Southern Company Services, Inc.
Post Office Box 2625
Birmingham, Alabama 35202
Telephone 205 870-6011

Southern Company Services
the southern electric system

August 10, 1993

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

Re: Revised Draft of the "Protocol for a Model Comparison of the UAM-IV and UAM-V Models"

Dear Ms. Johnson:

In response to EPA's comments of July 15, 1993 and our discussions during the August 5 conference call, Systems Applications International (SAI) has revised the draft protocol for determining the acceptability of UAM-V for use in the development of the State Implementation Plan for Atlanta, GA. The revised draft model comparison protocol is enclosed for your review.

You will notice that we have retained in the revised draft two related features of the original scoring system that were discussed at length and without resolution in our recent conference call -- the episode treatment and the best "2 out of 3" scoring approach for determining the acceptable model. After much reflection, we decided that using a scoring system based on separate primary episode days and a total combined score would be less robust, and, indeed, technically unsound, compared to a system based on treating each episode separately and determining acceptability on a best "2 out of 3" basis. We conclude this without any preconceived notion as to the scoring system under which UAM-V would be more likely to win. Rather, we base our reasoning solely on technical grounds.

Consideration of separate episodes and the use of the best "2 out of 3" scoring avoids giving any one episode too much weight in the determination. If the SOS episode produced a very high score for one model, for example, it could determine the winning model under a total combined scoring system, even if that model lost for the two regulatory episodes. This could not happen in the proposed scoring system. The system ensures that the chosen model must win for at least one of the two regulatory episodes.

Moreover, we continue to believe that the statistical tests should be performed on the 1987 episode as a whole, rather than separately for the two episode days in that episode. By splitting the days, the 1987 episode is given more weight than the 1988 and SOS episodes, and this is inappropriate because of the correlation between the two days. The argument for treating separate days in the scoring because the attainment demonstration will look at each day separately is not a strong one. In reality, attainment is shown for the days in one continuous simulation -- the model is not run for each day. Accordingly, the proposed scoring system more closely reflects the way in which the 1987 episode will be used for demonstrating attainment. Indeed, all of the statistical measures in the scoring system will be calculated with information from both days in the episode.

In summary, we continue to believe that the proposed scoring system will more appropriately determine the better of the two models for use in the attainment demonstration.

Since time is short, we request your comments as soon as possible. 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 Jay Haney at 415/507-7164.

Sincerely,

John J. Jansen
Principal Scientist

cc: Environmental Protection Agency
Joseph A. Tikvart

Georgia Environmental Protection Division
Robert H. Collom, Jr.
Dale J. Kemmerick

Systems Application International
J. L. Haney

Georgia Power Company
N. H. Hirshberg
S. D. Holder
M. E. Wilder

Southern Company Services
W. D. Herrin
S. S. Vasa

RESPONSE TO EPA'S COMMENTS ON THE ATLANTA UAM-IV/UAM-V COMPARISON PROTOCOL

9 August 1993

Prepared by

Systems Applications International
101 Lucas Valley Road
San Rafael, CA 94903

RESPONSE TO GENERAL COMMENTS

- Additional information has been added to the protocol document to support the contention that the UAM-V model is scientifically superior to UAM-IV.

- The scope of the protocol has been reduced so that it only specifically addresses the UAM-IV/UAM-V comparison. Following the comparison, the SIP demonstration protocol submitted by the State of Georgia will be revised if UAM-V is the model chosen for the attainment demonstration.

- In the event that the UAM-V is selected for application to the Atlanta nonattainment area and the UAM-V simulated ozone concentrations are biased low compared to both the observations and the UAM-IV simulated concentrations, the reasons for this bias will be investigated and the results of the investigation will be provided as part of the comparison documentation. A statement to this effect has been added to the protocol (page 3-4).

RESPONSE TO SPECIFIC COMMENTS

1. Text has been modified as indicated.

2. Additional description of the UAM-V features including some explanation as to why these features render UAM-V technically superior to UAM-IV has been added to the protocol.

3. The words "reactive" and "plume" should be hyphenated. Text has been modified.

4. Per EPA's suggestion, two protocols will be prepared. Consequently, this statement has been omitted from the text.

5. Use of the ROM output will depend on the availability and reliability (relative to other methods of estimating boundary conditions) of the ROM simulation results.

Because of the uncertainties regarding the ROM schedule, specific dates have not been incorporated into the UAM-IV/UAM-V comparison schedule.

6. The schedule and the list of deliverables have been modified to reflect the reduced scope of the protocol document. Specific dates for the deliverables have been provided.

7. The roles of the technical work groups have been more explicitly stated. In so far as the comparison will provide the basis for the attainment demonstration (whether UAM-IV or UAM-V is used) the work groups identified in the protocol should review the model inputs and performance evaluation. It is recognized that the Region IV representative is the EPA spokesperson for decisions concerning the model evaluation protocol.

