DRAFT

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BRIEFING PAPER
OZONE MODELING IN THE LAKE MICHIGAN AREA

This briefing paper is intended to provide decision makers and the interested public with information on the photochemical grid model being developed for the Lake Michigan Ozone Study (LMOS), so that they may have realistic expectations of what the model can and cannot do.

What is a Photochemical Grid Model?

*The model, which relates ozone precursor emissions (i.e., VOC and NOx) to ambient ozone concentrations, can be thought of as a sophisticated bookkeeping system; tracking emissions, simulating atmospheric processes (transport, diffusion, chemical reactions, and removal), and ensuring that mass is conserved within each grid cell in the modeling region.

*It is expected that there will be over 30,000 grid cells in the LMOS modeling region. In the vicinity of Lake Michigan, the grid cells will be 4 km on a side and there will be 7 vertical layers. In the outer portions of the modeling region, the grid cells will be 16 km on a side and there will be 4 vertical layers.

*The LMOS model will also be able to treat up to 1-2 dozen major sources (primarily, NOx sources) as individual point sources. This sub-grid scale resolution provides the best representation of the impacts of NOx emissions from point sources and, as such, will improve our ability to ascertain the effectiveness of NOx controls.

How Accurate Are Photochemical Grid Models?

*Previous evaluations of the model for the base case (i.e., an actual present day ozone episode) indicate that: (a) peak concentrations are reproduced within ±15-20%, (b) model bias ("signed" concentration differences between model and observations) is about ±5-15%, and (c) gross model error ("unsigned" differences) is about ±30-35%. USEPA has adopted these ranges as representing acceptable model performance.

*Accurate base case performance does not, however, necessarily guarantee accurate model performance for other conditions. If compensatory errors are present, then the model may appear to produce the right answer, but for the wrong reason. Consequently, the model may not respond properly (and may yield erroneous results) when applied to a future year emission control scenario.

*Past model evaluations have likely been affected by compensatory errors. For example, it is now generally accepted that the motor vehicle emission estimates were low a factor of 2 or more. Despite such significant underestimation, researchers reported surprisingly good agreement between modeled and observed concentrations. This suggests that there were compensating factors (e.g., inflated boundary conditions, or underestimated mixing heights).

*A major goal of the LMOS is to identify and minimize compensatory errors. We will attempt to do this through the stressful testing of the modeling system, including sensitivity and uncertainty analyses, and evaluation of individual model components. This testing is only possible if supported by a "rich" data base, such as that collected during the 1991 field program.

*It is also important to keep the performance standards noted above in perspective. The peak values to be simulated here are on the order of 50% above the ambient standard (or about 0.06 ppm). If the model is off by, say, -20% (or about 0.04 ppm), this represents a significant fraction of the air quality increment of concern.

What Are the Advantages of Photochemical Grid Models and What Information Do They Provide?

*Most advanced modeling system available for regulatory application including state-of-the-science representation of the emissions and atmospheric processes that lead to ozone formation in the region

*Generally accepted as the most technically credible planning tool to support the development of ozone SIP control programs and to assess the relative benefits of VOC and NOx control (Note: use of the model for other regulatory applications, such as new source permitting, is unclear at this time.)

*Modular design provides a framework within which to embed our current understanding of the emissions and atmospheric processes; the model can be modified to reflect improved understanding of these processes as new information emerges in the future

*Resolves emissions and concentrations spatially (individual, adjacent grid cells) and temporally (individual, consecutive hours)

*Improves spatial understanding of ozone concentrations throughout the region because it will provide hourly estimates of ozone (and other primary and secondary species) for each grid cell, while monitoring data are only available for a few locations

*The model can tell us: (a) how much each geographic area or grid cell contributes to predicted ozone concentrations (i.e., culpability), and (b) how much emissions need to be reduced to achieve attainment. (To obtain this information, multiple model iterations are generally necessary.)

*Example model output are provided in Attachment #1

How are Photochemical Grid Models Different from Models Used for Other Regulatory Programs (e.g., SO2 Models)?

