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RESULTS OF PHOTOCHEMICAL MODELING SENSITIVITY ANALYSES IN THE LAKE MICHIGAN REGION: CURRENT STATUS OF LAKE MICHIGAN OZONE CONTROL PROGRAM (LMOP) MODELING

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1. INTRODUCTION

The four states that border Lake Michigan are cooperatively applying a state-of-the-art nested photochemical grid model to assess the effects of potential emission control strategies on reducing elevated tropospheric ozone concentrations in the region to levels below the national ambient air quality standard. In order to provide an extensive database to support the application of the photochemical model, a substantial data collection effort known as the Lake Michigan Ozone Study (LMOS) was completed during the summer of 1991 (Koerber, 1993). The Lake Michigan Ozone Control Program (LMOP) was established by the States of Illinois, Wisconsin, Michigan, and Indiana to carry out the application of the modeling system developed from the LMOS, in terms of developing the attainment demonstrations required from this area by the Clean Air Act Amendments of 1990.

In order to help focus the efforts of the control strategy developers, one portion of the LMOP modeling will be set aside for the consideration of simplified, across-the-board type emissions reductions. The purpose of this paper is to describe the manner in which the emissions sensitivity portion of the LMOP modeling will be conducted, as well as to provide a status report and some preliminary results from the modeling to date. As will be discussed in the remainder of this text, the identification of the best estimate inputs to the model has been in flux to this point in the LMOS/LMOP modeling and as a result the modeling system has not yet been shown to replicate historical ozone episodes within the performance bounds set by LMOS or the United States Environmental Protection Agency (USEPA). Thus, one is cautioned not to reach conclusions regarding eventual control strategy decisions in the region based on the preliminary results presented herein.

2. THE LMOS MODELING SYSTEM

The focal point of the LMOS modeling system is the Urban Airshed Model, Version V (UAM-V), as described in Morris et al. (1992), which solves the species continuity equations over time for ozone and its precursors across a three-dimensional grid. While the model uses the Carbon Bond IV chemistry mechanism (Gery et al., 1989), UAM-V has numerous enhancements above and beyond the current regulatory version of the Urban Airshed Model (UAM-IV) that allow for better simulation of ozone formation. The most important of which are: 1) grid nesting is available to allow higher resolution in areas where emissions patterns and meteorological conditions are most important to the formation, transport, and dissipation of ozone (e.g., the lake breeze phenomenon in the LMOS domain), while still considering photochemical patterns over a regional scale; 2) subgrid scale plumes from major point sources are treated explicitly; and 3) the number of vertical layers in the model and their locations and properties can be user-defined, as opposed to having the model's vertical representation of the atmosphere being restrained to the determination of mixing heights.

Other components of the LMOS modeling system provide the inputs to UAM-V. The Chicago And Lake Michigan configuration of the Regional Atmospheric Modeling System (CAL●RAMS) is the prognostic numerical model used to prescribe the meteorological inputs for the LMOS UAM-V simulations (Lyons, ????). Day-specific and typical summer day anthropogenic emissions estimates prepared by the States for point and area sources are processed by the Geocoded Emissions Modeling and Projections (GEMAP) system to provide the

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photochemical model with a temporally and spatially allocated set of speciated emissions. GEMAP contains submodules which attempt the determine the appropriate motor vehicle emissions factors and amount of biogenic emissions for the modeling domain. (Emissions for the outermost, coarsest resolution grid are derived from the National Acid Precipitation Assessment Program database.) The USEPA Regional Oxidant Model was used to set the initial conditions of the model and may also be used to assign the boundary conditions for future year runs. Surface and aircraft measurements taken near the upwind domain boundary in the 1991 field study were the basis for the basecase boundary inputs.

3. EMISSIONS SENSITIVITY MODELING

The primary objective of the emissions sensitivity tests is to provide qualitative information to the LMOP control strategy developers on the effects of general emissions reduction scenarios while the regional attainment strategy process is still in its formative stages. Based on the knowledge gained from the sensitivity simulations, strategies will be constructed from those control measures determined to be the most effective in reducing ozone. These strategies will, in turn, be simulated by UAM-V to determine whether attainment would be achieved in the domain based on that particular set of controls.