8. Text has been modified as indicated.

9. Text has been modified as indicated.

10. Text has been modified as indicated.

11. For the attainment demonstration, two simulation periods (29 July - 1 August 1987 and 7-8 July 1988) and three primary episode days (31 July 1987, 1 August 1987, and 8 July 1988) have been identified. The 1987 days are part of multi-day ozone episode. Within this episode, the first two days of the selected simulation period represent "build-up" days, the third is the day on which the maximum ozone concentration for the episode was recorded, and the fourth day is a "clean-out" day. One consideration in selecting the simulation period is to allow sufficient time at the beginning of the simulation for the model to simulate the ozone "build-up" that often precedes the peak exceedance and to minimize the effects of the initial conditions, which are not well known, on the simulation. Because high ozone concentrations were observed on 29 and 30 July both of these days were selected as start-up days for the simulation of 31 July (the maximum observed ozone concentration increases steadily throughout the three-day period from 13.5 pphm on 29 July to 15.5 pphm on 30 July to 20.1 pphm on 31 July). Another consideration in the episode-selection process is that the modeling episodes should be chosen to represent the various types of meteorological conditions that are associated with ozone episodes in the nonattainment area. Although 1 August can be characterized as somewhat of a "clean-out" day, the meteorological conditions are sufficiently different from 31 July and the ozone concentrations are sufficiently high (the maximum is 16.9 pphm) that this day has been chosen as a second primary episode day.

    For the model comparison, model performance will be assessed on a per episode basis (for the 1987, 1988, and 1992 (SOS) episodes). Thus, the number of primary episode days is inconsequential. Comparing model performance for two episode days that are part of the same simulation period could confound the comparison as model performance on back-to-back simulation days may be correlated.

Clarification has been added to the protocol.

12. Due to time and resource constraints, the model comparison will be limited to the 4 km grid.

    The vertical structure for the UAM-V grid will be consistent with that of the prognostic meteorological model and will be determined upon analysis of the upper-air meteorological data. The same vertical structure will be used for all episodes. The top of the UAM-V modeling domain will be the same as the top of the UAM-IV modeling domain. Additional information regarding specification of the vertical structure of the modeling domain has been added to the protocol.

    This grid structure will also be utilized if UAM-V is selected for use in the attainment demonstration.

13. Text has been modified as indicated.

14. A discussion of the non-road mobile emissions has been added to the protocol.

15. The comparison assumes that the performance of the "winning" model will not only be better than that of the other model but will also meet the EPA-recommended criteria for acceptable model performance.

    The use of prognostic meteorological modeling as a tool for preparing meteorological inputs for photochemical modeling has only recently become widely discussed and used within the air quality modeling community. As with any "new" methodology, there have been some successes and some failures (as well as some misuses and some misinterpretations). One problem with using a prognostic model to simulate day-specific meteorology is that the meteorological fields generated by the prognostic meteorological model may not always agree with observations. Numerical approximations, physical parameterizations, and initialization errors represent a few of the potential sources of error in prognostic meteorological models that can cause the model solution to deviate from actual atmospheric behavior. Another issue is the interfacing of the meteorological and photochemical models. Interpolation or averaging of the prognostic-model-generated fields to the photochemical model vertical grid can result in inadequate representation of the simulated meteorological features. For this study, use of four-dimensional data assimilation (FDDA) will ensure agreement between the simulated fields and the observations and the SAIMM and the UAM-V vertical grids will be compatible. Several previous applications, to which we believe the reviewer must be referring, either did not use the available observational data (e.g. FDDA) or suffered from problems posed by the use of the UAM-IV vertical grid structure.

    Our experience in using the SAIMM to prepare meteorological fields for photochemical modeling (for Los Angeles, Sacramento, and Houston) has been encouraging. Accordingly, we feel that a contingency plan to use the DWM is unnecessary at this time.

16. The SAIMM will be applied to each of the episodes and the available data will be incorporated into the meteorological model using the Newtonian nudging approach to four-dimensional data assimilation (FDDA). The fields will then be postprocessed for input into the UAM-IV and UAM-V. This involves extraction of the required meteorological variables and interpolation or averaging of the fields to the UAM-IV and UAM-V grids. No further "adjustment" of the meteorological fields is anticipated. Any modification of the meteorological fields (which would involve re-running the model with different input parameters or reinterpolating the fields to the photochemical model grids using a different set of assumptions) will be based on physical principles and would not contradict available meteorological data. Any changes to the model inputs will be completely justified. Clarification has been added to the protocol.

17. Further justification to support the use of the SAIMM has been provided in the protocol.

18. The methodology will depend upon the meteorology associated with each of the episodes (e.g. is the episode a stagnation event or can a possible pollutant transport pathway be identified?) as well as the availability of ROM outputs. When used, background concentrations will be specified according to EPA-recommended values. Clarification of the methodologies to be used for specifying the BOUNDARY and TOPCONC concentrations has been provided in the protocol.

19. Additional information regarding the PiG treatment has been added to the protocol. Since the PiG treatment does not increase the simulation time substantially, there is no practical upper limit to the number of sources that can be treated. All major point sources (NO_x and VOC) will be treated with the PiG treatment. The cut-offs will be determined following inspection of the emissions data (i.e. ranking of the sources by emission totals) and may be different for NO_x and VOC sources.

20. See response #12.

21. The intention to use EPS 2.0 has been added to the protocol.

22. This information has been included.

23. Further detail regarding the diagnostic analysis section has been added to the protocol. There is, in fact, no minimum set of diagnostic and sensitivity experiments that should be applied to every episode to ensure that "discrepancies between simulated and observed data are minimized". Two diagnostic/sensitivity simulations that will definitely be performed are: zero emissions and clean boundary conditions. The full set of diagnostic and sensitivity simulations will be appropriately chosen for each episode, with input from the Technical Work Group, to address those considerations that are especially important and/or troublesome for the episode, the simulation, and

the nonattainment area.

