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The Ozone Transport Assessment Group: Modeling Activities

Michael Koerber
Lake Michigan Air Directors Consortium
Des Plaines, Illinois

Joseph Tikvart
U.S. Environmental Protection Agency
Research Triangle Park, North Carolina

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INTRODUCTION

Summertime weather conditions can lead to elevated ozone concentrations which approach or exceed the National Ambient Air Quality Standards (NAAQS) for ozone across a large portion of the eastern U.S.[1,2,3] These elevated concentrations, through transport, make it difficult for individual urban areas to demonstrate attainment of the ozone NAAQS. These urban areas have found that it will take significant reductions in both local ozone precursor emissions and incoming (transported) ozone and ozone precursor concentrations in order to show attainment.

In recognition of the transport problem, the U.S. Environmental Protection Agency (USEPA) established a two-phase program for states to develop approvable ozone State Implementation Plans (SIPs). In a policy memorandum dated March 2, 1995, USEPA outlined the major elements of this program.[4] Phase I requires states to complete pre-November 1994 SIP requirements, submit regulations sufficient to meet the initial Rate of Progress requirements, and submit modeling analyses. Phase II calls for a two-year (1995-1996) consultative process to assess national and regional strategies to deal with ozone transport in the eastern U.S., and subsequent revisions of local control plans, as necessary, based on any new national or regional strategies.

To accomplish the Phase II consultative process, the Environmental Council of the States (ECOS), in conjunction with USEPA, established the Ozone Transport Assessment Group (OTAG). The goal of OTAG is to identify and recommend a strategy to reduce transported ozone and its precursors which, in combination with other measures, will enable attainment and maintenance of the ozone NAAQS in the eastern U.S. A number of criteria will be used to select the strategy including, but not limited to, cost-effectiveness, feasibility, and impacts on ozone levels. A modeling study will be performed to quantify the ozone impacts. This study consists of the following five tasks:

* prepare appropriate photochemical model inputs for several periods of elevated ozone concentrations (i.e., ozone episodes);
* perform basecase photochemical model simulations for these episodes;
* perform an operational evaluation of the basecase simulation to assess model performance;
* perform sensitivity tests to examine the response of the model to changes in certain model inputs; and
* apply the model to examine the effect of current, expected, and possible additional national and regional control strategies on the transport of

ozone and ozone precursors in the eastern U.S.

The purpose of this paper is to summarize the plans for the OTAG modeling study.

EXPECTATIONS

The expectations of those using the OTAG modeling results should be consistent with the following key points:

* The modeling will focus on interstate and interregional transport. Consequently, the results should not be used to address local regulatory issues, such as individual urban area attainment demonstrations. (Individual states/regions are responsible for performing the necessary urban modeling analyses.)

* The modeling will not provide future year boundary conditions for every episode and future year of interest for every urban modeling domain. (Individual states/regions are responsible for preparing the specific boundary conditions for any subsequent urban modeling analyses.)

* The limited number of episodes which will be modeled may not represent all possible transport patterns or all possible nonattainment conditions.

* Models are tools for helping decision makers understand air quality problems and evaluate potential control strategies. Models are most reliable for directional and relative assessments.

* The decision to apply the models for this study is an attempt to take advantage of their capabilities at their current state of development. Evolution and improvement of the models and the underlying data bases in the future should be expected.

OVERVIEW OF MODELING SYSTEM

The modeling study will employ the following models:

EMS-95 The EMS-95 emissions model will be used to provide emissions inputs for the photochemical models.[5] EMS-95 spatially distributes, temporally allocates, and chemically speciates user-supplied emissions for point and anthropogenic area sources; and calculates emissions for motor vehicles for each grid cell and each hour, and then chemically speciates them.

The primary emissions database is USEPA's new National Inventory, which is the product of a recent effort initiated by USEPA and ECOS. Biogenic emissions will be prepared using either BEIS or BEIS2. Base year inventories for each episode year (for basecase modeling) and future year inventories for 1999 and 2007 (for strategy modeling) will be derived from the National Inventory, which reflects 1990 conditions.

RAMS

The RAMS prognostic meteorological model will be used to provide meteorological inputs for the photochemical models.[6] Observed meteorological data will be incorporated into the RAMS predictions using a four-dimensional data assimilation (FDDA) procedure.