*Longer computer run times: Over the next year or so, the run times for the model on the available State computers are expected to remain on the order of 2:1 (i.e, it will take 6 days to simulate a 3-day episode). Because such significant run times will limit the number of alternative control strategies which can be examined, modifications to the computer code and the computers used should be sought in the future to lower run times.

*Very data hungry: The model requires information on emissions, air quality, and meteorology for the thousands of model grid cells. The accuracy of model output demands that considerable resources be spent to develop accurate model inputs. Recent advancements in model formulation have probably exceeded the quality of the available data bases. In a complicated area, such as the Lake Michigan region, it has been necessary to spend several years and several million dollars to compile a "rich" data base to run and evaluate the model.

*Need to evaluate performance: While the use of measurements to assess the accuracy of model estimates is generally encouraged, USEPA does not require its other models to be evaluated for each and every application. Given the substantial costs and potential societal changes associated with control programs for ozone, however, formal model evaluation is considered essential for photochemical grid models to ensure that they are reliable and that the resulting control programs will be effective.

What are Some of the Key Issues Related to Using Photochemical Grid Models to Evaluate Control Strategies?

*The need to develop and use a "rich" data base here has implications on the ability to model episodes from other years (with higher ozone levels, but only "routine" data bases). Because we will not be examining model performance with a routine data base, we will have much less confidence in applying the model to episodes from other years. Consequently, it is assumed that the same episodes will be used to establish acceptable model performance and to demonstrate attainment. The modeled episodes, however, must be shown to be representative of these historical episodes to ensure that control strategies are developed for worst-case conditions.

*Resource limitations preclude examination of all possible combinations of control measures. It is, therefore, necessary to identify a short list of alternative control strategies that will be modeled. Development of this list will need to consider emission reduction potential, environmental benefits, technical feasibility, economic reasonableness, and public acceptability.

*Despite our best efforts to develop a technically credible model and compile a comprehensive, accurate data base, some degree of uncertainty and bias are still likely to exist. This may be due to errors in model input values, errors in measurements, or inadequate model representation of the atmospheric processes. To develop control strategies which really work, we must understand fully what the model results mean and be prepared to deal with uncertainty and bias.

How Should Uncertainty and Bias Be Dealt With?

*Current USEPA guidance implies that the LMOS modeling system should produce a single set of ozone concentration values ("best estimate") for a given emission control scenario. Any information on uncertainty and bias, within the regulatory context of the LMOS, must, therefore, be presented in terms of characterizing the accuracy and reliability of the single set of results (and not in terms of other possible sets of results). One of the challenges of the LMOS will be to present this information in an accurate, persuasive way such that it can be used by decision makers.