24. Text has been modified as indicated.

25. Equations for measures (4) - (6) have been provided as well as some additional clarification.

26. The subscript "i" references a monitoring site and is therefore not appropriate for the unpaired accuracy of the peak concentration.

27. The shift represents the spatial and temporal shift required to minimize the RMS error between the simulated and observed values and is episode-day specific. Clarification has been added.

28. If the comparison for a given measure is not "too close to call", the measure indicates that model performance is "clearly better" for one model and "clearly worse" for the other.

29. Most of the SOS data have already been made available; it is anticipated that the full SOS data set will be available in time for this study.

30. Calculation of fractional bias and the final model outputs will be provided to EPA.

31. (See comment 11). Summing the scores of the two models introduces the possibility that the success or failure of UAM-V could be determined based on the simulation of a single episode. It seems that this possibility should be avoided given that we have two episodes for which limited air quality and meteorological data are available and one episode for which both routine and supplemental data are available. For example, one of the models might perform extremely well for the SOS episode, worse than the other model for the other two episodes, and end up with the highest combined score. It would be inappropriate in this case to use the "winning" model for the attainment demonstration. Thus, "two out of three" seems to be the more robust scoring approach.

    The second part of this comment, regarding the "too close to call" criterion, has been addressed in the following way in the protocol document. If the score for UAM-V for a given episode is the same as or better than that for UAM-IV, UAM-V will be awarded a point for the episode.

32. Separate protocols will be prepared, the section on attainment demonstration has been omitted, and the title of the comparison protocol document has been changed as indicated.

33. Except where noted in the protocol, all aspects of the modeling analyses will be carried out in accordance with EPA guidance.

Revised Draft

PROTOCOL FOR A COMPARISON OF THE UAM-IV AND UAM-V MODELS

SYSAPP-93/085

9 August 1993

Prepared by

Systems Applications International
101 Lucas Valley Road
San Rafael, California 94903
(415) 507-7100

M6701 93094

Contents

1 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, as well as performance evaluation and model comparison procedures. (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. The boundary condition information for many applications of UAM-IV will be supported with the use of EPA's Regional Oxidant Model (ROM).

OVERVIEW OF UAM-V

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. A summary of these features follows.

1. Structured modular computer code: The UAM computer code has been rewritten so that new modules can be easily included and the code can be vectorized to take advantage of modern computer architecture.

2. Vertical Grid Structure: The vertical layer structure in UAM-V is defined by the user and is no longer based on the diffusion break (mixing height). This allows for higher resolution vertical layers near the surface and better matching with output from prognostic meteorological models, which typically use a terrain-following coordinate system with fixed levels above ground. The variable vertical structure of UAM-V permits more realistic treatment of night-time vertical structures and entrainment of elevated plumes into the grid calculations.

3. Three-dimensional Inputs: Several meteorological variables that were considered spatially constant in the UAM (METSCALARS) now vary temporally and spatially (e.g., temperature, water vapor, pressure, and photolysis rates). Furthermore, the horizontal diffusivities and vertical turbulent exchange coefficients are now required as input and are usually obtained from a prognostic meteorological model. This feature provides for the use of more realistic meteorological fields that may vary spatially over the region being simulated.

4. Two-way nested grid capability: A fine grid can be imbedded in a coarser grid for more detailed representation of advection/diffusion, chemistry, and emissions. Several levels of both horizontal and vertical nesting can be accommodated. UAM-V's nested grid structure also allows high grid resolution where it is needed without the computational cost of carrying this high grid resolution over much larger areas where it is not needed.

5. New Dry Deposition Algorithm: An updated dry deposition algorithm formulated by Wesely (1989) has been implemented in the UAM-V. This algorithm is similar to that used by the Regional Acid Deposition Model (RADM).

6. Plume-in-Grid (P-i-G) Capability: The updated model is capable of treating the subgrid-scale chemistry and plume dynamics of user-selected point-source plumes. A Lagrangian photochemical model will simulate emissions from a point source until the plume size is commensurate with the size of a grid cell of the UAM-V. In particular, 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 P-i-G 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.

7. Emission Injections Aloft: Improved treatment of emission injections aloft (elevated sources) is also a feature of UAM-V. This feature includes penetration of multiple layers of varying stabilities in the plume-rise calculations.

The UAM-V model is currently being used in the regulatory ozone attainment demonstration for the Lake Michigan area and for the assessment of the impacts of petroleum development activities on air quality in the Texas-Louisiana Gulf Coast area.

OBJECTIVES

The objectives of the modeling analysis described in this protocol are to (1) apply UAM-IV and UAM-V for three ozone episodes in Atlanta (two 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 (3) determine the acceptability of UAM-V.

PURPOSE OF THE PROTOCOL DOCUMENT

This protocol is intended to serve as the basis for determining the acceptability of UAM-V for use in 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, and model acceptance criteria. 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.

This protocol only specifically addresses the UAM-IV/UAM-V comparison. Following the comparison, the SIP demonstration protocol submitted by the State of Georgia will be revised if UAM-V is the model chosen for the attainment demonstration.

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 model comparison.

2. Development of baseline emission inventories for the Atlanta modeling domain.

3. Identification of 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. Documentation of the model comparison and submittal of the results for EPA review and approval.

