



June 7, 1993

Ms. Brenda Johnson
Air, Pesticides and Toxics Management Division
Region IV
U.S. Environmental Protection Agency
345 Courtland Street
Atlanta, Georgia 30365

Re: Draft Protocol for UAM-V

Dear Ms. Johnson:

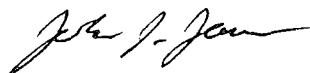
As was agreed at the May 11th meeting discussing the possible use of UAM-V for Atlanta, Systems Applications International (SAI) has prepared a draft protocol for applying UAM-V to the Atlanta area. The draft modeling protocol is enclosed for your review.

Where appropriate, the draft protocol adopts language from the EPA-approved modeling protocol prepared by the Georgia Environmental Protection Division (EPD). New material has been added describing the procedure for evaluating UAM-V against UAM-IV and for determining the acceptability of UAM-V for the Atlanta ozone attainment demonstration. Pursuant to EPA's suggestions, SAI has proposed a scoring system to judge UAM-V's performance against UAM-IV's performance for the relevant regulatory episodes and for one SOS episode (contingent upon SOS data availability).

As we discussed last Friday, we will be expecting comments back from EPA by June 30, 1993. We will then revise the protocol and, if all parties agree, the Georgia EPD will submit the final version to you for formal EPA Region IV approval.

In the meantime, if you have any questions about the draft protocol, please feel free to call me at 205/877-7698 or SAI's Shep Burton at 415/507-7101.

Sincerely,



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**PROTOCOL FOR APPLYING UAM-V TO THE ATLANTA AREA
TO SUPPORT THE DEVELOPMENT OF THE OZONE SIP**

June 4, 1993

Prepared by

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INTRODUCTION

This protocol outlines the methodologies to be followed in applying a modified version of the Urban Airshed Model (UAM), known as UAM-V, to the Atlanta ozone nonattainment area to support the development of the State Implementation Plan (SIP). Because the UAM-V model is being proposed as an alternative to the current regulatory version, UAM-IV, the protocol presents the procedures to be followed in (1) applying both UAM-V and UAM-IV for selected episodes, (2) assessing and comparing the performance of the models, and (3) determining the acceptability of UAM-V as a replacement for UAM-IV. Included in the protocol are details regarding the management structure of the modeling study, participating organizations, specifications for input preparation procedures, domain size and resolution specifications, performance evaluation and model comparison procedures, and the evaluation of emission reduction strategies for the attainment demonstration. (It should be noted that sections of this protocol have been obtained from the original September 1992 version of the UAM-IV protocol developed by the State of Georgia, (GDNR, 1992)).

BACKGROUND

The Clean Air Act Amendments of 1990 mandate that certain ozone nonattainment areas support the development of SIPs with photochemical models, such as EPA's Urban Airshed Model (UAM). Because Atlanta has been designated a serious ozone nonattainment area by the EPA, the State of Georgia has committed to performing an attainment demonstration using UAM. Under the 1990 Clean Air Act Amendments, photochemical grid modeling is required for serious, severe, and extreme ozone nonattainment areas and multi-state moderate ozone nonattainment areas. In accordance with the CAAA, all nonattainment areas designated moderate or above, have until November 1993 to submit a plan reflecting a 15 percent reduction in volatile organic compound (VOC) emissions from 1990 to 1996, and for those areas required to do modeling, until November 1994 to submit a revised SIP demonstrating, through modeling, attainment of the NAAQS for ozone. Serious nonattainment areas have until 1999 to reach attainment of the ozone standard.

The current regulatory version of the UAM (UAM IV, Version 6.2) incorporates the latest version of the Carbon-Bond Mechanism and other modifications that have been made to the model since its release in 1990. When applied in urban areas, the UAM typically employs a horizontal grid resolution of 4-6 km and 4 or 5 vertical layers with varying thicknesses. Depending on the meteorological conditions of the episode being simulated and the size of the UAM modeling domain, any transport of ozone or ozone precursors into the modeling domain must be estimated by the boundary condition concentrations. Prescription of boundary condition information for many applications of UAM-IV will be supported with the use of EPA's Regional Oxidant Model (ROM).

The latest version of the UAM (UAM-V) incorporates many new features including variable nested grids, a user-defined fixed vertical grid structure; the use of three-dimensional inputs for temperature, water vapor, pressure, photolysis rates, horizontal diffusivities and vertical turbulent exchange coefficients; updated dry deposition; and a plume-in-grid (P-i-G) algorithm. Because of these features, UAM-V represents a significant technical advance beyond the UAM-IV. In particular, UAM-V's two-way interactive nesting of grids is much better suited to the exploration of control strategies in the urban or high emission density areas within a region, than are the fixed grid or one-way nesting methods used previously in UAM-IV and ROM, because the effects of regional transport or recirculation of pollutants can be simulated within one large domain. UAM-V's nested grid structure also allows high grid resolution where it is needed without the cost of carrying this high grid resolution over much larger areas where it is not needed. The variable vertical structure of UAM-V permits more realistic treatment of nighttime vertical structures and entrainment of large elevated plumes into the grid calculations. Additionally, the reactive plume P-i-G algorithm treats emissions as a series of multi-layered ellipsoidal puffs in which ambient air is entrained, chemistry takes place, and concentrations are "shed" from the outer shells into the grid as the puff size grows to match the limiting cross sectional area (X-Y or X-Z) of the grid cell. This reactive plume-in-grid treatment avoids the premature- and over-dilution problems that previous urban- and regional-scale photochemical grid models (such as ROM and UAM-IV) suffer with large point sources.

OBJECTIVES

The objectives of the modeling analysis are to (1) apply UAM-IV and UAM-V for three ozone episodes in Atlanta (two multiday regulatory episodes and one episode from the 1992 Southern Oxidants Study (SOS)), (2) assess and compare the performance of UAM-V with UAM-IV for these episodes, and determine the acceptability of UAM-V, and (3) if accepted, apply UAM-V to evaluate alternative control strategies, using the regulatory episodes, for bringing the area into attainment and to provide guidance for the preparation of the Atlanta SIP.

PURPOSE OF THE PROTOCOL DOCUMENT

This protocol is intended to serve as the basis for the performance and successful completion of photochemical modeling to support the development of the Atlanta SIP. The purpose of the protocol is to describe the methodologies to be followed throughout the study, including domain selection, input preparation procedures, performance evaluation procedures, model acceptance criteria, and control strategy evaluation procedures. It should be viewed as a set of general guidelines that provide focus, consistency, and a basis for consensus for all parties involved in the study.