Another prognostic meteorological model, SAIMM (which is derived from an earlier version of RAMS), has already been used to prepare meteorological fields for the July 1988 episode. Given the similar lineage of RAMS and SAIMM and the limited resources of this project, the existing SAIMM fields will be used for this episode.

UAM-V

Version 1.23 of the UAM-V regional/superregional photochemical grid model will be used to predict ozone and ozone precursor concentrations.[7] This is essentially the same model used in the MOCA modeling study.[8] UAM-V is an enhanced version of the current USEPA guideline version of the UAM model. It incorporates many new features including variable nested-grids, a user-defined vertical grid structure, updated dry deposition, updated photolysis rates, a Plume-in-Grid (PiG) algorithm for treating point source plumes, and use of three-dimensional inputs for meteorological variables, such as, temperature, water, vapor, and pressure.

A select number of simulations will also be performed with ROM to confirm the UAM-V results and to provide a "bridge" to the extensive set of ROM results which have been used by a number of states to support their current SIP development efforts.

EPISODES

The OTAG modeling will examine transport during periods of elevated ozone concentrations in the eastern U.S. Due to time constraints and the limited level of ozone and ozone precursors in the eastern U.S.

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EPISODES

The OTAG modeling will examine transport during periods of elevated ozone concentrations in the eastern U.S. Due to time constraints and the limited level of resources currently identified, the modeling will only be able to consider four episodes. The primary criteria for selecting these episodes are consistency with current SIP modeling and existence of interregional transport. The following four episodes have been selected for modeling (see Figure 1):

July 1 - 15, 1988

July 13 - 21, 1991

July 20 - 30, 1993

July 7 - 18, 1995

Examination of surface ozone concentration maps, synoptic weather maps, and trajectory analyses show that these episodes all involve intraregional and interregional transport.

MODELING DOMAIN AND GRID CONFIGURATION

The modeling domain must be large enough to minimize the influence of boundary conditions, encompass the relevant synoptic scale weather systems, and include all possibly culpable emission source regions. Based on prior experience with superregional modeling in the eastern U.S., the SUPROXA domain appears to fulfill these requirements adequately and will be used for this study.

UAM-V can use either a Cartesian or latitude/longitude coordinate system. A latitude/longitude coordinate system is preferable for large domains, such as SUPROXA, to avoid distortion along the edges of the domain. Although EMS-95 can use a latitude/longitude coordinate system, RAMS uses a polar stereographic projection coordinate system. Thus, the RAMS output must be mapped to the latitude/longitude system.

The UAM-V modeling domain includes two grids (see Figure 2):

Grid A: 1/9° latitude, 1/6° longitude (approx. 12 km) horizontal spacing and 7 vertical layers over the eastern U.S. (137 x 110 x 7 grid cells)

SW Corner: -92 °W, 32°N
NE Corner: -69.5°W, 44°N

Grid B: 1/3° latitude, 1/2° longitude (approx. 36 km) horizontal spacing and 5 vertical layers over the SUPROXA domain (64 x 63 x 5 grid cells)

SW Corner: -99°W, 26°N
NE Corner: -67°W, 47°N

This grid configuration will result in 19,102 grid cells in the surface layer and 125,650 grid cells in total. (Subsequent references to the horizontal grid resolution will be expressed in terms of the UTM equivalents because they are easier to comprehend.)

The vertical layer structure for UAM-V is as follows:

Five Layers	0-100 m, 100-500 m, 500-1500 m, 1500-2500 m, and 2500-4000 m
Seven Layers	0-50 m, 50-100 m, 100-250 m, 250-500 m, 500-1500 m, 1500-2500 m, and 2500-4000 m

The top of the modeling domain (4000 m) is specified to be higher than the typical summertime mixing height in this part of the country.

Hourly, gridded, speciated estimates of ozone precursor emissions will be prepared for this domain with 12 km resolution. Emissions for Grid B will be developed by aggregating the 12 km resolution emissions to the 36 km grid.

Meteorological fields will be prepared for this domain by applying RAMS with a 108 km grid over the continental U.S., and nested 36 km and 12 km grids which roughly correspond to Grids A and B. Vertical resolution will consist of 29, 24, and 20 layers in the 108 km, 36 km, and 12 km grids, respectively.

MODEL APPLICATION

Three types of modeling analyses are planned. First, basecase simulations will be performed and compared to ambient measurements for the purpose of evaluating model performance. A number of numerical and graphical performance measures will be considered. The performance evaluation will focus on the model's ability to reproduce the magnitude, spatial pattern, and temporal profile of observed ozone and ozone precursor concentrations.