SCHEDULE

The estimated schedule for performing model comparison is as follows:

• **Prepare protocol**	**May-August 1993**
• **Assemble Met/AQ data**	**July-August 1993**
• **Develop base-year inventories**	**May-August 1993**
• **UAM base case modeling analysis**	**July-November 1993**
• **UAM-V acceptability recommendation**	**November 1993**

DELIVERABLES

Documentation describing UAM input preparation, model performance evaluation, and performance intercomparison will be provided to the EPA at appropriate times during the model comparison study. Deliverables include:

- **Model Comparison Protocol** **31 August 1993**
- **Acceptability Recommendation (Technical Memorandum)** **30 November 1993**
- **Model Comparison Report** **1 January 1994**

MANAGEMENT STRUCTURE/TECHNICAL COMMITTEES

This section presents an overview of the management and technical committees that will be established to oversee the model comparison analysis. Systems Applications International (SAI) will perform the UAM-IV and UAM-V modeling work. The State of Georgia's Environmental Protection Division will prepare the emission inventories to be used in the comparison. The Georgia Institute of Technology will assist the state in preparing episode-specific emission inventories for 1992. The model comparison will be reviewed by three committees, the Modeling Policy Oversight Group, the Technical Work Group, and the Emission Inventory Work Group.

Modeling Policy Oversight Group

The Policy Oversight Group consists of Robert Collom, William Estes, and Marvin Lowry of the Georgia Environmental Protection Division (EPD), Kay Prince of EPA Region IV, Richard Scheffee of EPA OAQPS, Nancy Hirshberg of Georgia Power Company, John Jansen of Southern Company Services, and Dr. William Chameides of the Georgia Institute of Technology. This group will review the results of the model comparison study and participate in the UAM-V acceptability decision.

Technical Work Group

The Technical Work Group for this modeling project consists of Dale Kemmerick and Kenneth Powell of the Georgia EPD, Brenda Johnson of EPA Region IV, Richard Scheffee of EPA OAQPS, Nancy Hirshberg of Georgia Power Company, John Jansen of 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 Work Group will review the work performed by SAI and the state including selection of the UAM-V modeling domain, specification of initial and boundary conditions, diagnostic analysis, performance evaluation, comparison of UAM-IV and UAM-V performance, and determination of acceptability for UAM-V.

Emission Inventory Work Group

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 the group's responsibility to monitor the work performed by Georgia Environmental Protection Division and the Georgia Institute of Technology to assure conformity to the "Inventory Preparation Plan - 31 July 1991." Members of this group are: Ron Methier and Thomas Teston of Georgia EPD, Joey Levasseur of EPA Region IV, Chet Wayland of EPA OAQPS, Nancy Hirshberg of Georgia Power Company, John Jansen of 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 (the base year inventories for 1987, 1988, and 1992). This review will ensure that the inventory preparation procedures conform to those 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 Oxidant 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. Use of the ROM output will depend on the availability and reliability (relative to other methods of estimating boundary conditions) of the ROM simulation results.

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

Information regarding the modeling episodes; UAM-IV and UAM-V modeling domains; air quality, meteorological, and emission data bases; and the input preparation procedures that will be followed in the UAM-IV and UAM-V applications is provided in this section.

EPISODE SELECTION

For the attainment demonstration, two simulation periods (29 July - 1 August 1987 and 7-8 July 1988) and three primary episode days (31 July 1987, 1 August 1987, and 8 July 1988) have been identified. The 1987 days are part of a multi-day ozone episode. Within this episode, the first two days of the selected simulation period represent "build-up" days, the third is the day on which the maximum ozone concentration for the episode was recorded, and the fourth day is a "clean-out" day. One consideration in selecting the simulation period is to allow sufficient time at the beginning of the simulation for the model to simulate the ozone "build-up" that often precedes the peak exceedance and to minimize the effects of the initial conditions, which are not well known, on the simulation. Because high ozone concentrations were observed on 29 and 30 July, both of these days were selected as start-up days for the simulation of 31 July (the maximum observed ozone concentration increases steadily throughout the three-day period from 13.5 pphm on 29 July to 15.5 pphm on 30 July to 20.1 pphm on 31 July). Another consideration in the episode-selection process is that the modeling episodes should be chosen to represent the various types of meteorological conditions that are associated with ozone episodes in the nonattainment area. Although 1 August can be characterized as somewhat of a "clean-out" day, the meteorological conditions are sufficiently different from 31 July and the ozone concentrations are sufficiently high (the maximum is 16.9 pphm) that this day has been chosen as a second primary episode day.

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. 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; it will only be used to assess and compare the performance of UAM-IV and UAM-V.

In contrast to the attainment demonstration, model performance will be assessed on a per episode basis (for the 1987, 1988, and 1992 (SOS) episodes). The reason for this is that comparing model performance for two episode days that are part of the same simulation period could confound the comparison as model performance on back-to-back simulation days may be correlated.

If UAM-V is deemed acceptable, then all future-year modeling will be performed with 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 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, CO, and hydrocarbons; and supplemental meteorological measurements of winds, temperatures, and 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 SO_2 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 tethersondes 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 tethersondes, 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.

