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Project Summary

Final Evaluation of Urban-Scale Photochemical Air Quality Simulation Models

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The research study discussed here is a continuation of previous work whose goal was to determine the accuracy of several selected urban photochemical air quality simulation models using data from the Regional Air Pollution Study in St. Louis. This work reports on the testing of three models with a sample size of 20 days. The models evaluated here are: The Photochemical Box Model (PBM), The Lagrangian Photochemical Model (LPM), and the Urban Airshed Model (UAM). Emphasis in this report is directed at the ability of the models to reproduce the maximum 1-hour ozone concentrations observed on 20 days selected from nearly 2 years of data. The PBM, LPM, and UAM have been evaluated using statistical methods and graphical techniques and all show potential as air quality management tools. The standard deviation of the differences between observed ozone maxima and predicted concentrations at the same place and time ranged from 0.04 to 0.06 ppm for maxima of 0.16 to 0.26 ppm. This measure of uncertainty should be recognized by decision-makers using these models in regulatory and planning processes.

This Project Summary was developed by EPA's Environmental Sciences Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The Regional Air Pollution Study (RAPS) was conducted in the St. Louis region over the period 1974-1977. RAPS was designed to provide a comprehensive data set for the testing and evaluation of numerical air quality simulation models on an urban scale. While the RAPS field measurements were in progress EPA surveyed the available, state-of-the-art, photochemical air quality simulation models, and selected three for evaluation. In addition, a simple box-model approach was constructed by EPA and included in the study.

The following models were investigated in the evaluation program.

Photochemical Box Model (PBM) - a single cell Eulerian model constructed by EPA.

Lagrangian Photochemical Model (LPM)- a multi-level parcel model developed by Environmental Research and Technology, Inc.

Livermore Regional Air Quality Model (LIRAQ) - a single-level Eulerian grid model developed by Lawrence Livermore Laboratory.

Urban Airshed Model (UAM) - a multi-level, Eulerian grid model developed by Systems Applications, Inc.

LIRAQ was dropped from the evaluation because of a series of technical and logistics problems detailed in our first evaluation report.* LIRAQ was unable to produce significant ozone levels for St. Louis, but no specific correctable error could be identified.

The remaining models were tested extensively and corrections of obvious errors

*Shreffler, J.H. and K.L. Schere, 1982: Evaluation of four urban-scale photochemical air quality simulation models. EPA Report, U.S. Environmental Protection Agency, Research Triangle Park, NC (in press).

or deficiencies were made. No effort was made to adjust or tune the model predictions to observed concentration values. The prevailing philosophy behind the evaluation effort was to use the models in an off-the-shelf mode, much as they eventually would be applied by a user in a regulatory situation. However, great care was taken in preparation of data sets and model executions. Although model assumptions vary, effort was made to use data in similar manners in all models. Data preparation and actual execution of the models was accomplished solely by the authors at EPA. The goal of the evaluation was to provide a fair and objective determination of the accuracy of a set of photochemical models when tested in an operational mode against a comprehensive urban data base.

The only reasonable method of determining accuracy is to test a model against an extensive observational data base. Providing such a data base was the purpose behind the RAPS. Since the level of the ozone maximum for each day is of paramount importance relative to the National Ambient Air Quality Standards the comparison between its observed value and the model prediction at the same time and place would be of central interest. The method of evaluation consists of selecting a set of test days, executing model simulations, and computing residual concentrations (observed-predicted). The specific outcome of the evaluation is a presentation of information on residuals under the given circumstances. Conclusions about model acceptability require further assumptions and judgements.

As an integral part of the RAPS a network of 25 surface stations was established in and around St. Louis and comprised the Regional Air Monitoring System (RAMS). The RAMS stations continually monitored various meteorological variables as well as ambient concentrations of pollutant gases. In addition to the RAMS, upper air balloons were released each hour from urban and rural sites to provide wind profiles for modeling purposes.