Second, several sensitivity tests will be performed to provide some general information to guide the development of control strategies. A desirable feature of these tests is that the model inputs can usually be prepared quickly and easily; thereby, allowing many model simulations to be conducted. A list of the expected first round of sensitivity tests is provided in Table 1.

Third, actual control strategies will be modeled. Two sets of strategies will be identified: Phase I and post-Phase I. The Phase I strategy includes all existing (or expected) national, regional, and nonattainment area control measures. Examples of these measures are national programs for motor vehicles, commercial and consumer solvents, architectural coatings, and small engines; the low emission vehicle and NOx control initiatives in the Ozone Transport Region; and individual state 15% plans. The post-Phase I strategies include candidate additional national and regional control measures.

Because the focus of the OTAG modeling is on transport, and not on demonstrating attainment, a number of different metrics will be used to summarize the modeling results. Table 2 identifies the list of metrics to be used for this study.

ORGANIZATIONAL STRUCTURE AND RESPONSIBILITIES

The OTAG modeling organizational structure, which is shown in Figure 3, identifies the models to be used and the responsibilities for each portion of the modeling work. The Co-Chairs of the Regional and Urban Scale Modeling (RUSM) Workgroup will provide day-to-day management of the study.

All model inputs will be developed centrally. A contractor will prepare inputs for the emissions model. The State of Wisconsin will perform prognostic meteorological modeling to prepare meteorological inputs for the photochemical model.

Individual modeling centers will perform all emissions and photochemical modeling for a given episode. July 1988 will be modeled by the USEPA modeling center, July 1991 by the Midwest modeling center, July 1993 by the Southeast modeling center, and July 1995 by the Northeast modeling and analysis center. A number of coordination activities have been identified to ensure consistency between the modeling centers.

To accommodate other groups wishing to perform superregional modeling, the following ground rules have been established to ensure acceptance of these results in the OTAG process:

(1) **PROTOCOL:** Provide written summary of modeling plans (or agree to follow OTAG modeling protocol)

(2) **INPUTS:** Use OTAG-generated model inputs (or improved inputs, as

determined by the RUSM co-chairs)

(3) **MODELS:** Use same version/configuration of OTAG emissions, meteorological, and photochemical models, and pass a benchmark simulation

If proposing to use a different model (or a different version/configuration of an OTAG model), then it will be necessary to provide both: (a) an acceptable explanation on how these modeling results will be coordinated/reconciled with the OTAG modeling results; and (b) a model performance evaluation conducted in accordance with the OTAG procedures.

(4) **OUTPUT:** Provide hardcopy of certain outputs (to be specified by the RUSM Workgroup co-chairs) and electronic copy of inputs and outputs

DATA AVAILABILITY

A data clearinghouse will be established to ensure the ready availability of key emissions, observed, and modeling data. The basic goal of the clearinghouse is to provide reliable, centralized data management which fosters exchange of key data elements. It is the responsibility of each Modeling Center to provide data to the clearinghouse. These data will consist of electronic versions of basic model input and output files. It is the responsibility of the clearinghouse to receive data; store and provide open access to data; and provide copies of data, upon request.

SCHEDULE

The OTAG modeling study must be completed by September 30, 1996. This deadline is necessary to allow the Policy Group sufficient time to formulate strategies recommendations by the end of 1996, in accordance with the schedule for the two-year consultative process established in USEPA's March 2, 1995 memo. To ensure timely completion of the modeling, the following interim milestones have been proposed.

MODEL SET-UP

August 1995	Select first set of episodes to model
October 1995	Recommend modeling system and select final set of episodes to model
Jan - Feb 1996	Develop basecase model inputs (emissions and meteorology)

BASECASE MODELING

Jan - Mar 1996	Perform basecase modeling
April 1996	Perform analysis and interpretation of basecase modeling
Mar - May 1996	Perform sensitivity analyses with basecase modeling

STRATEGY MODELING (PHASE I MEASURES)

May - June 1996	Perform strategy modeling with Phase I controls
June 1996	Perform analysis and interpretation of strategy modeling with Phase I controls

STRATEGY MODELING (POST-PHASE I MEASURES)

June - Sept 1996	Perform strategy modeling with post-Phase I controls
September 1996	Complete final analysis and interpretation of strategy modeling with post-Phase I controls

CONCLUSIONS

The OTAG modeling study will provide information to help answer questions about the significance of ozone and ozone precursor transport, and the relative effectiveness of controls (on both a pollutant and geographic basis) in reducing transported ozone and ozone precursor concentrations in the eastern U.S. based on present understanding of the science. The study is unique in its attempt to both bring together the numerous stakeholders and employ state-of-the-art models and up-to-date data bases, which should enhance the political and technical acceptability of the modeling results.