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

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	Mlk-EKMA, Atlanta	O_3

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

Site Name	Location UTM (Zone 16) UTMX	UTMY	Variables Measured
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

93094.03

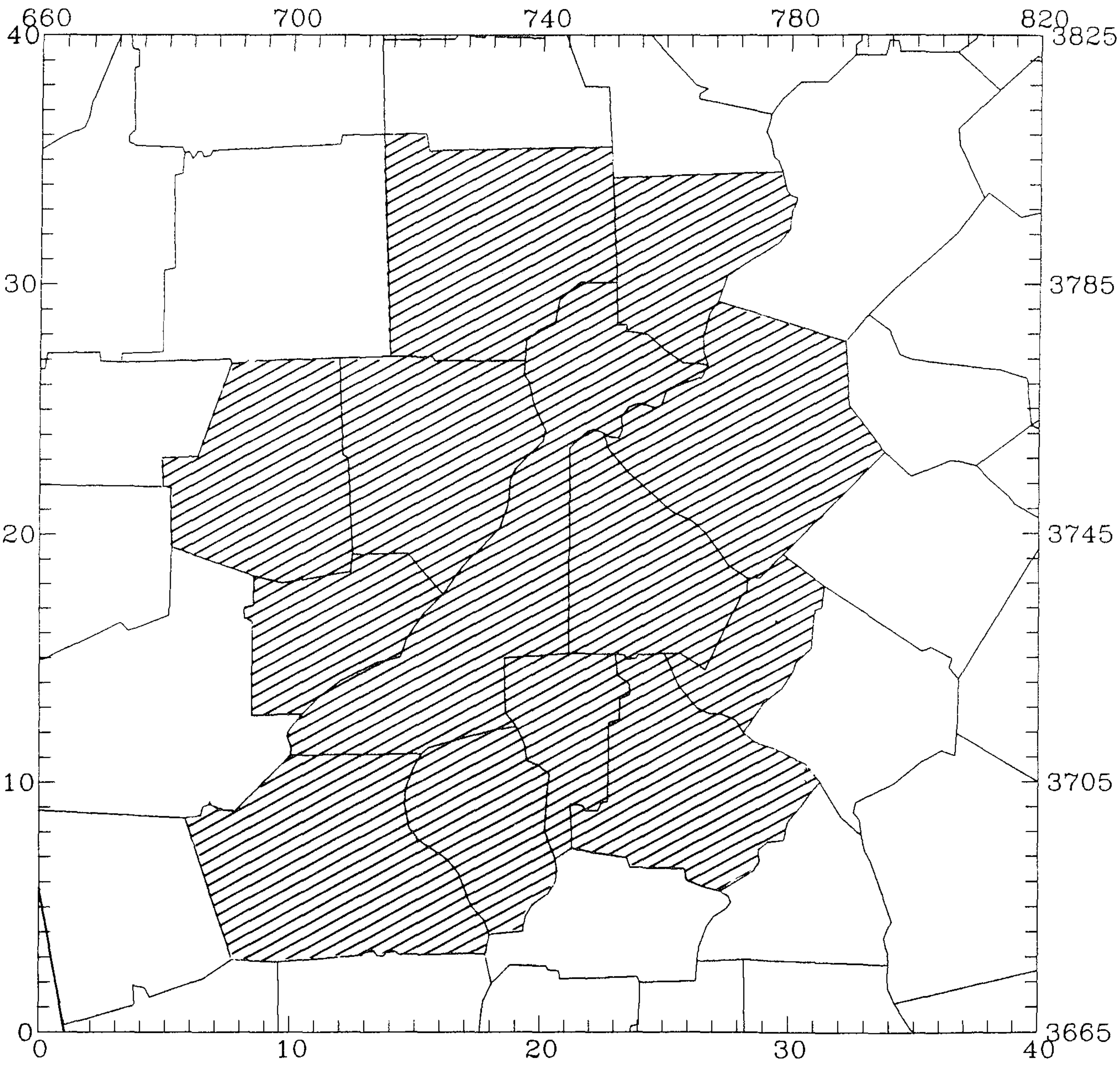

Figure 2-1. UAM-IV modeling domain for Atlanta. Domain consists of a 40 by 40 array of 4 km grid cell with an origin at UTM coordinates 660 km easting, 3665 km northing, zone 16. Stippled area depicts nonattainment area.