For the emission sensitivity studies, UAM-V will be applied over the domain shown in Figure 1 using the 16 km grid A and 8 km grid B. An innermost, higher resolution (4 km) Grid C will not be employed for the sensitivity tests in order to minimize run times. Previous simulations have suggested that addition of the 4 km grid does not appreciably affect the simulated ozone concentrations (Morris et al., 1993). These tests will be performed for two ozone episodes that occurred during the most intensive data collection period of the field study: June 24-28, 1991 and July 15-19, 1991. The first two days of each of these episodic simulations are considered as ramp-up days to lessen the unwanted influence of initial conditions on the eventual simulated concentration patterns, and as such, results from these initialization days will not be considered. According to Hanna (1993), these two episodes are synoptically characteristic of approximately 80% of ozone episodes in the midwestern United States. Both episodes were associated with strong subsidence inversions, temperatures in excess of 22 C, and winds from 180 to 270 degrees. Another rationale for applying the generic emissions tests over Episodes 1 and 2 is that while both are representative of typical Lake Michigan ozone transport conditions, they differ somewhat in their source-receptor relationships. The June episode was marked initially by southerly winds and an early afternoon lake breeze which served to advect high levels of ozone northward over the stable Lake and then onshore along the east coast of Wisconsin (peak value = 175 ppb at Manitowoc on the 26th) Later in the episode, the winds became more southwesterly resulting in ozone peaks along the Michigan shoreline. The July episode featured predominantly southwesterly winds during most of the period which resulted in the highest impacts along the Michigan shoreline (peak value = 170 ppb at Borculo on the 18th and Sleeping Bear Dunes on the 19th).

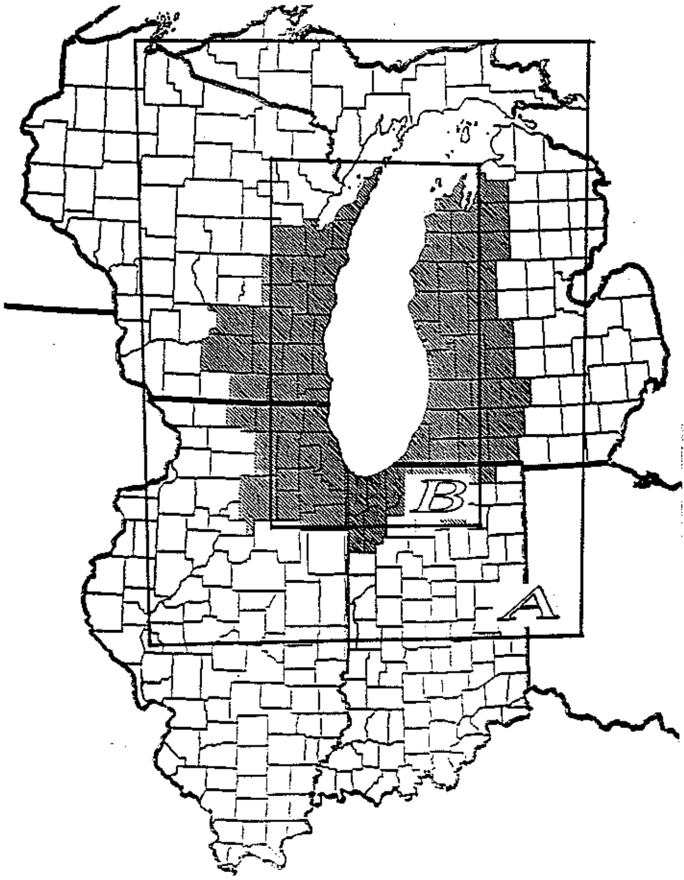

Figure 1. Lake Michigan Ozone Study modeling domain for the sensitivity studies. Grid A consists of a 35 by 50 mesh of 16 km sided grid cells. Grid B consist of a 34 by 60 mesh of 8km sided cells. The shaded area represents counties for which high resolution emissions estimates were prepared.

Table 1 lists the specific simulations that are planned to qualitatively assess the sensitivity of ozone formation, as predicted by UAM-V, to large scale changes in anthropogenic emissions magnitudes and patterns. The primary goal of the simulations is to answer the question of whether nitrogen oxide (NO_x) control is beneficial in the Lake Michigan basin and if so, to what degree. Secondary goals of the exercise are to determine: 1) where volatile organic compound (VOC) controls should be emphasized, 2) where NO_x controls could be most effectively implemented, 3) the benefits of elevated NO_x control versus surface level NO_x reductions, 4) the relative culpability of transport-influenced areas classified by USEPA as moderate nonattainment areas to their own ozone problem, as well as to elevated ozone concentrations throughout the region, and 5) the relative culpabilities of major source groups (motor vehicles, point sources, etc.) to the pervasive degree of smog in the domain. It is anticipated that a solid "first-guess" generic control strategy will result from this series of trial and error runs.