REFERENCES

1. "Rethinking the Ozone Problem in Urban and Regional Air Pollution", National Research Council, 1991.

2. "The State of the Southern Oxidants Study (SOS): Policy-Relevant Findings in Ozone Pollution Research, 1988-1994", prepared by W.L. Chameides and Ellis B. Cowling on behalf of the SOS Science Team and the SOS Coordinating Council, April 1995.

3. "Air Quality Data Analysis for the 1991 Lake Michigan Ozone Study", Final Report STI-92022-1410-FR, September 1994, Sonoma Technology Incorporated, Santa Rosa, California.

4. Memorandum entitled "Ozone Attainment Demonstration" from Mary Nichols (Director, Office of Air and Radiation) to Regional Administrators dated March 2, 1995.

5. "The Emissions Modeling System (EMS-95) User's Guide", July 1, 1995, Alpine Geophysics, Boulder, Colorado.

6. "RAMS, The Regional Atmospheric Modeling System, Version 3a, User's Guide", November 1993, ASTeR, Inc., Fort Collins, Colorado.

7. "User's Guide, Lake Michigan Ozone Study, Photochemical Modeling System", Volumes I - III, October 1993, Systems Applications International, San Rafael, California.

8. "Application of UAM-V to the Northeast as Part of Phase I of the Modeling Ozone Cooperative (MOCA)", Draft Final Report SYSAPP-95/049d, August 8, 1995, Systems Applications International, San Rafael, California.

Table 1. First Round of Sensitivity Tests

Biogenic Emission Runs

A Basecase w/BEIS and w/BEIS2

A Basecase w/BEIS and w/BEIS2 for -0% VOC(anthropogenic)/-50% NOx

A Basecase w/BEIS and w/BEIS2 for -50% VOC(anthropogenic)/-0% NOx

1. Phase I (or Proxy)

B a. Phase I (or proxy) with 0% VOC/0% NO_x

2. Nonattainment/Urban Attainment/Rural Attainment

F a. Phase I (or proxy) with -30% VOC (all anthropogenic)/-15% NO_x (all low level emissions) in urban attainment areas

F b. Phase I (or proxy) with -30% VOC (all anthropogenic)/-15% NO_x (all low level emissions) in all attainment areas

F c. Phase I (or proxy) with -30% VOC (all anthropogenic)/-15% NO_x (all low level emissions) in all areas

3. Point Source Impacts

D a. Phase I (or proxy) with 0% VOC (all anthropogenic)/-60% NO_x (elevated point source emissions)

D b. Phase I (or proxy) with 0% VOC (all anthropogenic)/-30% NO_x (elevated point source emissions)

D c. Phase I (or proxy) with 0% VOC (all anthropogenic)/-30% NO_x (low level point source emissions)

4. Mobile Source Impacts

E a. Phase I (or proxy) with -30% VOC (mobile source emissions)/-15% NO_x (mobile source emissions)

5. Mixed Impacts

E a. Phase I (or proxy) with -30% VOC (mobile source emissions)/-15% NO_x (mobile source emissions) and -60% NO_x (elevated point source emissions)

E b. Phase I (or proxy) with -30% VOC (mobile source emissions)/-15% NO_x (mobile source emissions) and -30% NO_x (elevated point source emissions)

B c. Phase I (or proxy) with -30% VOC (all anthropogenic)/-60% NO_x (elevated point source emissions) and -30% NO_x (all low level emissions)

B d. Phase I (or proxy) with -30% VOC (all anthropogenic)/0% NO_x

B e. Phase I (or proxy) with 0% VOC/-60% NO_x (elevated point source emissions) and -30% NO_x (all low level emissions)