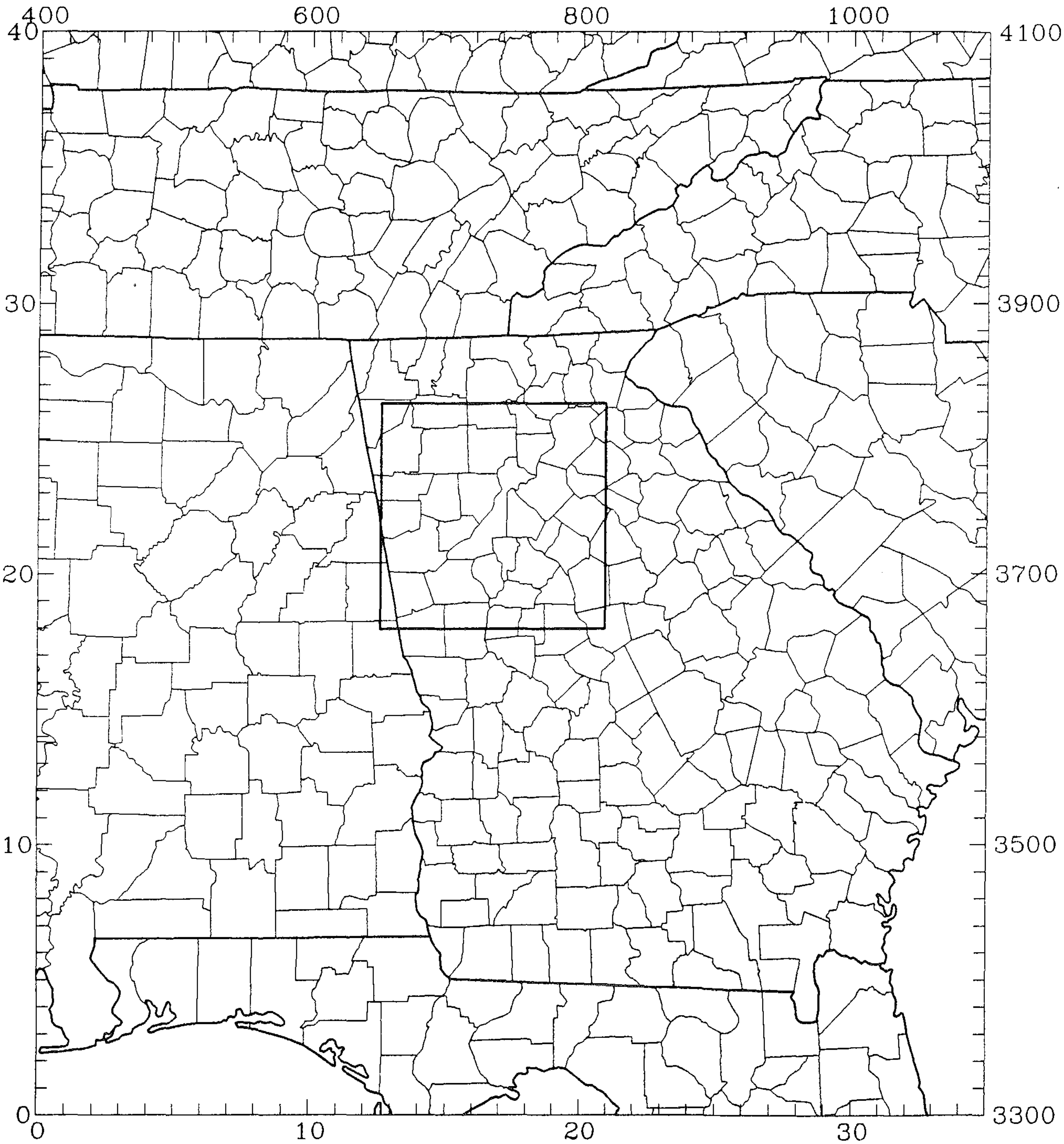

FIGURE 2-2. Geographical location of the UAM-IV modeling domain for Atlanta.

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.

The vertical structure for the UAM-V grid will be consistent with that of the prognostic meteorological model and will be determined upon analysis of the upper-air meteorological data. The same vertical structure will be used for all episodes. The top of the UAM-V modeling domain will be the same as the top of the UAM-IV modeling domain.

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 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 1990 modeling emission inventory which is under development for the UAM-IV domain will form the basis for both the UAM-IV and UAM-V modeling inventories. Those counties in the regional domain of UAM-V will use the EPA interim inventory. 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.