OVERVIEW OF THE ATLANTA UAM APPLICATION

The photochemical modeling study outlined in this document will include the following elements:

1. Preparation of a protocol (this document) that describes the background, objectives, and procedures to be followed in the modeling analysis. (If UAM-V is accepted for use in Atlanta, this document will replace the existing UAM-IV protocol that has already been approved by EPA (GDNR, 1992)).
2. Development of baseline, projected baseline, and control scenario emission inventories for the Atlanta modeling domain.
3. Identification of multi-day regulatory ozone episodes that include at least three primary episode days for UAM application, and an additional episode selected from the 1992 SOS field program.
4. Preparation of UAM-IV and UAM-V meteorological and air quality inputs for each of the episodes.
5. Application of the UAM-IV and UAM-V, evaluation of each model's performance for each of the episodes, and determination of UAM-V acceptability.
6. Future-year application of UAM-V for each regulatory episode to establish future-year baseline conditions.
7. Development of future-year emission control strategies for the Atlanta area.
8. Application of UAM-V to evaluate selected control scenarios to demonstrate attainment of the NAAQS for ozone.
9. Documentation of the entire UAM application process, including input preparation methodologies, performance evaluation, and future-year analysis and submittal of results for EPA review and approval.

SCHEDULE

The estimated schedule for performing the UAM application and SIP development for Atlanta is the following:

- | | |
|------------------------------------|----------------------------|
| 1. Prepare protocol | May-June 1993 |
| 2. Assemble Met/AQ data | June-July 1993 |
| 3. Develop base year inventories | May-August 1993 |
| 4. UAM base case modeling analysis | July-November 1993 |
| 5. UAM-V acceptability decision | November 1993 |
| 6. Develop 1999 inventory | September-November 1993 |
| 7. Attainment demonstration | December 1993 - April 1994 |
| 8. SIP preparation | January-November 1994 |
| 9. SIP submittal | November 15, 1994 |

DELIVERABLES

Documentation describing UAM input preparation, model performance evaluation, performance intercomparison, control strategy development, and attainment demonstration will be provided to the EPA at appropriate times during the modeling analysis.

MANAGEMENT STRUCTURE/TECHNICAL COMMITTEES

This section presents an overview of the management and technical committees that will be established to oversee the modeling analysis. The State of Georgia's Environmental Protection Division is the agency responsible for conducting the UAM analysis and developing the ozone SIP. The state will be assisted by Systems Applications International (SAI), in performing the UAM-V and UAM-IV modeling work. The Georgia Institute of Technology is assisting the state in preparing episode-specific emission inventories. The modeling analysis will be managed and reviewed by three committees, the Modeling Policy Oversight Group, the Technical Work Group, and the Emission Inventory Work Group.

Modeling Policy Oversight Group (taken from existing UAM-IV protocol and modified)

Because the proposed UAM-IV and UAM-V modeling domains do not overlap other ozone nonattainment areas, involvement of any other state or local government agency is not

anticipated in either the Policy or Technical Oversight Groups. Emission inventory information for parts of the extended UAM-V domain in Alabama will be obtained from EPA's Interim 1990 inventory. The Policy Oversight Group includes representatives from the EPA Region IV Office, Georgia Environmental Protection Division, the regulated community, and public interest groups. Representatives were chosen for their direct involvement in environmental protection policy.

The Policy Oversight Group consists of Robert Collom, William Estes, and Marvin Lowry of the Georgia Environmental Protection Division (EPD), Stuart Perry of EPA Region IV, Richard Scheffee of EPA OAQPS, Nancy Hirshberg of Georgia Power Company, John Jansen of the Southern Company Services, and Dr. William Chameides of the Georgia Institute of Technology. This group will set the objectives of the study, provide the schedule, determine resource needs, and implement any modification to the modeling protocol as the analysis proceeds.

This group will be actively involved in determining the control strategy necessary to demonstrate attainment of the O₃ standard and will establish the cost-effectiveness criteria that produces attainment at lowest cost.

The Policy Oversight Group will convene on an as-needed basis to develop progress reports and discuss issues pertaining to the Atlanta UAM development.

Technical Work Group (taken from existing UAM-IV protocol and modified)

The Technical Working Group for this modeling project consists of Dale Kemmerick and Kenneth Powell for the Georgia EPD, Brenda Johnson of EPA Region IV, and Richard Scheffee of EPA OAQPS, Nancy Hirshberg of Georgia Power Company, John Jansen of the Southern Company Services, and Carlos Cardelino of the Georgia Institute of Technology. This group will review all work to make sure that all technical aspects are performed satisfactorily and conform to the methodologies specified in this protocol, and to ensure that EPA Guidance for UAM application is followed.

The Technical Working Group will review the work performed by SAI including this protocol, the selection of the UAM-V modeling domain, the specification of initial and boundary conditions, the diagnostic analyses, the performance evaluations, the comparison of UAM-IV and UAM-V performance, the determination of acceptability for UAM-V, and the application of UAM-V for attainment strategy evaluation.

Emission Inventory Work Group (taken from existing UAM-IV protocol and modified)

The Emission Inventory Work Group will have the responsibility of overseeing and reviewing the development of the emission inventory of VOC, NOX, and CO for point, area, mobile, and biogenic sources used in modeling the UAM episodes. It is their responsibility to monitor the work performed by Georgia Air Protection Branch and the Georgia Institute of Technology to assure conformity to the "Inventory Preparation Plan - 31 July 1991."

Members of this group consists of Ron Methier and Thomas Teston of Georgia EPD, Yasmin Yorker of EPA Region IV, Chet Wayland of EPA RTP, Nancy Hirshberg of Georgia Power Company, John Jansen of the Southern Company Services, and Carlos Cardelino of the Georgia Institute of Technology.

The Emission Inventory Group will have responsibility for reviewing the emission inventories developed by the state and/or Georgia Tech that will be used in the modeling exercise, including base year inventories for 1987, 1988, and 1992. The Emission Inventory Group will also be responsible for the reviewing the development of both growth and control factors used to project the future year modeling inventory for 1999, and to review the associated documentation. These activities will conform to the procedures contained in this protocol and various EPA guidance documents.

Participating Organizations

The organizations that will be involved in the Atlanta ozone UAM Analysis are the Georgia Environmental Protection Division, EPA Region IV, Atlanta Regional Commission, the Georgia Institute of Technology, Georgia Power Company, and Southern Company Services. Georgia EPD may request assistance from, or use information from other participating members of the Southern Oxidants Study (SOS) Group.

Relationship to Regional Modeling Protocols

The Georgia EPD has reviewed EPA's Regional Modeling Protocol for ROM and generally agrees with this plan. The dates of the candidate Atlanta UAM episodes have been provided to EPA so that ROM simulations can be performed for these periods. The output from ROM for the selected modeling episodes will be examined and may be used to estimate boundary conditions for the UAM-IV domain.