TABLE 1

A. Matrix runs to determine whether NO_x control is beneficial

1. Reduce NO_x emissions 30% throughout Grid B.
2. Reduce NO_x emissions 60% throughout Grid B.
3. Reduce NO_x emissions 30% & VOC emissions 30% throughout Grid B.
4. Reduce NO_x emissions 30% & VOC emissions 60% throughout Grid B.
5. Reduce NO_x emissions 60% & VOC emissions 30% throughout Grid B.
6. Reduce NO_x emissions 60% & VOC emissions 60% throughout Grid B.
7. Reduce VOC emissions 30% throughout Grid B.
8. Reduce VOC emissions 60% throughout Grid B.

9-12. Supplementary runs of varying NO_x and VOC reductions to help more fully characterize the ozone isopleth curves as exemplified in Figure 2.

B. Geographic emphasis of VOC control

13. Reduce NO_x emissions x% & VOC emissions by y% (where percentages are determined from the previous matrix runs to be approximate levels of control necessary for attainment) in the urban and suburban areas of the domain.

14. Reduce NO_x emissions x% & VOC emissions by y% (where percentages are determined from the previous matrix runs to be approximate levels of control necessary for attainment) only in the urban areas of the domain.

C. Geographic and source level emphasis of NO_x control

15. Reduce VOC emissions by y% in a chosen area (from preceding runs) and reduce NO_x emissions by x% in urban areas only.

16. Reduce VOC emissions by y% in a chosen area (from preceding runs) and reduce NO_x emissions by x% in all non-urban areas.

17. Reduce NO_x emissions x% in the elevated point source input file and 0% in the surface input file; reduce VOC emissions by y% in the selected area.

18. Same as 17, but 0% NO_x control in the elevated point source file in x% in the surface input file.

D. What is the relative contribution of the downwind moderate nonattainment areas to ozone concentrations in their particular areas, as well as regionally

19-21. 100% control of all emissions in all moderate nonattainment areas, all Michigan moderate areas, and all Wisconsin moderate areas.

E. What are the relative culpabilities of major source groups

22. Reduce motor vehicle VOC by y% (in areas chosen from preceding runs).
23. Reduce low-level points NO_x by x%.
24. Reduce area source NO_x and VOC by x% and y%, respectively.

4. DISCUSSION/PRELIMINARY RESULTS

The sensitivity portion of LMOP modeling will consist of nearly fifty simulations and is expected to take approximately 3 months to complete once started. The series of simulations will be initiated once a basecase set of inputs has been chosen for which UAM-V has been demonstrated to be accurately replicating the observed ozone and precursor patterns. As part of the basecase identification process for the LMOS modeling system, significant effort has been put into diagnostic analyses via UAM-V of various inputs into the model. Not unexpectedly, a number of input deficiencies have been identified which have required correction before model performance could be evaluated for that basecase. Boundary conditions, wind directions, and turbulent exchange coefficients in the model have been the subjects of most focus and some revision. Despite the best efforts to accurately characterize the meteorological and air quality input fields, the basecase modeling to date still demonstrates substantial underprediction of the observed peaks. This underprediction is assumed to be symptomatic of a flawed emissions inventory.

Varying degrees of uncertainty exist in all of the model inputs, but given the intended use of the LMOP modeling system to develop ozone-reducing emission reduction plans, it is critical that the emissions estimates match as closely as possible actual conditions. By applying similar methodology as in Wagner et al. (1992), the LMOP emissions reductions matrix simulations (runs 1-12) also are intended to assess the effect of inventory uncertainties on the signal of UAM-V resulting from controls.

As part of LMOS, a comparison was made between the ambient VOC/NO_x ratios at several sites in the domain and the inventory VOC/NO_x ratios for the grid cells believed to be impacting the monitors. Korc et al. (1993) concluded that the ambient data had a ratio 1.2 to 1.8 times higher than that of the inventory data, depending on site and day of comparison. This implies that either: 1) VOC emissions are underestimated, 2) NO_x emissions are overestimated, 3) some combination of 1) and 2), or 4) both VOC and NO_x emissions are underestimated with inventory VOC being underestimated by a larger magnitude than the NO_x. The model, however, is reproducing observed patterns of NO (and NO_x) fairly well, suggesting that the inventory problem is attributable to an underestimation of VOCs. Figure 2 shows time series plots of nitric oxide (NO) ambient concentrations and simulated UAM-V values for a representative sample of urban LMOS sites (presumably the most valid location for ambient/emissions comparisons). Photochemical models have in the past tended to underestimate NO_x concentrations when compared against monitored observations (Roth et al., 1989). The good NO_x agreement here is evidence that the NO_x inventory is probably valid. The observation that hydrocarbons are apparently underestimated has prompted the project to thoroughly re-evaluate the procedures by which the VOC inventory was derived to try to reconcile the differences between the inventory and ambient data.