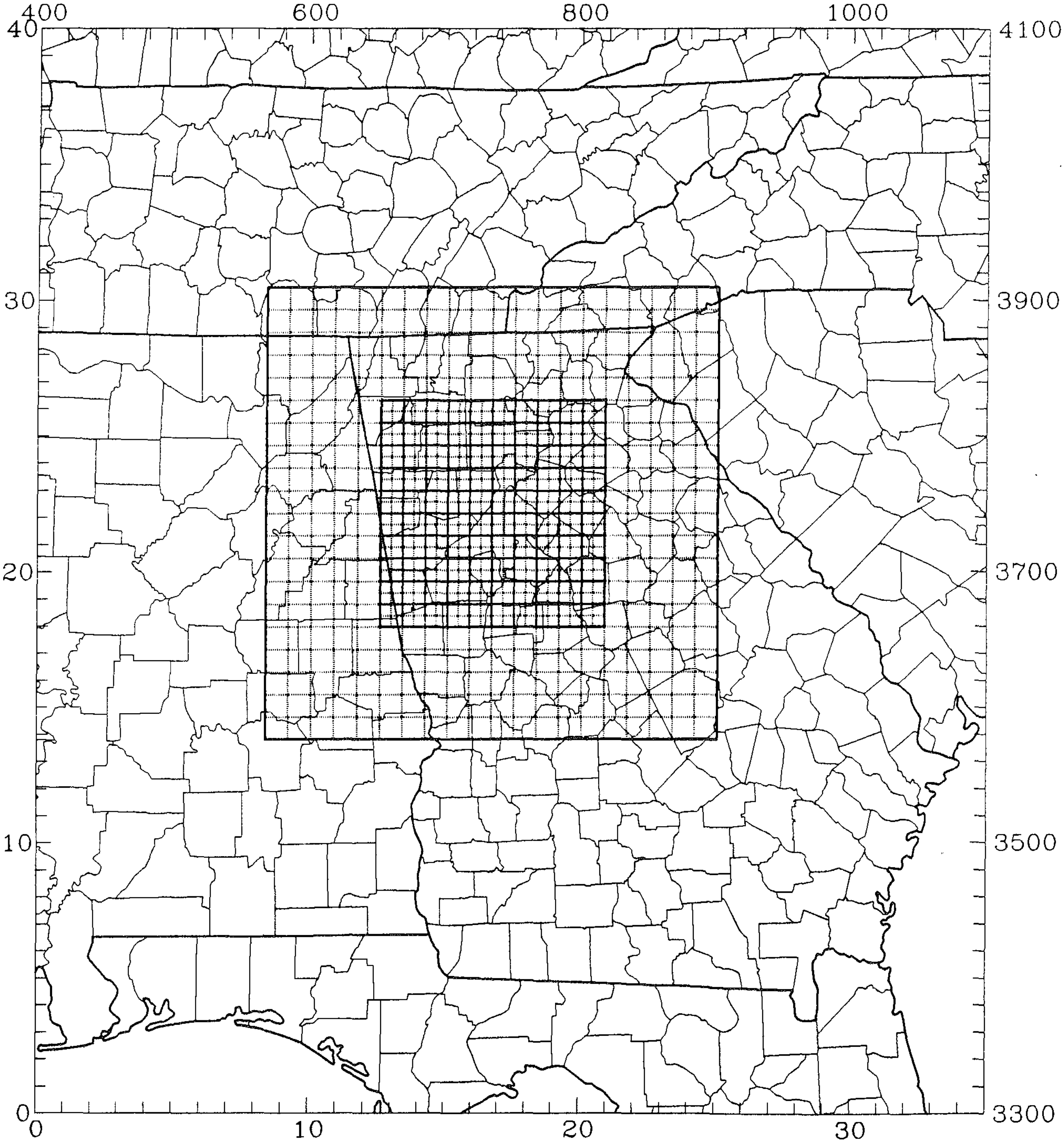

Figure 2-3. Preliminary UAM-V nested modeling domain for Atlanta. (Actual inner grid will consist of 40 by 40, 4 km cells, with 8 km cells in outer grid. For clarity of presentation, the size of the grid cells depicted in this figure are 8 km for inner grid and 16 km for outer grid)

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.

Non-road motor vehicles: Non-road motor vehicle emission estimates for the nonattainment counties will be obtained from the Aerometric Information Retrieval System (AIRS). Estimates for those counties that are outside of the nonattainment area will be extracted from the EPA 1990 interim inventory.

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.

In order to provide a dynamically consistent, physically realistic representation of the meteorological fields and, thus, to utilize the enhanced capabilities of the UAM-V (e.g., three-dimensional temperature and moisture fields, direct specification of the vertical exchange coefficients), the meteorological input preparation procedures will deviate from those outlined in the EPA UAM guidance document (EPA, 1991). The meteorological inputs will be prepared using the SAI Mesoscale Model (SAIMM), a prognostic, data-assimilating mesoscale meteorological model. To ensure agreement between the simulated fields and the observed meteorological data, observations will be incorporated into the prognostic model using a four-dimensional data assimilation (FDDA) procedure.

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

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.

<u>UAM-IV</u>: Not applicable.

<u>UAM-V</u>: Prepare based on UAM-V grid structure.

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

<u>UAM-IV</u>: Interpolate observed data to UAM-IV grid.

<u>UAM-V</u>: 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.

<u>UAM-IV</u>: Specify based on a regional analysis of air quality data, ROM output, or use EPA-recommended background concentrations.

<u>UAM-V</u>: Use EPA-recommended 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.

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.

EMISSIONS This file contains the ground-level emissions of all emitted species to be simulated for each hour and grid cell. Emissions will be processed using the Version 2.0 of the Emissions Preprocessing System (EPS). 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.

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: The vertical structure for the UAM-V grid will be consistent with that of the prognostic meteorological model and will be determined upon analysis of the upper-air meteorological data.

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.

METSCALARS

This file contains hourly values of the following spatially invariant meteorological parameters: NO_2 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.

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. The cut-offs will be determined following inspection of the emissions data (i.e., ranking of the sources by emission totals) and may be different for NO_x and VOC sources.

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.

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.

<u>UAM-IV</u>: Specify based on maximum mixing heights estimated for each episode.

<u>UAM-V</u>: Not applicable.

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

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

<u>UAM-V</u>: Derive from USGS data.

TEMPERATURE This file contains hourly, gridded temperatures.

<u>UAM-IV</u>: Only surface temperature is required; obtain from SAIMM output.

<u>UAM-V</u>: Three-dimensional array of temperatures is required; obtain from SAIMM output.

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.

<u>UAM-IV</u>: Obtain from USGS data.

<u>UAM-V</u>: Obtain from USGS data.

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

<u>UAM-IV</u>: Specify based on a regional analysis of air quality data, ROM output, or use EPA-recommended background concentrations.

<u>UAM-V</u>: Use EPA-recommended 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).

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.

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.

DIAGNOSTIC ANALYSIS

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. At a minimum, two diagnostic simulations will be performed. These include a simulation in which the emissions are set equal to zero and a simulation in which clean boundary conditions are imposed. As part of the diagnostic analysis a variety of graphical analysis techniques will be used to analyze the UAM simulation results. These will include (1) time-series plots of the observed and simulated pollutant concentrations, (2) contour plots showing isopleths of simulated pollutant concentrations and, where available, observed values for the surface monitors, and (3) vertical cross sections illustrating how the vertical profiles of pollutant concentrations vary in space and in time.