Relationship to Other Area Modeling Protocols

The UAM-IV and UAM-V domains do not overlap any other urban areas for which UAM will be applied, and, therefore, no specific coordination will be necessary with any other state.

Relationship to Planning/Strategy Groups

The Atlanta Regional Commission and the Georgia Department of Transportation will be important contributors to the mobile emissions inventory by providing detailed traffic data. The latest version of the Mobile Emissions Factor Program will be used to calculate emissions totals. Present plans involve the use of MOBILE5a.

2 UAM-IV AND UAM-V MODELING METHODOLOGY

This section provides a summary of the selected ozone episodes to be simulated, the specification of the UAM-IV and UAM-V modeling domains, the air quality, meteorological, and emission data bases that are available for input, and the input preparation procedures that will be followed for the UAM-IV and UAM-V applications.

EPISODE SELECTION

An analysis of high ozone events that occurred during the period 1987-91 has resulted in the selection of two multi-day periods for UAM application - 29 July through 1 August 1987 and 7-8 July 1988. During the four-day 1987 multiday episode, exceedances of the ozone standard were recorded at all 5 monitors and two meteorological regimes were identified. Therefore, the 31st of July and the 1st of August are considered "primary" episode days as defined in the UAM guidance document. The 8th of July 1988 has been identified as the third primary episode day as required by the EPA for regulatory application of the UAM. During this episode, ozone violations were also recorded at all 5 monitoring sites operating in the Atlanta area. In addition, these episodes include ozone concentrations that are either the maximum or within 95% of the maximum concentrations measured during the 1987-1991 period for all 5 sites.

These regulatory episodes will be simulated with UAM-IV and UAM-V and a comparison of model performance will be made to determine if UAM-V is acceptable to evaluate future year attainment strategies. If UAM-V is deemed acceptable, then all future-year modeling will be performed with UAM-V. To further assess and compare the performance of UAM-IV and UAM-V, one episode selected from the 1992 Southern Oxidants Study (SOS) (9-10 August 1992) will be simulated. The enhanced data base available for the 1992 episode will provide further assurance that UAM-V is performing as well as or better than UAM-IV. Because very few ozone exceedances were recorded and the observed maximum ozone concentration on 10 August was only 140 ppb, this episode does not qualify as an appropriate SIP episode and no future year modeling will be performed for the episode. It will only be used to assess and compare the performance of UAM-IV and UAM-V.

AVAILABLE METEOROLOGICAL AND AIR QUALITY DATA BASES

The air quality data base for the 1987 and 1988 episodes consists of all NAMS, SLAMS, and SPMS monitoring sites in the Atlanta area. Those sites monitoring Ozone, NO_x, and CO will be included in this study and are listed in Table 2-1. Available meteorological data for the 1987 and 1988 episodes are presented in Table 2-2. Information about winds and temperatures aloft will be derived from the twice-daily National Weather Service radiosonde

TABLE 2-1

Atlanta Area Monitoring Sites

13	0891002	11	1640002	F01	56	DeKalb Tech, Clarkston	CO
13	1210054	11	4420001	F01	55	Holcomb Bridge Rd., Atlanta	CO
13	0890002	11	1600002	F01	56	S. DeKalb College, Decatur	NO ₂
13	1210048	11	0200048	F01	56	Ga. Tech Power Sub-Station, Atlanta	NO ₂
13	2230002	11	4020002	F03	55	DOT, Dallas	O ₃
13	0970002	11	1800001	F01	56	Sweetwater Creek St., Pk, Lith. Springs	O ₃
13	0890002	11	1600002	F01	56	S. DeKalb College, Decatur	O ₃
13	2470001	11	4340001	F03	56	Monastery, Hwy 212, Conyers	O ₃
13	0850001	11	1580001	F01	56	Georgia Forestry Station, Dawsonville	O ₃
13	1210055	11	0200055	F01	56	Confederate Avenue, Atlanta	O ₃
13	1210050	11	0200050	F01	56	Midtown, Atlanta	CO
13	1210051	11	0200051	F01	56	Peachtree Center, Atlanta	CO
13	1210052	11	0200052	F01	56	Brookwood, Atlanta	CO
13	1210053	11	0200053	F01	56	Mik-EKMA, Atlanta	O ₃

Table 2-2. Surface meteorological observation sites, locations, and variables in the Atlanta region.

Site Name	Location UTM (Zone 16)		Variables Measured
	UTMX	UTMY	
Atlanta Hartsfield International Airport	739.580	3726.148	WS, WD, T, T _D , P
Dobbins Naval Air Station	729.590	3755.498	WS, WD, T, T _D , P
Fulton County (Charlie Brown) Airport	729.947	3740.709	WS, WD, T, T _D
Dekalb Peachtree Airport	749.724	3752.306	WS, WD, T, T _D
Conyers Monastery Monitor	772.248	3719.869	WS, WD
South Dekalb Panthersville Monitor	752.780	3730.991	WS, WD, T, T _D

launched from Athens, Georgia which is located just outside the proposed UAM-IV domain but within the proposed UAM-V domain.

During the summer of 1992, a field measurement program was conducted in the Greater Atlanta area as part of the Southern Oxidants Study (SOS). Supplemental air quality measurements have been acquired and should be available for ozone, NO_x, and hydrocarbons, and supplemental meteorological measurements of winds, temperatures, solar radiation are available from additional ground sites and upper-air platforms (i.e. radar profilers). Continuous surface air quality measurements were obtained for 23 ozone sites, 7 SO₂ sites, 6 CO sites, and 12 NO_x/NO_y sites; and intermittent measurements of reactive hydrocarbons were obtained for 28 sites. Vertical measurements of ozone and VOCs were obtained from tether sondes at 4 sites. Meteorological measurements consisted of surface wind speed/direction and temperature measurements at 12 sites (in addition to those available from NWS sites), and solar radiation at 6 sites. Measurement of meteorological variables aloft were obtained using one lidar, one radiosonde, 4 tether sondes, and 4 radar profilers. This enhanced data set will be used to prepare inputs to the UAM-IV and UAM-V and to assess the performance of the model in replicating observed ozone concentrations for the 1992 episode. Because of scheduling considerations, if the 1992 SOS data set is not available by July 15, 1993, it may not be possible to include the 1992 episode in the modeling analysis.