This report presents the results of model simulations for 20 individual days chosen from the RAPS data base, twice the number from the initial evaluation detailed in the first evaluation report. These days, eleven from 1975 and nine from 1966, account for some of the higher O_3 measurements observed in the RAPS surface monitoring network. Maximum hour-average single station O_3 values all exceeded 0.16 ppm on the 20 days.

Results and Discussion

The Photochemical Box Model (PBM), a single cell Eulerian air quality simulation model, simulates the transport and chemical transformation of air pollutants in smog-prone urban atmospheres. The model's domain is set in a variable volume, well-mixed reacting cell where the physical and chemical processes responsible for the generation of ozone (O_3) by its hydrocarbon (HC) and oxides of nitrogen (NO_x) precursors are mathematically created. To apply the model to the St. Louis RAPS data base the horizontal scale of the single cell was 20 km and the vertical scale was time-varying, proportional to the depth of the mixed layer. The model domain was centered on downtown St. Louis such that the 20 x 20 km area encompassed most of the major emissions sources on either side of the Mississippi River. A uniform distribution of source emissions was assumed across the surface of the cell. Twelve of the RAMS surface monitoring stations were located within the cell's boundaries and nine others were available for determining model boundary concentrations.

The following statistics summarize the differences between the observed hourly maximum concentration of O_3 for each day and the PBM prediction at the same time. The concentrations are averages over the PBM domain.

$$\Delta C = \text{Obs - Pred (ppm)}$$
$$\overline{\Delta C} = -0.012$$
$$\text{s.d.}(\Delta C) = 0.039$$
$$\overline{|\Delta C|} = 0.029$$

Evidence shows that the PBM is a useful tool in assessing the urban air quality for photochemically reactive pollutants, especially in stagnation conditions. The PBM is relatively simple to use and its data requirements are far less stringent than most other numerical air quality simulation models. The areas of further study that should be pursued include: (a) the relationship between the average O_3 concentration observed within the model domain and the maximum O_3 level observed at a single station, (b) the continued testing and refinement of the chemical kinetic mechanism within the PBM, and (c) the sensitivity of the model to variations in selected parameters such as initial and boundary concentrations, initial cell depth, emissions, wind speed, and solar radiation.

The Lagrangian Photochemical Model (LPM) was developed by Environmental Research and Technology, Inc. and adapted under contract with EPA for use with the RAPS data base. The LPM considers a portion of the atmosphere as an identifiable parcel which can be tracked from early morning to the late afternoon. As the parcel moves over the various emissions sources, pollutants are assimilated, vertically mixed, and subjected to photochemical reactions in the presense of solar radiation. The model has recently been modified for this study to include a Gaussian-type lateral spread of the parcel. The following statistics summarize the differences between the observed hourly maximum O_3 concentration and the LPM predictions at the first vertical model level for the same time and place.

$$\Delta C = \text{Obs - Pred (ppm)}$$
$$\overline{\Delta C} = -0.023$$
$$\text{s.d.}(\Delta C) = 0.058$$
$$\overline{|\Delta C|} = 0.052$$

Compared to the results presented in the first evaluation report, the LPM has shown considerable improvement in its predictive capabilities resulting from changes made to allow parcel expansion and in the method of initialization. The model shows promise as an effective tool to understand O_3 production in an urban region. It is relatively easy to use, inexpensive to execute, and seems immune to various execution errors which tend to arise unexpectedly in complex computations of this sort. An area of further research may include a study of the vertical diffusivity as it relates to unrealistic build-up of pollutants at ground level.

The Urban Airshed Model (UAM) is a 3-D grid-type photochemical air quality simulation model developed by Systems Applications, Inc. (SAI) of San Rafael, California. The model structure consists of a lattice array of cells, arranged so that the total volume represents an urban domain and in which the physical and chemical processes responsible for photochemical smog are mathematically simulated. The horizontal dimensions of each cell are constant but the heights of the cells vary throughout a model simulation according to changes in the depth of the mixed layer. To apply the model to the St. Louis RAPS data base, the area modeled was 60 km wide and 80 km long. Each individual cell was 4 km on a horizontal side. Vertically, there were four layers of cells in total; the bottom two layers simulated the mixed layer and the top two represented the region immediately above the mixed layer. The domain of the UAM was centered just west of downtown St. Louis and included the entire metropolitan area. Of the 25 RAMS monitoring stations, 21 are situated within the model domain area and the remaining 4 are available for determining boundary concentrations.