Any corrections or modifications to the model inputs resulting from the diagnostic analysis will be based on sound scientific principles, will not conflict with observed data, and will be thoroughly documented.

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).

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. Because the 1987 episode contains two "primary" episode days, the calculation of statistics for this episode will be slightly different than for the 1988 and 1992 episodes as noted below.

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

1) Unpaired accuracy of the peak (A_u) - (EPA goal: within $\pm$ 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:

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

where O_{max} and S_{max}, the observed and simulated maxima, respectively, are taken over all locations and times for the episode (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). For the 1987 episode, S_{max} will be the maximum simulated concentration for the simulation day on which the observed maximum occurs. The mean relative error (MRE) and mean unsigned relative error (MURE) are defined as follows:

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

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

where O_i is the i^{th} observation greater than or equal to 60 ppb, S_i is the i^{th} simulated value, and N is the number of observed hourly values greater than or equal to 60 ppb across all observation sites.

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 for each episode by calculating the following:

4) Spatially-paired average peak accuracy ($A_{avg,s}$)
   - all monitors, paired in space, not time (± 2 hours)

$$\textit{Spatially Paired Average Peak Accuracy} = \frac{\sum_{i=1}^{N} \frac{O_{\max,i} - S_{\max_{/\Delta t/ \leq 2},i}}{O_{\max,i}}}{N}$$

where $O_{\max,i}$ is the observed maximum concentration at monitoring site i, $S_{\max_{/\Delta t/ \leq 2},i}$ is the simulated maximum concentration of monitoring site i that occurs within two hours of the time of the observed maximum, and N is the number of monitoring sites. For the 1987 episode, a two-day average will be computed, thus *N* represents the number of monitoring sites times two.

5) Temporally-paired average peak accuracy ($A_{avg,t}$)
   - all monitors, paired in time, not space (9 grid cells)

$$\textit{Temporally Paired Average Peak Accuracy} = \frac{\sum_{i=1}^{N} \frac{O_{\max,i} - S_{\max,i \pm \Delta x}}{O_{\max,i}}}{N}$$

where $O_{\max,i}$ is the observed maximum concentration at monitoring site i, $S_{\max,i + \Delta x}$ is the simulated maximum concentration selected from the nine grid cells surrounding monitoring site i, and N is the number of monitoring sites. For the 1987 episode, a two-day average will be computed, thus *N* represents the number of monitoring sites times two.

6) Unpaired station average peak accuracy ($A_{avg,u}$)
   - all monitors, unpaired in time or space (± 2 hours, 9 grid cells)

$$\textit{Unpaired Average Peak Accuracy} = \frac{\sum_{i=1}^{N} \frac{O_{\max,i} - S_{\max_{/\Delta t/ \leq 2},i \pm \Delta x}}{O_{\max,i}}}{N}$$

where $O_{\max,i}$ is the observed maximum concentration at monitoring site i, $S_{\max_{/\Delta t/ \leq 2},i}$ is the simulated maximum concentration within two hours of the observed maximum and selected from the nine grid cells surrounding monitoring site i, and N is the number of monitoring sites. For the 1987 episode, a two-day average will be computed, thus *N* represents the number of monitoring sites times two.

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 $\pm$ 2 hours and 20 km. The optimal temporal and spatial shift calculated for each episode day are those that minimize the root mean square error. Averages of these measures will be computed for the 1987 episodes. 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, scores for measures 4-6 will be averaged together, and scores for 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):

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

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

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

Accuracy parameters (ACCURACY):

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

Spatial shift (Δx):

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

Temporal shift (Δt):

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

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 when the comparison is "too close to call." The total score for each model will then be calculated as follows:

$$SCORE = POINTS_{Au} + POINTS_{MRE} + POINTS_{MURE} +$$

$$(POINTS_{Aavg,s} + POINTS_{Aavg,t} + POINTS_{Aavg,u})/3. +$$

$$(POINTS_{\Delta x} + POINTS_{\Delta t} + POINTS_{MREopt} + POINTS_{MUREopt})/4.$$

Scores will be computed and compared for each of the episodes separately.* If $SCORE_{UAM\text{-}V}$ is the same as or better than $SCORE_{UAM\text{-}IV}$, then UAM-V will be judged to perform acceptably for the episode. Judgement in favor of UAM-V in the case of a "tie" score reflects consideration of technical merit. To determine the acceptability of UAM-V, the model would have to perform better than UAM-IV for two of the three episodes.

In the event that the UAM-V is selected for application to the Atlanta nonattainment area and the UAM-V simulated ozone concentrations are biased low compared to both the observations and the UAM-IV simulated concentrations, the reasons for this bias will be investigated and the results of the investigation will be provided as part of the comparison documentation.

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* 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 the primary episode day of the 1988 and 1992 episodes.

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Morris, R. E., T. C. Myers, E. L. Carr, M. C. Causley, S. G. Douglas, and J. L. Haney. 1990. *User's Guide for the Urban Airshed Model, Volume II: User's Manual for the UAM (CB-IV) Modeling System.* U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park (EPA/4-90-007B) (NTIS No: PB91-131235).