MODELING DOMAIN SPECIFICATION

The 160 x 160 km, 4 km resolution modeling domain that has been used in all previous UAM modeling work for Atlanta will be used for the UAM-IV modeling. This domain is depicted in Figure 2-1. The proposed UAM-V modeling domain will be comprised of an outer, coarse-resolution grid that extends approximately 80 km beyond the current UAM-IV domain and a nested, higher-resolution grid that is identical to the UAM-IV domain. The coarse-grid cell size will be approximately 8 km. The overall domain size will be approximately 320 x 320 km. By including these additional grid cells, boundary condition information for the nested, urban grid will be simulated, rather than specified by the user. The location of the 40 by 40 UAM-IV domain is presented in Figure 2-2 and the preliminary UAM-V domain is presented in Figure 2-3. Final specification of the outer UAM-V grid will be determined following analysis of the meteorological conditions for each of the episodes. If appropriate, consideration may be given to adding an additional higher resolution nested grid (e.g. 2 km by 2 km cells) in certain high emission density areas near Atlanta.

EMISSION INVENTORY DEVELOPMENT

Because photochemical grid models simulate the hour-by-hour photochemistry occurring for each grid cell comprising the modeling domain, the input emissions data must be similarly resolved. Total VOC and NO_x emissions must be chemically speciated into the chemical classes employed by the model. Additionally, the emissions data must be spatially allocated

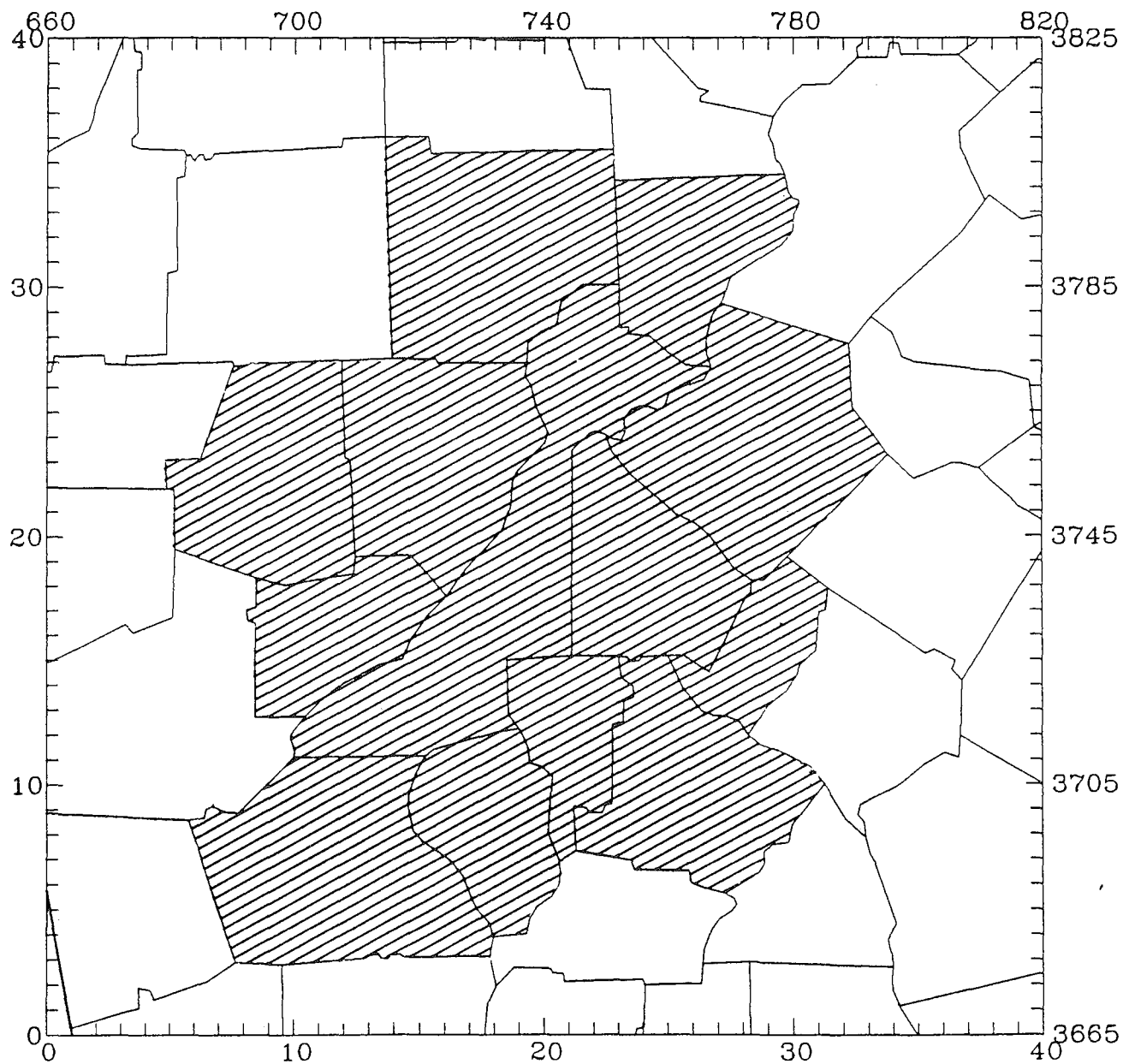


Figure 2-1. UAM-IV modeling domain for Atlanta. Domain consists of a 40 by 40 array of 4 km grid cell with an origin at UTM coordinates 660 km easting, 3665 km northing, zone 16. Stippled area depicts nonattainment area.