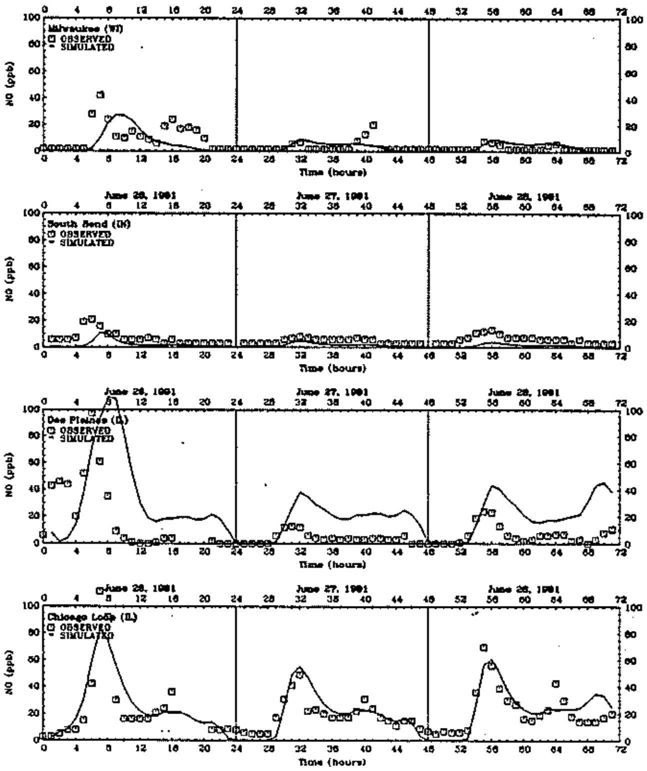

Figure 2. Time series comparisons between model predicted NO (solid line) and ambient NO observations (boxes) at several urban LMOS locations.

Figure 3 demonstrates the means by which the effect of emissions uncertainty on the response of the modeled ozone will be assessed. The graph is normalized by the current LMOS emissions inventory at 100% VOC and 100% NO_x (Point A). The base LMOS inventory totals 3,700 tons per day of VOC emissions, 2,600tons of which are anthropogenic; total anthropogenic NO_x emissions equal 2,500 tons per day. The solid line *BC* denotes the ambient ratio of VOC/NO_x, the dotted lines to either side show the possible uncertainty bounds suggested by the ambient ratio/emissions ratio comparison analysis. The hatched area on the graph indicates a zone of plausible actual emitted VOC and NO_x tonnages, according to the analysis of inventory bias and the competent model reproduction of observed NO_x concentrations (for purposes of graph, assume base NO_x emissions are accurate to approximately 20%). In order to effect the goals of the sensitivity tests, as presented in Section 3, the 24 runs listed on Table 1 will employ the adjusted base LMOS emissions inputs (i.e., about a 50 percent increase in total anthropogenic VOC emissions which appears to be a reasonable approximation of the actual inventory).

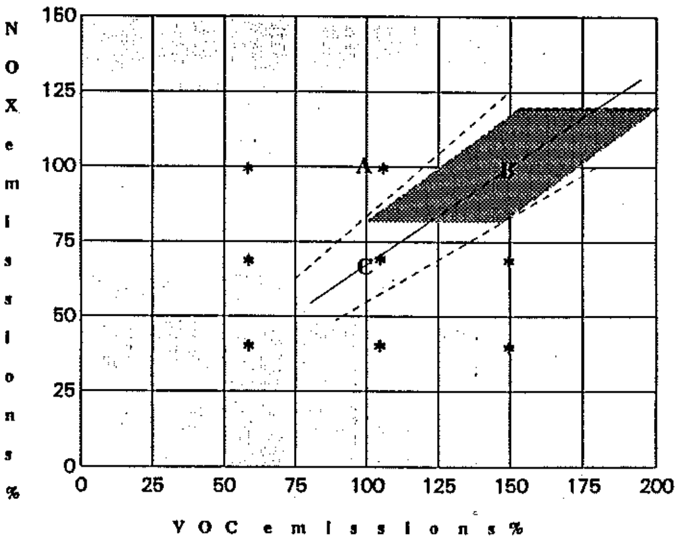

Figure 3. Base graph for ozone isopleth diagrams. The shaded area represents plausible LMOS inventory totals as total VOC and NO_x perecentage changes from the current LMOS emissions base (Point A). Asterisks represent emissions scenarios that will be tested in sensitivity runs 1-8.

