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Project Summary

Evaluation of Four Urban-Scale Photochemical Air Quality Simulation Models

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This research was initiated with the intent of determining the accuracy of four photochemical air quality simulation models using data from the Regional Air Pollution Study in St. Louis. The models evaluated in this report are: The Photochemical Box Model (PBM), The Lagrangian Photochemical Model (LPM), The Urban Airshed Model (UAM), and The Livermore Regional Air Quality Model (LIRAQ). Emphasis is directed at the ability of the models to reproduce the maximum 1-hour ozone concentrations observed on 10 days selected from nearly two years of data. The PBM, LPM, and UAM have been tested successfully and show potential as air quality management tools. LIRAQ does not show potential as a model for general use, irrespective of its accuracy, which was impossible to judge at this time. For the three other models, the standard deviations of the differences between observed ozone maxima and predicted concentrations at the same place and time tend to be large, ranging 0.04 to 0.1 ppm for maxima of 0.19 to 0.26 ppm. Possible resolution of this high variability might improve performance of the latter three models.

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 to 1977. RAPS was designed to provide a comprehensive data set to test and evaluate numerical air quality simulation models for an urban area. While the RAPS field measurements were in progress, EPA surveyed the available, state-of-the-art, photochemical air quality simulations models, and selected three for evaluation. Since no existing model embodied a simple box-model approach, a box model was constructed by EPA. The four models evaluated by EPA and described herein are as follows:

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.

The final report describes the results of simulations for 10 days when maximum measured O_3 concentrations were 0.19 ppm to 0.26 ppm in St. Louis. Generally, these days exhibit stagnation conditions with little cloud cover and represent situations conducive to the production of photochemical oxidant from local emissions.

The models were tested extensively, and obvious errors or deficiencies were corrected. However, no effort was made to adjust or tune the model predictions to observed concentration values. The approach to the evaluation was to use off-the-shelf models, much as they would be used in a regulatory situation. Even so, great care was taken in preparation of data sets and model executions. Although model assumptions varied, the authors were careful to use data in similar manners in all models. Data preparation and actual execution of the models was accomplished solely 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.

An integral part of RAPS, was establishment of a network of 25 surface stations in and around St. Louis, known as the Regional Air Monitoring System (RAMS). The RAMS stations continually monitores various meteorological variables as well as ambient concentrations of pollutant gases, providing observational data for comparison with model predictions.

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 in such a manner that the 20 x 20 km area encompassed most of the major emissions sources on either side of the Mississippi River . 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.

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.

$$\Delta C = \text{Obs.} - \text{Pred (ppm)}$$

$$\overline{\Delta C} = -0.033$$

$$\text{s.d.}(\Delta C) = 0.041$$

$$|\overline{\Delta C}| = 0.039$$

The evaluation of the PBM is continuing in EPA's Meteorology Division. This analysis is the first major step toward a thorough understanding of model performance. Initial evidence shows that the model 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 hysteresis problem during advection conditions, (b) the relationship between the average O_3 concentration observed within the model domain and the maximum O_3 level observed at a single station, (c) the continued testing and refinement of the chemical kinetic mechanism within the PBM, and (d) 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 for use with the RAPS data base. (The LPM is essentially identical to the general-use model named ELSTAR). The LPM considers a portion of the atmosphere as an identifiable parcel which can be tracked from early morning to late afternoon. As the parcel moves over the various emission sources, pollutants are assimilated, vertically mixed, and subjected to photochemical reactions in the presence of solar radiation.

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

$$\Delta C = \text{Obs} - \text{Pred (ppm)}$$

$$\overline{\Delta C} = -0.004$$

$$\text{s.d.}(\Delta C) = 0.11$$

$$|\overline{\Delta C}| = 0.080$$

The LPM has shown promise as an effective tool to understand O_3 production in an urban region. The model 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. Areas of further research should incude the following: (a) the importance of the initial conditions versus the emissions accumulated in the parcel, (b) reasonable methods to include horizontal diffusion, (c) the vertical diffusivity as it relates to unrealistic build-up of pollutants at ground level.