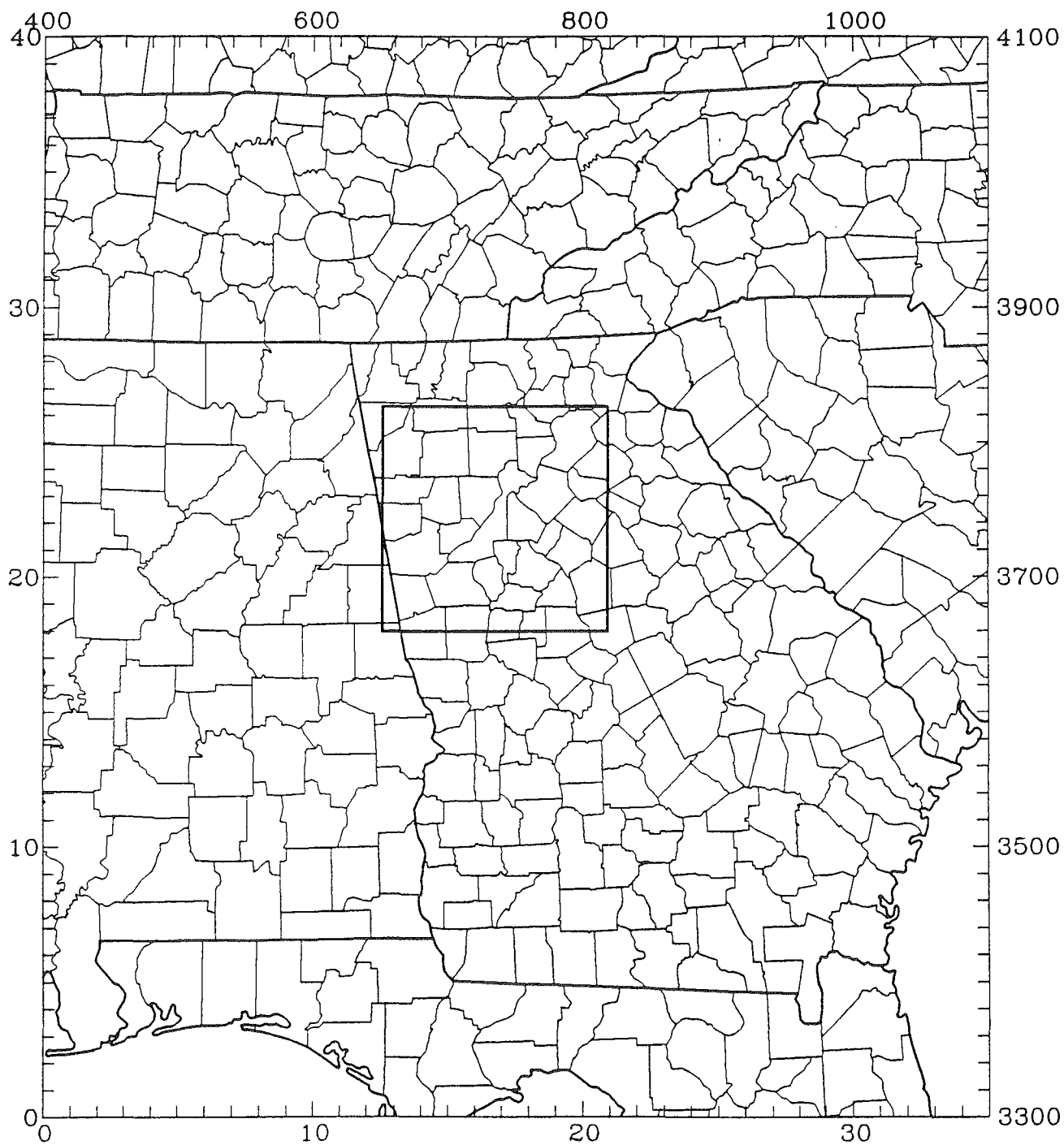


FIGURE 2-2. Geographical location of the UAM-IV modeling domain for Atlanta.

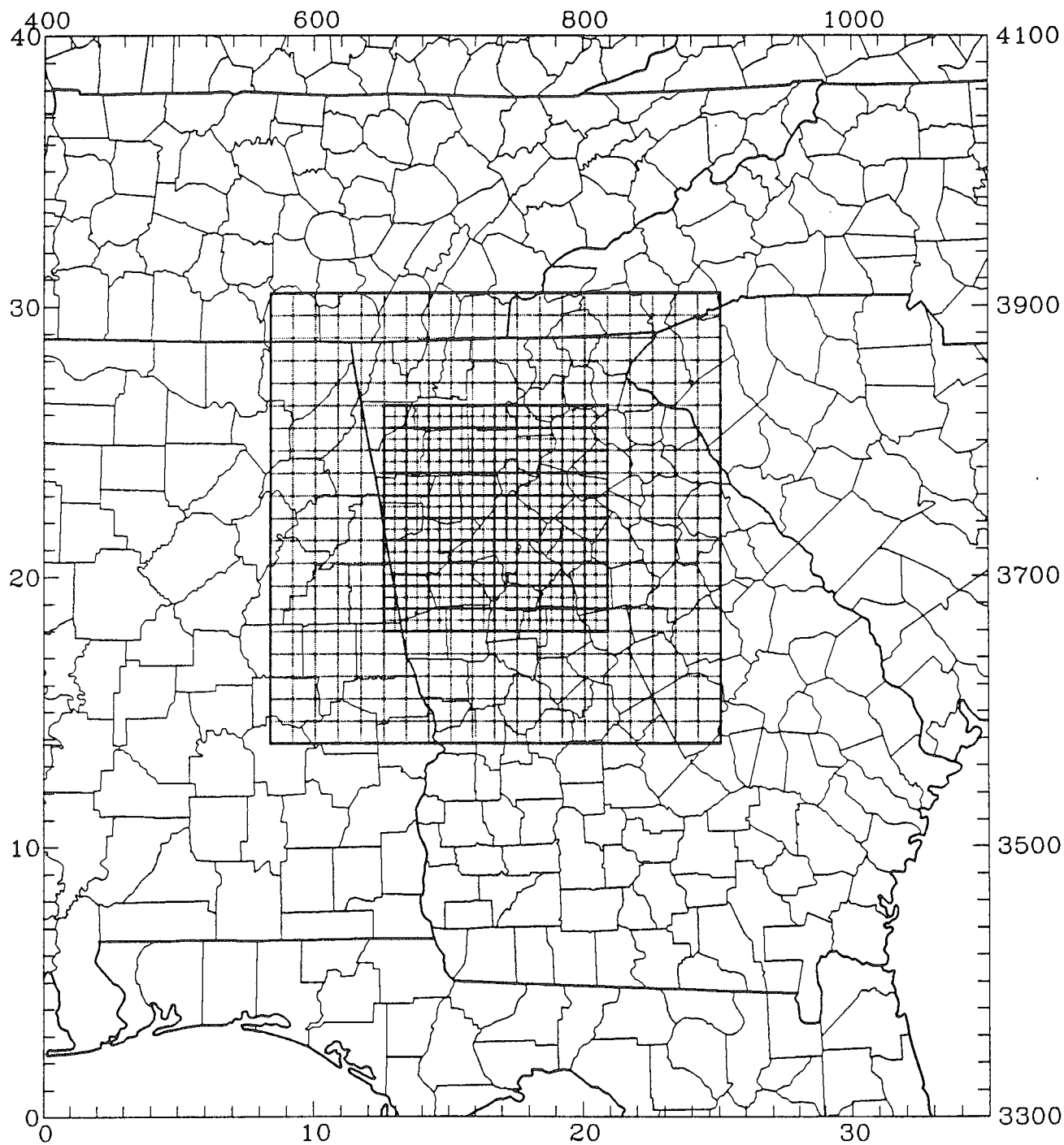


Figure 2-3. Preliminary UAM-V nested modeling domain for Atlanta. (Actual inner grid will consist of 40 by 40, 4 km cells, with 8 km cells in outer grid. For clarity of presentation, the size of the grid cells depicted in this figure are 8 km for inner grid and 16 km for outer grid)

by grid cell on an hourly basis for each hour of the modeling episode. If photochemical modeling is being performed to evaluate potential control strategies, future year inventories must be projected which incorporate anticipated changes in emissions levels in addition to the chemical, spatial, and temporal resolution mentioned above.

