

A primary objective of the weight of evidence analyses is to use other methods to corroborate the modeling results or to independently assess the potential for attainment. Considerations in designing these analyses include:

- potential or expected effects of model performance problems or other modeling related uncertainties (e.g., emission projection factors) on the outcome of the modeled attainment and screening tests
- representativeness of days as characterized by the episode selection analysis (e.g., are all key regimes represented? are days for which attainment is not simulated included among the key regimes/design-value days?)
- other uses of the observational data (e.g., trends analysis).

## Use of Modeling and Corroborative Evidence to Demonstrate Attainment

The attainment demonstration for each area will require an integrated analysis of the modeling results and any corroborative evidence. The relative "weight" of each will be based on an assessment of the confidence (or degree of uncertainty) in the analysis procedures and results (e.g., data completeness, reliability of the methodology, relevant assumptions, credibility of the results), to the extent this can be established.

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# 10. Documentation

A final report describing the modeling/analysis methods and results will be prepared. A single report will be prepared; however, the results for the individual areas of interest will be presented separately. Preparation of this document is described in this section.

## EPA Recommended Elements

Each of the recommended subject areas will be addressed in the final report. These include:

- modeling/analysis protocol
- emissions preparations and results
- air quality/meteorology preparations and results
- performance evaluation for air quality simulation model (and other analyses)
- diagnostic tests
- description of the strategy demonstrating attainment
- data access
- weight of evidence determination
- review procedures used.

The purpose of and issues associated with each subject area is summarized in the EPA guidance document (EPA, 1999).

## Outline for Final Report

A draft outline for the final report follows:

Executive Summary (including a discussion of the conceptual description of the 8-hour ozone nonattainment problem for each area of interest)

**I. Introduction**
  A. Background and objectives
  B. Modeling grid specification
  C. Episode selection/simulation periods
  D. Characterization of meteorology and air quality of the modeling episodes
**II. Modeling Protocol**
**III. Base-Case Modeling Emission Inventory Preparation**
  A. Emissions data
  B. Overview of emissions processing procedures
  C. Preparation of the area and non-road emission inventory component
  D. Preparation of the mobile-source emission inventory component
  E. Preparation of point-source emission inventory component

- F. Estimation of biogenic emissions
- G. Quality Assurance
- H. Summary of the Modeling Emission Inventories

**IV. Meteorological Modeling and Input Preparation**

- A. Overview of the MM5 meteorological modeling system and application procedures
- B. Presentation of results/model performance evaluation
- C. Preparation of UAM-V ready meteorological fields
- D. Quality assurance

**V. Air Quality, Land-Use, and Chemistry Input Preparation**

- A. Air quality related inputs
- B. Land-use inputs
- C. Albedo/haze/ozone column
- D. Chemistry parameters
- E. Quality assurance

**VI. Model Performance Evaluation**

- A. Initial simulation results
- B. Diagnostic and sensitivity analysis
- C. Summary of base-case model performance

**VII. Future-Year Modeling Exercises**

- A. Future-year emission inventory preparation
- B. Future-year boundary conditions preparation
- C. Future-year baseline simulation results
- D. Emission sensitivity simulation results
- E. Control-strategy simulation results

**VIII. Attainment Demonstration** *(this will include a subsection for each area of interest and will be completed based on the attainment demonstration runs following final EPA guidance)*

- A. Description of the attainment strategy
- B. Modeled attainment and screening test results
- C. Additional analysis
- D. Methods
- E. Results
- F. Repeat for each type of additional analysis
- G. Integrated weight of evidence analysis

**IX. Summary of review procedures used**

**X. Data access procedures**

**References**

# 11. Summary of Deliverables and Schedule

The following is a list of major deliverables and a schedule for their completion:

| | |
|---|---|
| Draft modeling protocol document | 23 May 2003 |
| Final modeling protocol document | 2 weeks after receipt of final comments from EPA (20 June 2003?) |
| Updated modeling protocol document | As needed |
| Draft final report | 1 December 2003 |
| Final report | 4 weeks following receipt of comments from ATMOS technical committee |
| Modeling tools and databases | 31 December 2003 |

A schedule for the modeling analysis was provided in Figure 1-2.

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# 12. Archival/Data Acquisition Procedures

The data, input, and output files for the modeling analysis will be available in electronic format. Interested parties should contact the ATMOS Operations Committee chairpersons for information on how to obtain these files. The modeling tools to be used for this study (with the exception of the BEIS and MOBILE models and the CART statistical analysis software, which can be obtained from EPA or other sources) will be included in the deliverables from SAI.

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