The Livermore Regional Air Quality Model (LIRAQ) was developed at Lawrence Livermore Laboratory (LLL) under funding of the National Science Foundation. The model is an Eulerian grid type and was specifically constructed for use in the San Francisco Bay area, where the Bay Area Quality Management District (BAAQMD) retains an interest in LIRAQ applications. Reflecting the originally intended region of study, the model has provision for generating mass-consistent wind fields in complex terrain but allows only one grid cell vertically. In 1975, EPA entered into an Interagency Agreement (IAG) with LLL to have LIRAQ adapted for use with the RAPS data base in St. Louis. Because LIRAQ uses special features of the CDC 7600 computing system, adapting it to run on the EPA's UNIVAC 1110 was deemed impractical. Therefore, LIRAQ was transferred to the Lawrence Berkely Laboratory (LBL) computing facility where EPA could have direct access to the model.

The effort to evaluate LIRAQ performance was beset with difficulties, and EPA is considering eliminating the model from its evaluation program. With limited testing, LIRAQ did not produce significant concentrations of ozone, suggesting errors in the emission and/or chemistry module. Presently, three days (195, 226, and 275 of 1976) have been tested on the LBL system by EPA. The Day 275 simulation produced an error in LIRAQ execution of unknown origin. On Days 195 and 226, little ozone was generated by the model, and nitrogen oxides seemed to totally dominate the photochemical system. Even if current problems are resolved, there are cost-benefit considerations centered on the adequacy of the model's theoretical framework (single vertical cell), cost, and inaccessibility for general use. The LIRAQ conversion was initiated with the intent of having a complete spectrum of state-of-art models in existence in 1975 for testing by EPA. Reconsiderations of its eventual utility have made LIRAQ less than attractive for further research. Since LIRAQ is tied to a specific computer system, its prospects for use in a general regulatory setting - the ultimate goal of the model evaluation program - are extremely dim.

The Urban Airshed Model (UAM) is a three-dimensional (3-D) grid-type or Eulerian, photochemical air quality simulation model developed by Systems Applications, Inc. (SAI) of San Rafael, California. The structure of the model 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.

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

$$\Delta C = \text{Obs - Pred (ppm)}$$

$$\overline{\Delta C} = -0.074$$

$$\text{s.d.}(\Delta C) = 0.033$$

$$|\overline{\Delta C}| = 0.074$$

The evaluation of the UAM is continuing at the Meteorology Division of EPA, and additional test days may be chosen to add to those already done. From the work performed to this point, 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. Areas of further study that should be pursued include: (a) the adequacy of the wind-field methodology, and (b) the sensitivity of the model to variations in selected parameters such as initial and boundary concentrations, emissions, wind fields, and solar radiation.

Conclusions

The evaluations of urban photochemical air quality simulation models presented in this report represent the first comprehensive effort to examine model performance under controlled conditions. Great care was taken in establishing the same data base and impartial running procedures for all models. The following points briefly summarize the general conclusions emerging from the study.

1. The PBM model performs the best in near-stagnation conditions.
2. The LPM fixed-box formulation for the air parcel needs modification. Unrealistically high ozone predictions result under certain circumstances.
3. LIRAQ lacks potential as a model for general-use for a variety of reasons and might be phased out of the evaluation program. No decision was made on use by specialized groups for specific locales.
4. The UAM tends to consistently underpredict ozone. the effect possibly results from spurious numerical diffusion.
5. For all models, the user should have a strong scientific background and be extremely careful in implementing air quality simulations.
6. For all models, there is substantial variabilty between specific 1-hour predicted and observed concentrations at a particular location. Decision makers in regulatory agencies should be cognizant of this variability.

Using the results described in this report and the possible model problems they elucidate, a final investigation of the structure of each model should be carried out. If any further problems are identified, with workable solutions, they should be corrected. Model modifications should be based on sound scientific judgements and not solely on a desire to improve the results. A decision should be made on whether to pursue further development and testing in the special case of LIRAQ. When model changes are final, another set of runs should be made and analyzed. Up to 10 additional days from the RAPS could be included in the final analyses.

*The EPA authors **Jack H. Shreffler** (also the EPA Project Officer, see below) and **Kenneth L. Schere** are with the Environmental Sciences Research Laboratory, Research Triangle Park, NC 27711.*

The complete report, entitled "Evaluation of Four Urban-Scale Photochemical Air Quality Simulation Models," (Order No. PB 82-239 278; Cost: $16.50, subject to change) will be available only from:

National Technical Information Service
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