The Atlanta 1990 base year emission inventory will serve as the basis for the modeling inventories developed for this application. (For the UAM-V domain, those areas outside the domain of the 1990 Atlanta inventory will use EPA's 1990 interim inventory, which is the same inventory being used in the ROM simulations). These inventories will be developed in accordance with the Inventory Preparation Plan and guidance from a memo from William Laxton, December 26, 1991 on emissions and modeling related issues. The adjustments made to the 1990 SIP inventory will consist of expanding the geographical coverage to encompass the entire modeling domain rather than just the ozone nonattainment area, adjusting emission rates for episodic conditions, and projecting attainment-year emissions levels that account for both anticipated changes in activity levels and the effects of proposed control measures.

For this application, the inventories will be reviewed and summarized, and quality assurance checks will be made prior to being used in the UAM analysis.

The following paragraphs identify issues to be addressed by the Emissions Inventory Group in developing the modeling inventories.

Point sources: Emissions cut-off levels for differentiating between point and area sources have been stated in the Inventory Preparation Plan as 10 TPY for VOC in the nonattainment area and 100 TPY for VOC in the 25 mile area outside of the nonattainment area. NO_x cutoff levels are 100 TPY. Other issues relating to the point source modeling inventory include the plume rise level to be used for selecting sources for elevated source treatment in the UAM and the type and sources of data to be utilized in constructing activity and emission projections (e.g., ARC, BEA, or survey results).

Area sources: Emissions will be developed as outlined in the Inventory Preparation Plan from the use of questionnaires, per capita estimates, and emission per employee factors. Additional issues include identification of the data to be used to construct activity projections, and whether sufficiently detailed data are available to estimate changes in activity levels by grid cell.

Onroad motor vehicles: Emissions will be determined from the TRANPLAN areawide transportation network model by ARC for an eight county area. For the remaining counties, motor vehicle emissions will be estimated based on county-level VMT provided by GDOT from the HPMS data base and emission factors from MOBILE5a. These procedures are described in the Inventory Preparation Plan. Other issues include identification of the transportation control measures planned for incorporation into the SIP and the methods to be used for measuring the effects of these TCM's on motor vehicle emissions.

Biogenic sources: Emissions from biogenic sources in the Atlanta modeling domain will be estimated using EPA's Biogenic Emission Inventory System (BEIS) and SOS data from the 1992 Atlanta Intensive study.

Other issues: In addition to the items listed above, available episode-specific data for point sources and sources affected by meteorological conditions will be identified and incorporated into the modeling inventories. Differences between weekday and Saturday emission levels must also be addressed, since one of the modeling episodes includes a Saturday. Spatial and temporal allocation factors must be developed to apportion county level emissions by grid cell and to allocate total daily emissions to the hours of the episode days. Appropriate speciation profiles must be identified for use in disaggregating VOC and NO_x emissions into the chemical classes required by the model. Additionally, if a high resolution nested grid is specified for certain areas of the domain, the inventory will have to be prepared to reflect this configuration.

The use of data from ARC for developing future year projection data will ensure compatibility with other regional projections, since ARC data is used for planning purposes in the Atlanta Metropolitan Area. The Emission Inventory Group will conduct comparative analyses of the ARC data with the BEA data to identify any potential biases with ARC data.

Once the future base case emissions have been developed and the performance evaluation tests show that the UAM-V simulation results are acceptable, the data sets will be frozen. These frozen data sets will be made available to other interested parties with UAM capabilities to perform attainment strategy evaluations. Currently it is anticipated that Southern Company Services and the Georgia Institute of Technology (GIT) will perform UAM attainment strategy evaluations in addition to EPD.

INPUT PREPARATION PROCEDURES

The procedures to be used in preparing model inputs will depend on the availability and appropriateness of the historical meteorological and air quality data. Due to differences in model structure and capabilities, the UAM-V requires several additional input files compared to UAM-IV. Input preparation for UAM-IV will follow EPA Guidance (EPA, 1991). For UAM-V, those features that are appropriate for the Atlanta area application, including the enhanced input preparation procedures, will be employed. Wherever possible, consistency between the UAM-IV and UAM-V inputs will be imposed (e.g., both sets of meteorological fields will be prepared using a prognostic meteorological model, the SAI Mesoscale Model (SAIMM)).

A brief description of the files required for UAM-IV and UAM-V and the procedures for preparing these files are presented below:

AIRQUALITY This file contains the initial concentrations of each of the CB-IV species for each grid cell at the start of the simulation.

UAM-IV: Interpolate observed data to UAM-IV grid.

UAM-V: Interpolate observed data to UAM-V grid.

BOUNDARY This file contains the location of the modeling domain boundaries and the concentration of each species used as the boundary condition along each lateral boundary for each level.

UAM-IV: Specify based on a regional analysis of air quality data, ROM output, or use background concentrations.

UAM-V: Use background concentrations or ROM output for outer grid boundaries (320 X 320 km domain) and UAM-V generated concentrations for the nested grid boundaries (160 x 160 km domain).

CHEMPARAM This file contains information regarding the chemical species to be simulated including reaction rate constants, upper and lower bounds, activation energy, reference temperature, and resistance to surface sinks. For photochemical applications, the file is supplied with the model.

UAM-IV: Use existing CB-IV file.

UAM-V: Use existing CB-IV file.

RATES This file includes the photolysis rates as function of solar zenith angle and altitude.

UAM-IV: Not applicable.

UAM-V: Use file provided with the model.

AGGMAP This file serves the dual purpose of defining the location of any nested, higher-resolution grids located within the modeling region and the location of cells to be treated as aggregates for the chemistry calculations.

UAM-IV: Not applicable.

UAM-V: Prepare based on UAM-V grid structure.

EMISSIONS This file contains the ground-level emissions of all emitted species to be simulated for each hour and grid cell. For UAM-V, a separate emissions file must be provided for each nested grid.

UAM-IV: Use existing episode-specific files for 160 x 160 km domain.

UAM-V: Use existing episode-specific UAM-IV files; prepare emissions for outer grid.

PTSOURCE This file contains the point source information, including stack height, temperature and flow rate, plume rise, grid cell into which the emissions are emitted, and emissions rates for all emitted CB-IV species for each point source for each hour.

