Technical Memorandum

SUGGESTED PROCEDURES FOR ESTABLISHING BOUNDARY CONCENTRATION INPUTS FOR URBAN AIRSHED MODEL APPLICATIONS IN THE LAKE MICHIGAN OZONE STUDY

Prepared for

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INTRODUCTION

This memorandum provides recommendations for establishing boundary concentration inputs for Urban Airshed Model (UAM) applications in the Lake Michigan Ozone Study (LMOS). These model inputs are important for two reasons. First, significant quantities of ozone and its precursors may be transported across the boundary of the UAM modeling region during the course of an ozone episode. Under such conditions, the success of model evaluation efforts will depend on the ability to accurately specify the spatial and temporal character of these inputs. Second, emission controls will very likely be implemented in source regions upwind of the LMOS study area. The effect of such controls on inflow pollutant levels in future years may have an important bearing on decision making in the LMOS.

In planning the LMOS, two approaches have been taken to address the boundary concentration issue. First, the design of the 1991 field measurement program contains provisions for collecting pollutant concentration data in upwind areas. These plans include the continuous operation of surface monitoring sites in the southern and western areas of the study region. In addition, instrumented aircraft will be used during episode conditions to characterize pollutant levels aloft along portions of the southern and western portions of the modeling region. When available, this combination of surface and airborne measurements should provide a good basis for establishing current boundary concentration levels. However, data aloft will not be collected on a continuous basis or along all portions of the upwind boundaries. Thus, other means must be identified for setting boundary concentration inputs when suitable data are not available. In addition, current measurements will be of limited value in setting future year boundary concentration levels, especially if significant changes occur in upwind emissions areas resulting from a combination of increases (or decreases) in emissions activity levels and the effects of emission controls.

In recognition of the regional character of the ozone problem, the EPA has developed the Regional Oxidant Model (ROM). This model is designed to study ozone formation over large subcontinental areas and will be applied by the EPA to a large region encompassing the LMOS study area. Simulations will be conducted for time periods that include the episodic periods to be modeled with the UAM. In principle, the ROM simulation results in the vicinity of the LMOS study area can be used to establish the boundary concentration inputs to the UAM. An important feature of ROM is that it can be used to explicitly treat the influence of future year emissions changes in the areas upwind of the LMOS study area on ozone and precursor levels at the LMOS modeling boundary. Thus, ROM also provides an attractive means for establishing future year boundary concentration inputs to the UAM.

Before the ROM results can be used to establish current or future boundary conditions, it must first be demonstrated that the model provides accurate concentration predictions, especially along the upwind boundaries. Since ROM has undergone only limited evaluation to date, a key issue is whether ROM model performance will be judged adequate for establishing boundary concentration inputs to the UAM. How boundary concentrations should be determined when the ROM model predictions do not agree with the available measurements collected along the boundary is another important technical issue.

The primary objective of this document is to describe a process for establishing UAM boundary concentration inputs. Note that a detailed specification of how boundary values should be determined must await the collection and analysis of the summer 1991 LMOS field data and the results of the ROM performance evaluation activity. The proposed approach for establishing boundary concentration inputs consists of three activities:

> Develop evaluative information concerning (1) the potential importance of boundary concentration inputs to UAM evaluation and application efforts and (2) the adequacy of ROM model performance.
>
> Determine the quality of available pollutant concentration data collected at the surface and aloft.
>
> Establish procedures for setting boundary concentration inputs.

The following sections elaborate on the scope of these three activities.

DEVELOP EVALUATIVE INFORMATION

The objectives of this activity are (1) to develop basic information concerning how potentially important boundary concentration inputs are to the determination of ozone and precursor levels within the LMOS study region, and (2) to assess the adequacy of the ROM model performance and its suitability for use in establishing boundary concentration inputs to the UAM.

A series of UAM sensitivity runs should be made to determine the potential importance of boundary concentration inputs on calculated ozone and precursor levels within the LMOS modeling domain. Estimates of uncertainties in boundary values will need to be developed. Data collected at upwind surface sites and from the instrumented aircraft should provide information with which to characterize the spatial and temporal variations of boundary concentration levels. In general, boundary ozone and precursor values may range from natural background levels to much higher values observed in and downwind of significant source areas.

The ROM performance evaluation results must be reviewed to determine whether the model is providing accurate pollutant concentration predictions. In general, the evaluation should be as stressful as the data will allow. If the model results are in good agreement with the observations (both at the boundary of the LMOS region and in areas upwind of the LMOS region), then some confidence can be placed in the usage of the results for specifying boundary concentration inputs to the UAM.

If the ROM results are not deemed fully adequate, then a set of comparative studies should be carried out to assess the relative importance of both formulation and data limitation issues. Model formulation issues may be related to the use of three vertical grid layers and a fixed horizontal grid resolution. Good agreement between ROM and UAM results for a similar situation will provide further credibility to the ROM results. To assess ROM model formulation limitations, the following comparison studies should be performed:

> Examine vertical grid limitations by applying both UAM and ROM to the LMOS study region using 3 vertical layers in each model. Then develop UAM results for the LMOS study region using six and eight vertical layers.
>
> Examine the importance of horizontal grid resolution by applying the UAM to the LMOS study region using both single resolution and nested, variable horizontal grid resolution.
>
> Assess the feasibility of applying the UAM to the ROM subcontinental modeling domain. If feasible, perform a model intercomparison study.