6. Regional Impacts

C a. 5c (or 5e)* in NE

C b. 5c (or 5e)* in MW

C c. 5c (or 5e)* in SE

C d. 5c (or 5e)* in SW

* = selection of 5c or 5e here to be made based on results of 5c and 5e runs

Table 2. Model Metrics

AREA	OBJECTIVE METRICS	SUBJECTIVE METRICS
SUPROXA - Grid B		* Map of peak 1-hour surface ozone * Map of peak 8-hour surface ozone * Map of 1-hour surface ozone differences (max diff) * Map of peak 1-hour aloft ozone (Layer 3: 500 - 1500 m) * Time series plots for key sites
SUPROXA - Grid A		
Regions (4)		
Subregions (13)	* Peak 1-hour surface ozone * Peak 8-hour surface ozone * Number of grid cells in the following ranges: <85, 85-124, 125-144, 145-164, >164 ppb * Daily "dosage" of ozone in the following ranges: <85, 85-124, 125-144, 145-164, > 164 ppb * Number of grid cells with ozone increases in the following ranges: <-10, -10 to -5, -5 to 0, 0 to +5, +5 to +10, > +10 ppb * Average daily ozone, NOy, and ROG for Layers 1-2 (0-100 m), Layers 3-4 (100-500 m), Layer 5 (500-1500 m), and Layers 6-7 (1500-4000 m) along each boundary of each subregion	