UAM-IV: Use existing episode-specific files for 160 by 160 km grid.

UAM-V: Use existing episode-specific UAM-IV files plus additional point sources in outer grid. All major point sources will be treated by plume-in-grid formulation.

HEIGHT This file contains a three dimensional array of values defining the heights of the tops of layers above ground at each grid location. It can vary both spatially and temporally, but the recommended practice is to define the layers to be constant in time and space. This file also contains the atmospheric pressure, which may also vary spatially and temporally.

UAM-IV: Not applicable.

UAM-V: Prepare according to UAM-V grid structure.

H2O This file contains a three-dimensional array of water vapor concentrations in ppm by volume. The data vary spatially and temporally.

UAM-IV: Not applicable.

UAM-V: Obtain from SAIMM output.

TEMPERATURE This file contains a three-dimensional array of ambient temperatures. The values vary spatially and temporally.

UAM-IV: Only surface temperature is required; obtain from SAIMM output.

UAM-V: Obtain from SAIMM output.

SURFACE This file contains landuse information for each grid cell in the region. It varies spatially, but not temporally.

UAM-IV: Derive from USGS data (designated file name is TERRAIN for UAM-IV).

UAM-V: Derive from USGS data.

TERRAIN For UAM-IV, this file contains landuse information for each grid cell in the region. It varies spatially, but not temporally. For UAM-V, this file contains a two-dimensional array of terrain heights above sea level. These data do not vary temporally.

UAM-IV: Obtain from USGS data.

UAM-V: Obtain from USGS data.

TOPCONC This file contains the concentration of each CB-IV species for the area above the modeling region.

UAM-IV: Use background estimates.

UAM-V: Use background estimates.

VDIFFUSION This file contains a three-dimensional array of vertical exchange coefficients for the top of each grid cell in the region. The data vary spatially and temporally. For UAM-V, separate data files may be provided for nested grids; otherwise, the coarse grid data will be interpolated to provide data for nested grids.

UAM-IV: Not applicable.

UAM-V: Derive from the SAIMM output.

WIND This file contains the x- and y- direction wind velocity components for every grid cell for each hour of the simulation. Also contained in this file are the surface wind speeds for the entire domain. For UAM-V, separate data files may be provided for nested grids; otherwise, the coarse grid data will be interpolated to provide data for nested grids.

UAM-IV: Prepare using the SAIMM.

UAM-V: Prepare using the SAIMM.

DIFFBREAK This file contains the daytime mixing height or nighttime inversion height for each column of cells at the beginning and end of each hour of the simulation.

UAM-IV: Obtain from SAIMM output.

UAM-V: Not used.

METSCALARS This file contains hourly values of the following spatially invariant meteorological parameters: NO₂ photolysis rate constant, water-vapor concentration, temperature gradient above and below the mixing height, atmospheric pressure, and exposure class (a measure of surface-layer atmospheric stability).

UAM-IV: Estimate using hourly observed meteorological data.

UAM-V: Not applicable.

REGIONTOP This file contains the height above ground of the top of the modeling region. It can vary both spatially and temporally, but the usual practice is to set it to a constant.

UAM-IV: Specify based on maximum mixing heights estimated for each episode.

UAM-V: Not applicable.

QUALITY ASSURANCE OF UAM INPUTS

The meteorological, air quality, and land-use inputs prepared for UAM-IV and UAM-V will be plotted and examined to ensure accurate representation of the observed data in the UAM-ready fields, temporal and spatial consistency, and reasonableness.

Quality assurance procedures that will be used to ensure the consistency and accuracy of the emissions inventories generated with the emissions preprocessing system include documentation of major assumptions, careful accounting of emissions totals throughout the development process, verification of spatial distribution of emissions against known source locations, and identification of missing or unreasonable data values. The final emissions inventory will be tabulated, plotted, and examined before any UAM simulations are performed.

Following the preparation of inputs and initial application of the UAM-IV and UAM-V to each episode, a series of diagnostic experiments will be conducted to examine the effects of uncertainty and identify inconsistencies and/or deficiencies in the model inputs.

3 ASSESSMENT AND COMPARISON OF MODEL PERFORMANCE

The modeling will be performed with the day-specific emission inventory assembled for each episode and the performance of UAM-IV and UAM-V will be evaluated to determine how well the historical ozone episodes are replicated. Graphical and statistical analyses will be used to evaluate and compare model performance for UAM-IV and UAM-V.

Graphical Analyses

Graphical analysis will be used to assist in the model performance evaluation. Graphical analysis products will include (1) time-series plots of observed and simulated ozone concentrations, (2) contour plots showing isopleths of simulated ozone concentrations and, where available, observed values for the surface, (3) scatter plots of the simulated and observed concentrations, and (4) frequency distribution plots of residuals (differences between simulated and observed concentrations).

*For
diagnostic
purposes?*

Statistical Measures of Performance

The statistical analysis to assess model performance of UAM-IV and UAM-V will include calculation of a number of statistical measures of bias and error. The same set of hourly ozone data from monitors located in the Atlanta nonattainment area will be used to evaluate the performance of the two models. In the calculation of these statistical measures, weighted interpolation of the simulated values in the four grid cells surrounding a monitoring site is performed to provide collocated pairs of simulated and observed values.

The three primary measures that will be calculated for UAM-IV and UAM-V, for which EPA has provided "acceptability" goals in the UAM guidance document (EPA, 1991), are the following:

- 1) Unpaired accuracy of the peak (A_p) - (EPA goal: within ± 20 percent)
 - unpaired in space or time - peak simulated versus peak observed
- 2) Mean relative error (MRE) (normalized bias) - (EPA goal: within ± 15 percent)
 - paired in space and time using pairs for which observation is above cutoff
- 3) Mean unsigned relative error (MURE) (gross error) - (EPA goal: less than 35 percent)
 - paired in space and time using pairs for which observation is above cutoff

The unpaired accuracy of the peak concentration is defined as:

$$\text{Unpaired Accuracy of the Peak Concentration} = \frac{S_{\max} - O_{\max}}{O_{\max}}$$

where $S_{\max}$ and $O_{\max}$, the simulated and observed maxima, respectively, are taken over all locations and times (the location and time of the maximum simulated value does not have to be the same as the site and time of the observed maximum). The mean relative error (MRE) and mean unsigned relative error (MURE) are defined as follows:

$$\text{Mean Relative Error} = \frac{\sum_{i=1}^N (S_i - O_i)/O_i}{N}$$

$$\text{Mean Unsigned Relative Error} = \frac{\sum_{i=1}^N |S_i - O_i|/O_i}{N}$$

where O_i is the i^{th} observation, S_i is the i^{th} simulated value, and N is the number of observed or simulated values.