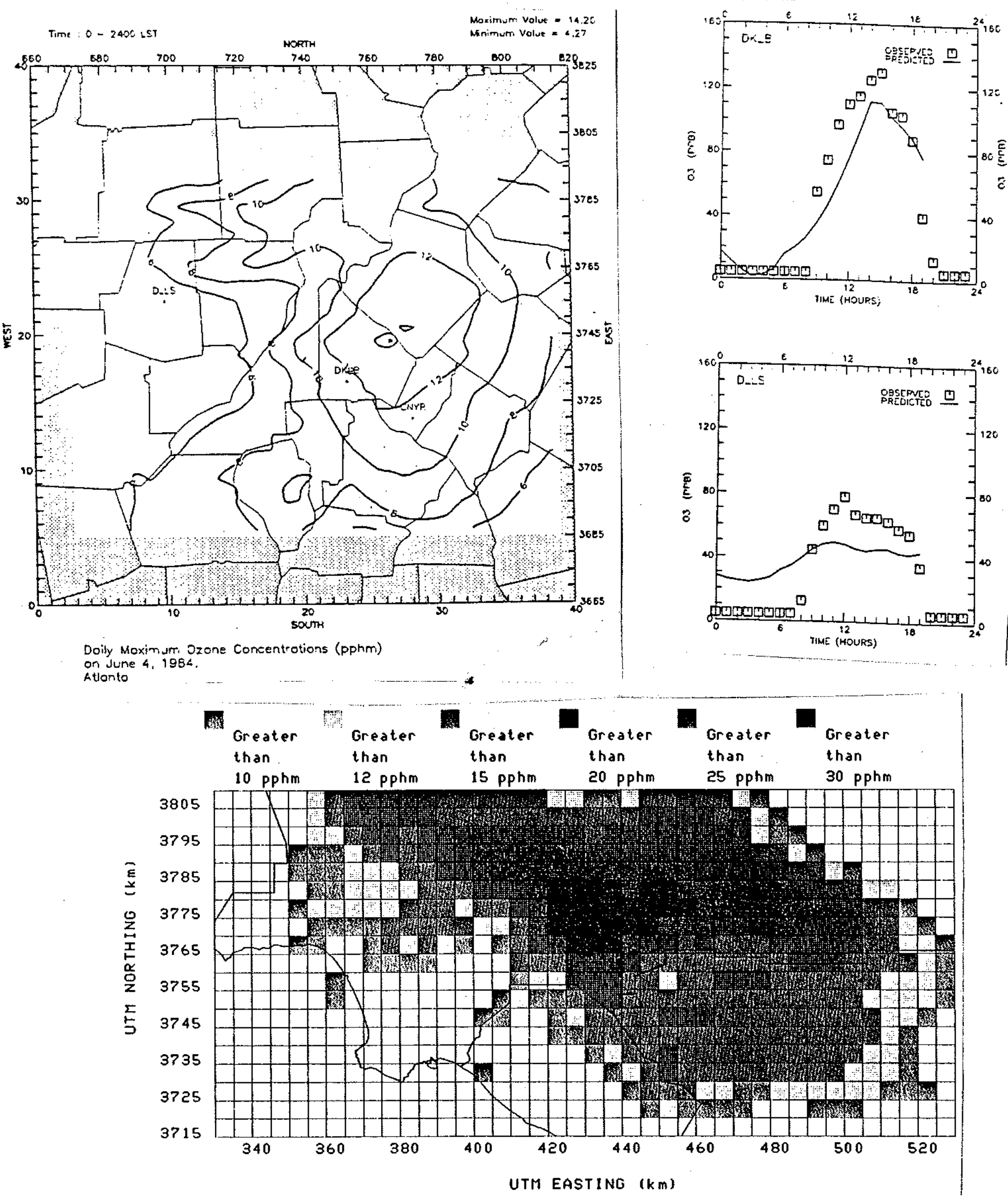
*A series of sensitivity/uncertainty analyses are planned to identify and quantify bias and uncertainty. In these analyses, model inputs (e.g., emissions, boundary conditions, and meteorology) will be varied over their range of uncertainty to provide an estimate of the uncertainty in model output due to these input uncertainties.

*Decision makers should be prepared to deal with this information. In particular, they must recognize the implications of either not adjusting the emissions inventory if significant bias is found to be present, or making empirical adjustments to the inventory that may not be rigorously supported by data (and, therefore, become open to inevitable criticism.)

*It must also be recognized that a possible outcome of the LMOS model evaluation effort is model failure (i.e., concluding that model performance is unacceptable). Past experience suggests that several evaluation cycles may be required to achieve adequate model performance and acceptance. The LMOS represents just the first attempt, albeit a very serious and expensive attempt, to apply a photochemical grid model in the Lake Michigan region. If unacceptable model performance is found here, then two options are possible. First, further study could be conducted. This would mean additional model development and field measurements, and would require more time and money. Second, the model could be applied "as is" (or possibly with some correction factors). There would be considerable doubt, however, about the adequacy of the resulting control strategies.

ATTACHMENT #1

EXAMPLE MODEL OUTPUT



Daily Maximum Ozone Concentrations (pphm) on June 4, 1984. Atlanta