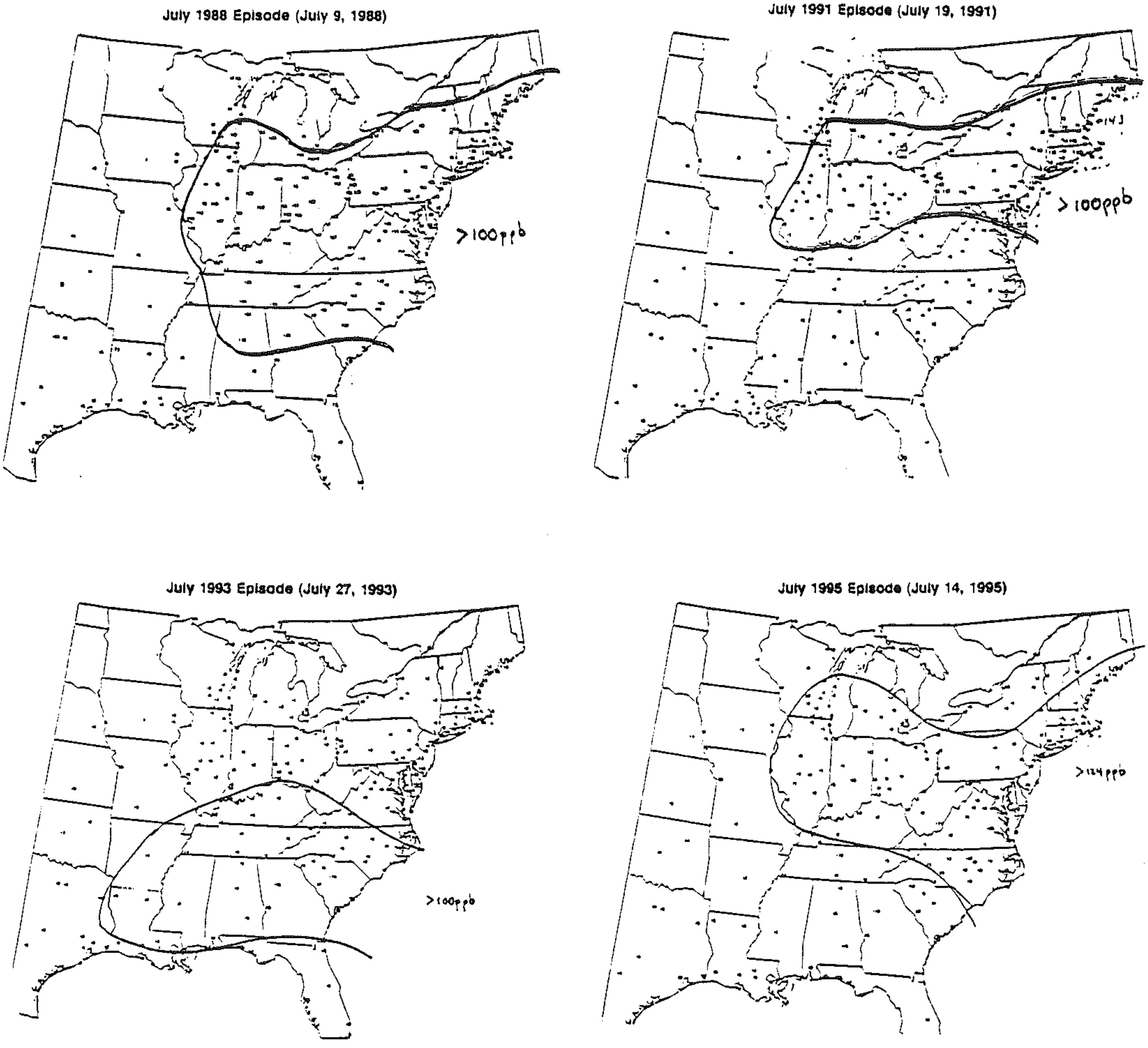

Figure 1. OTAG Modeling Episodes

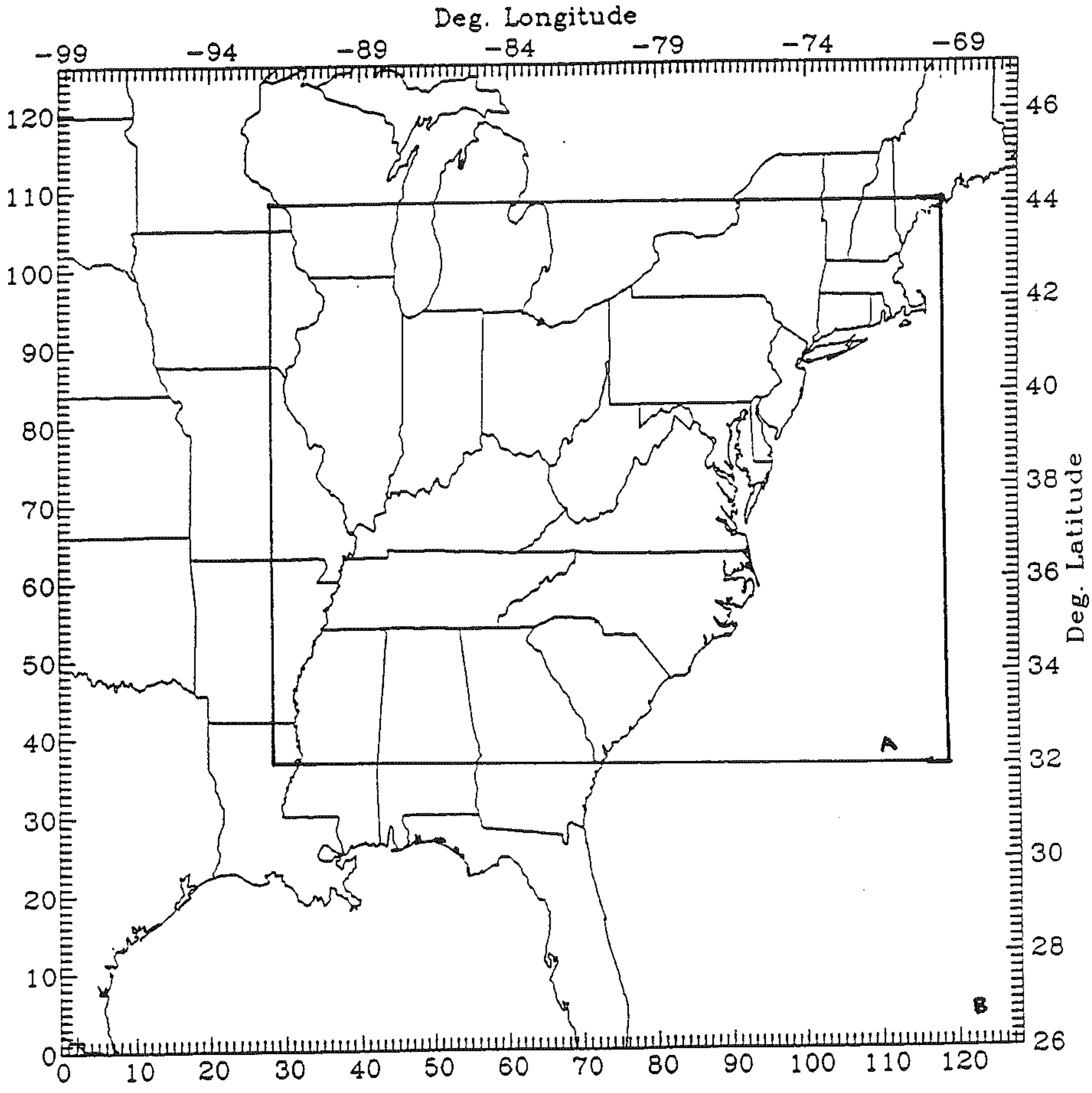