A lower bound of 60 ppb will be used for calculating the mean relative error and the mean unsigned relative error. The relative error will not be computed for observation and simulation pairs when the observed value is less than the lower bound to avoid excessive weighting of the relative means by low values and to avoid dividing by zero.

The performance of the model in replicating peaks will be further assessed by calculating the following:

- 4) Spatially-paired average peak accuracy ($A_{\text{avg},s}$) - all monitors, paired in space, not time (± 2 hours)
- 5) Temporally-paired average peak accuracy ($A_{\text{avg},t}$) - all monitors, paired in time, not space (9 grid cells)
- 6) Unpaired station average peak accuracy ($A_{\text{avg},u}$) - all monitors - unpaired in time or space (± 2 hours, 9 grid cells)

To provide additional insight regarding the temporal and spatial performance of the model, statistics will be computed for pairs that consist of the observations with the optimal simulated values (i.e., the simulated fields are shifted by a constant amount in time and space so that the agreement between the observed and simulated values is optimized). For this application, the temporal and spatial shifts will be limited to ± 2 hours and 20 km. The optimal temporal and spatial shift are the set of shifts that minimize the root mean square error. The measures to be calculated include:

- 7) Distance of spatial shift (Δx)
- 8) Length of temporal shift (Δt)
- 9) Bias calculated from optimized pairings after shift (MRE_{opt})
- 10) Gross error calculated from optimized pairings after shift ($MURE_{opt}$)

Determination of Acceptable Model Performance for UAM-V

The UAM-V is expected to provide a more reliable, scientifically justifiable means for evaluation of attainment strategies for the Atlanta area. The acceptability of UAM-V will be based on the model performance evaluation and comparison with UAM-IV performance results. To assess whether UAM-V performs as well as or better than UAM-IV, a comparison will be made for each performance measure. For scoring, performance measures 1-3 will be given equal weight, measures 4-6 will be averaged together, and measures 7-10 will also be averaged. With this approach, the comparisons may show differences that are "clearly better", "clearly worse", or "too close to call". The ranges for each measure that would be considered "too close to call" are:

Mean relative error before and after shift (MRE):

$$| |MRE_{UAM-IV}| - |MRE_{UAM-V}| | \leq 0.05 \text{ or } 5\%$$

Mean unsigned relative error before and after shift (MURE):

$$|MURE_{UAM-IV} - MURE_{UAM-V}| \leq 0.05 \text{ or } 5\%$$

Accuracy parameters (ACCURACY):

$$| |ACCURACY_{UAM-IV}| - |ACCURACY_{UAM-V}| | \leq 0.05 \text{ or } 5\%$$

Spatial shift (Δx):

$$| |\Delta x_{UAM-IV}| - |\Delta x_{UAM-V}| | \leq 2 \text{ km}$$

Temporal shift (Δt):

$$| |\Delta t_{UAM-IV}| - |\Delta t_{UAM-V}| | \leq 0.5 \text{ hr}$$

Following this approach, both models will be scored by giving 2 points for each measure to the model that performs clearly better, and no points for performance that is too close to call or is clearly worse. The total score for each model would then be calculated as follows:

$$\begin{aligned} \text{SCORE} = & \text{POINTS}_{\text{Au}} + \text{POINTS}_{\text{MRE}} + \text{POINTS}_{\text{MURE}} + \\ & (\text{POINTS}_{\text{Aavg,s}} + \text{POINTS}_{\text{Aavg,t}} + \text{POINTS}_{\text{Aavg,u}})/3. + \\ & (\text{POINTS}_{\Delta x} + \text{POINTS}_{\Delta t} + \text{POINTS}_{\text{MREopt}} + \text{POINTS}_{\text{MUREopt}})/4. \end{aligned}$$

If $\text{SCORE}_{\text{UAM-IV}} - \text{SCORE}_{\text{UAM-V}} \leq 1.5$, then UAM-V will be judged to perform acceptably. Because no points are given to either model when the performance is too close to call, the value of 1.5 provides recognition to the fact that in case of a tie or close score, UAM-V would be selected because many of the features of UAM-V are improvements over UAM-IV.

*Seem like
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the performance
2000 has been
double counted*

Scores will be computed and compared for each of the episodes separately. Although there are two "primary" episode days for the four-day 1987 episode, for model comparison purposes, statistics will be calculated using data from both days to determine overall performance for this episode. Scores will also be computed for each of the primary episode days of the 1988 and 1992 episodes. To determine the acceptability of UAM-V, the model would have to perform better than UAM-IV for two of the three episodes.

4 ATTAINMENT DEMONSTRATION

Attainment-Year Projections

Since the Atlanta O₃ Nonattainment Area has been classified as serious, UAM modeling will be conducted for an attainment year of 1999. The meteorological data for each base case episode will stay the same, but air quality (i.e., initial conditions) and emissions data will be projected to 1999. Current EPA guidance on the projection of future year emission inventories will be followed. Air quality data for boundary and initial conditions for 1999 will be derived from ROM results, if available. As the first step in demonstrating attainment, the UAM will be used to model 1999 using emission projections which include the effects of CAAA and other mandated control measures, along with projected changes in initial and boundary conditions.

Control Strategy Evaluation

Once the future attainment year (1999) base projection inventory (incorporating CAAA and other mandated controls) has been developed, Georgia EPD will prepare various emission reduction scenarios to address the potential impact of additional proposed control measures. These control strategy inventories will include NO_x controls only, VOC controls only, and various combinations of both NO_x and VOC controls.

Once the 1999 base year simulations for each of the regulatory episodes have been completed, it is anticipated that the UAM modeling data bases will be "frozen" and made available from the Policy Oversight Group to interested groups that may want to evaluate additional alternative control strategies, independently, to broaden the scope of the potential strategies identified. This will expand the possible range of modeled control strategies beyond the time and resource limitations of EPD, thus increasing the likelihood of identifying an optimal solution for achieving attainment. The use of frozen base case data sets will facilitate direct comparison of the effects of the control strategies developed by the various participants.

Procedures for Attainment Demonstration

Attainment of the ozone NAAQS will be demonstrated when UAM Modeling results show no predicted daily maximum ozone concentration greater than 120 ppb. Each grid in the domain must meet this standard for each of the three episode periods.

5 SUBMITTAL PROCEDURES

By November 15, 1994 the Georgia EPD will submit to EPA Region IV a State Implementation Plan and supporting documentation that demonstrate, through modeling, attainment of the ozone NAAQS for the Atlanta area for 1999. Copies of input data and modeling results will be available on various computer recording medium as requested.

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