The following statistics summarize the differences between the observed hourly maximum O_3 concentration and the UAM prediction at the same time and place.

$$\Delta C = \text{Obs - Pred (ppm)}$$
$$\overline{\Delta C} = -0.062$$
$$s.d.(\Delta C) = 0.035$$
$$\overline{|\Delta C|} = 0.062$$

The evaluation of the UAM by the Meteorology Division of EPA is now complete. It is clear that the potential use of a grid-type model such as the UAM is great, although the complexity of the model often makes solving the problems which arise more difficult. This model is a powerful tool available for use by the air quality analyst already experienced in working with complex simulation models. Model results should be carefully studied in each application and may not necessarily be used in an absolute sense in any given simulation. An area of future study that may be pursued is model sensitivity to variations in selected parameters such as initial and boundary concentrations, emissions, wind fields, and solar radiation.

Conclusions

The three models included in the final analysis span a wide range in complexity and sophistication but are all based on numerical solutions to mass-conservative equations. They are selected from the general categories of box, trajectory (Lagrangian), and grid (Eulerian) models. Emphasis in the model performance evaluations is placed on ozone, although results for other pollutant species are also discussed.

The PBM predictions for maximum O_3 for the average of the monitoring stations within the model domain were generally on the high side. The average O_3 residual showed a 23% overprediction over all test days. However, for the 5 stagnation-type days where the maximum observed O_3 occurred within the PBM domain the average overprediction was 8%, considerably better than for the entire sample. Only a slight tendency towards overprediction was indicated for the LPM. The biases of the residuals were relatively small, 11% of the average observations at Level-1 and only 2.5% at Level-3. The standard deviations of the residuals were the highest among the three models tested. The large variance in the residuals might be expected since the LPM generates a prediction which likely is the most specific to a particular place and time. Model predictions for maximum O_3 by the UAM in a specific sense (at the same time and location as the observed maximum) were consistently low for all evaluations with an average 32% underprediction over the sample. If the time and location of the model predictions are not constrained to be the same as those for the maximum observed O_3, the average model bias for the 20 days implied a 4% overprediction. This excellent agreement might suggest that the uncertainty in specifying a wind field for a grid model like the UAM could lead to large apparent errors in the model results.

The choice of which particular model to use in a specific application involves not only the accuracy of the model but also the resources required to operate it. The models tested here have resource requirements correlated with their level of complexity. In terms of man-months needed to set up a single day simulation and computer time expended (minutes of CPU on a UNIVAC 1100/82) the approximate requirements are:

PBM	--- 0.15 man-month ---	1 minute CPU
LPM	--- 0.20 man-month ---	10 minutes CPU
UAM	--- 0.50 man-month ---	110 minutes CPU

These models are now being made available to EPA's Office of Air Quality Planning and Standards for further statistical and sensitivity testing and ultimately for use in their regulatory decision-making process. Because model development is an evolving area of research it is very likely that subsequent "improved" versions of the models tested here will become available. A performance test with benchmark results, as described and tabulated in this report, now exists for future use in urban air quality model comparisons with any subsequent versions of the model.

K. L. Schere and J. H. Shreffler are on assignment to the U.S. Environmental Protection Agency from the National Oceanic and Atmospheric Administration, U.S. Department of Commerce.
J. H. ***Shreffler*** *is the EPA Project Officer (see below).*
The complete report, entitled "Final Evaluation of Urban-Scale Photochemical Air Quality Simulation Models," (Order No. PB 83-147 991; Cost: $22.00, subject to change) will be available only from:
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