The final refined LMOP control strategy modeling is expected to be based on the re-evaluated inventory. The asterisks on Figure 3 show the emissions totals to be simulated in the matrix runs 1-8. The supplementary runs 9-12 for each episode will be used to a) investigate the effects of applying similar across-the-board reductions as 1-8 to different emissions bases within the range of uncertainty in the inventory (i.e., other starting points within the hatched parallelogram) and/or b) attempt to define the region in the graph where ozone isopleths indicate NO_x-limited conditions.

Figure 4 shows an example of the type of analysis that will be possible as a result of the emission reduction matrix simulations. This figure is based on simulations performed by the LMOP Modeling Team and LMOS photochemical modeling contractor employing preliminary emissions and meteorological inputs and, thus, should not serve as anything more than an example of this type of diagram. The peak hourly simulated ozone value anywhere in the domain is plotted for each of 13 initial simulations as a function of their emissions base. In full, the analyses should also consider other metrics such as population exposure, areal coverage, and simulated ozone at specific locations. As in Figure 3, this graph is normalized such that the current LMOS inventory is denoted by 100% NO_x and VOC. The solid lines indicate the ozone isopleths that can be depicted based on the results of the 13 cases. As seen in the figure, not enough simulations were performed as part of this preliminary modeling to characterize key parts of the diagram (e.g., region of beneficial NO_x reductions, and the "ridgeline"). This figure is presented to illustrate one type of analysis resulting from the emissions sensitivity tests. Again, given the many qualifications associated with Figure 4 (i.e., problems with inputs, lack of a valid model performance evaluation to date, insufficient number of simulations, and failure to consider other metrics), the reader is cautioned not to draw any conclusions concerning possible LMOP control strategies (such as the benefit or liability of NO_x control) from this figure.

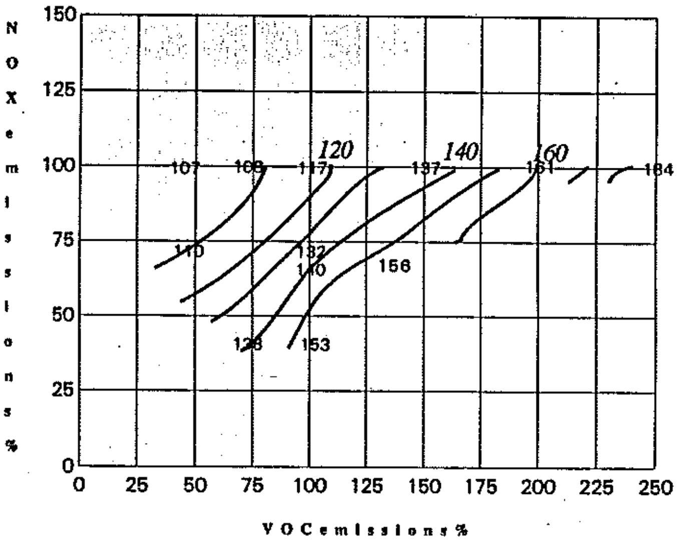

Figure 4. Ozone isopleth diagram derived from preliminary results of initial LMOP modeling. The foundation numbers indicate the peak simulated hourly ozone concentration for a simulation based on the fraction of baseline emissions. Numbers in italics are contour labels.

In summary, the sequence of sensitivity simulations described herein will be utilized to iteratively provide qualitative information to the LMOP decision makers as to the most effective control path to ozone attainment in the Lake Michigan region. It is anticipated that this roster of tests using UAM-V will provide answers to the broad technical questions facing the LMOS region in terms of approximate levels of control necessary for attainment and geographic culpabilities. A secondary goal of the runs listed in Table 1 is to attempt to quantify the effect of emissions inventory bias. It is possible that based on the results of these tests, that the model could show a different response, either in magnitude or in signal (worst-case), to ozone controls based on the range of uncertainty in the emissions estimates. In this case, the modeling results may be judged to be inconclusive for evaluating possible future year control strategies. Conversely, comparable model response to reductions from varying emission bases (within the identified bounds), would provide additional confidence in the effectiveness of developed control plans.

5. REFERENCES

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