The feasibility of the studies cited above should be carefully examined. Since the models employ different grid systems, it may be difficult to construct identical input data sets. In addition, these model comparison studies are likely to require significant labor and computer resources, which may necessitate the identification of supplemental sources of funding.

Inadequate performance of ROM may also be associated with shortcomings in the inputs to the model. The following ROM and UAM intercomparison studies may prove insightful:

> Apply both UAM and ROM to the LMOS study region and develop inputs using the LMOS data base. Good agreement with the

observations and comparable model results would provide confidence that ROM provides a good representation of the basic physical and chemical processes that influence ozone formation.

Apply both UAM and ROM to the subcontinental modeling region and perform a side-by-side performance evaluation and intercomparison.

Apply both UAM and ROM to the LMOS study region. Evaluate both models using the full LMOS data base. Then degrade the LMOS data base to represent data typically available at the regional scale and reevaluate model performance. Apply both models using three vertical levels; also apply the UAM using eight levels.

In all of the studies cited above, we recommend that (1) traditional comparisons of calculated and measured concentrations be made at the various observation sites, and (2) comparisons of results also be made at downwind "arbitrary" flux planes.

DETERMINE THE QUALITY OF DATA AT THE BOUNDARIES

The air quality data collected at surface stations and by the instrumented aircraft that are to fly along the southern and western boundaries of the LMOS study area will serve as an important source of information concerning boundary concentration levels. However, this information is also subject to measurement uncertainties. To effectively use this information in characterizing boundary concentrations, the measurement uncertainties should be quantified. For example, model predictions may be deemed acceptable if they fall within the range of uncertainty of the measurements.

Recommended activities to be carried out in this area include:

Develop quantitative estimates of data uncertainties based on an analysis of appropriate project QA information.

Assess the representativeness of data collected at surface stations situated near the boundary of the LMOS region.

Evaluate the consistency of surface and aircraft pollutant concentration data.

Analyze available data to determine under what conditions and to what heights surface data can be used to provide reasonable estimates of pollutant concentration levels aloft.

We recommend that the appropriate analyses be integrated into the activities to be conducted by the LMOS data analysis and quality assurance contractors.

SPECIFY PROCEDURES FOR ESTABLISHING BOUNDARY CONCENTRATION INPUTS

This section discusses a general approach for establishing boundary concentration inputs for both base case and future year UAM simulations. Ideally, the modeling contractor would establish boundary concentration inputs for the UAM using the ROM simulation results. However, it is unclear at this time that the performance of ROM will be deemed adequate. Thus, various alternatives are considered for setting boundary concentration inputs.

Specify Boundary Concentrations for Base Case Simulations

The recommended procedure for specifying boundary concentrations in base case (summer 1991) simulations is as follows. If ROM performance is judged acceptable, then use the model results along the LMOS study area boundary as inputs to the UAM. If ROM performance not acceptable, then employ available measurements. In situations where measurements are not available, employ some combination of ROM results and good technical judgement. Specific activities to be carried out include:

Perform model runs to see how sensitive calculated ozone levels are to the boundary concentration inputs.

Review findings of LMOS data analysis efforts as they pertain to the characterization of pollutant concentrations near the boundary of the LMOS study area. Note that the LMOS data analysis plan should include specific efforts to characterize boundary concentrations.

Develop a conceptual model characterizing the spatial and temporal characteristics of pollutant concentrations at the boundary.

Use results of conceptual model in conjunction with anticipated pollution patterns to develop high/medium/low estimates of boundary concentrations.

Perform UAM simulations using the three different settings of boundary concentration inputs (i.e., high, medium, and low).

Specify Boundary Concentrations for Future Year Simulations

The recommended procedure for specifying boundary concentration inputs in future year simulations is as follows. If ROM performance is judged acceptable, then use the model results for appropriate future year conditions along the LMOS study area boundary as inputs to the UAM. Note that it will be necessary to develop ROM outputs for a range of possible alternative future regional emission scenarios. If ROM performance is not acceptable, then develop boundary concentration inputs for future year simulations based on the results of the following activities:

Conduct UAM simulations to determine the sensitivity of calculated ozone concentrations to uncertainties in future year boundary concentration inputs. In particular, determine whether uncertainties in boundary concentration inputs could potentially mislead one concerning the possible directional effects of controls (i.e., does ozone increase or decrease with prescribed changes in VOC and NO_x emissions?). Particular attention must be given to specifying boundary concentration inputs if they influence the directional effects of controls.

Perform future year UAM simulations using a range of boundary concentration inputs selected to reflect their uncertainty.

Develop a conceptual model of future year boundary concentration behavior.

Perform future year UAM simulations using high, medium, and low settings of the boundary concentrations. The high setting might reflect current boundary values, and the low setting might reflect background values. The medium setting might be developed based on trajectory analyses. For example, back trajectories could be developed from selected points on the boundary of the LMOS study area to determine the upwind source areas contributing to pollutant levels at the boundary. Base year boundary values might be scaled based on the changes in emissions experienced in the upwind areas.