Figure 2. UAM-V Modeling Grid Configuration

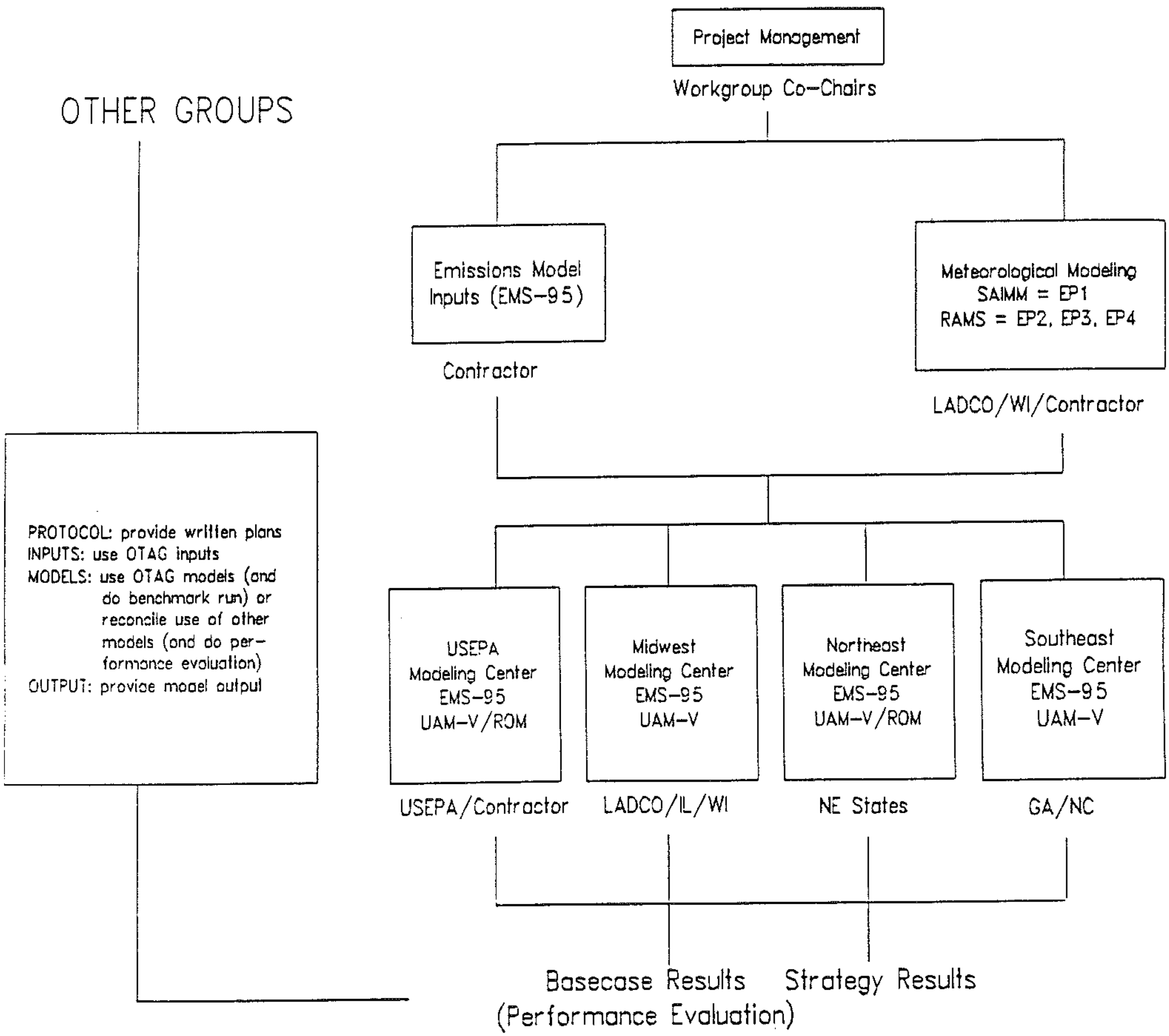

Figure 3. OTAG Modeling Organizational Structure