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# Project Summary

# A Regional Scale Model (1000 km) of Photochemical Air Pollution: Part 1. Theoretical Formulation

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**A theoretical framework for a multi-day, 1000-km scale simulation model of photochemical oxidant is developed. It is structured in a highly modular form so that eventually the model can be applied through straightforward modifications to simulations of particulates, visibility and acid rain.**

**The model structure is based on phenomenological concepts and consists of three and one-half layers. The interface surfaces separating the layers are functions of both space and time that respond to variations in the meteorological phenomena that each layer is intended to treat. Among the physical and chemical processes affecting passage and distribution of photochemical concentrations that the model is designed to handle are: horizontal transport, photochemistry, nighttime wind shear and the nocturnal jet; cumulus cloud effects; mesoscale vertical motion; mesoscale eddy effects; terrain effects; subgrid scale chemistry processes; natural sources of hydrocarbons, $NO_x$, and stratospheric ozone; and wet and dry removal processes, e.g., washout and deposition.**

**The predictability of pollutant concentrations at long range is considered, along with such related problems as the parameterization of "mesoscale" diffusion and the design of model "validation" experiments. A basis is established for estimating quantitatively the levels of uncertainty associated with dispersion model predictions.**

**This report focuses on theoretical aspects of the model and the question of predictability. Results of the model's performance and quantitative assessments of its predictability will be presented in subsequent parts of this report.**

***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

This project was begun in 1977 with the objective of developing a model for guiding the formulation of regional emissions control strategies. Initially the principal concern was with the photochemical oxidant; but in the course of its development, the model was constructed in a highly modular form that would allow straightforward applications to fine particulates, visibility, and, possibly, acid deposition as well.

When this project was begun, there did not exist an air pollution model that could simulate all the physical and chemical phenomena that are believed to control the fate of photochemical pollutants over large time and space domains. Among these phenomena are (not necessarily in order of importance):

1) Horizontal transport
2) Photochemistry, including the very slow reactions
3) Nighttime chemistry of the products and precursors of photochemical reactions

4) Nighttime wind shear, stability stratification, and turbulence "episodes" associated with the nocturnal jet
5) Cumulus cloud effects. Venting pollutants from the mixed layer, perturbing photochemical reactions rates in the shadows, providing sites for liquid phase reactions, influencing changes in the mixed layer depth, perturbing horizontal flow
6) Mesoscale eddy effects on urban plume trajectories and growth rates
7) Terrain effects on horizontal flows, removal, diffusion
8) Subgrid scale chemistry processes -- resulting from emissions from sources smaller than the model's grid can resolve
9) Natural sources of hydrocarbons, $NO_x$, and stratospheric ozone
10) Wet and dry removal processes, e.g., washout and deposition

A necessary condition for the credibility of a long range transport model is that all of these phenomena be taken into account, at least until it has been demonstrated that some of these processes play a negligible role.

Of similar concern are several questions regarding fundamental aspects of modeling itself. Following are three questions that are relevant not only to the utility of pollution models in regulatory, decision-making roles, but also to the meaningful implementation of the model itself.

(1) What aspects of pollutant concentrations are models capable of predicting?
(2) Given our present state of knowledge, what are the theoretical limits on the accuracy with which these quantities can be predicted (assuming perfect emissions data, chemical information, etc.)?
(3) How does one assess the accuracy of a given model?

These questions must be resolved before a model can be verified or used in any meaningful way.

## Procedure

In order to design a viable model framework consistent with all the anticipated applications noted above, an attempt was made to derive from the observational evidence available at the time this program was initiated an estimate of the minimum vertical and horizontal resolutions necessary to describe regional scale air pollution phenomena. The aim was to arrive at the best compromise between the restrictions imposed upon the model by computer time and memory limitations and the need to describe as accurately as possible all of the important physical and chemical processes. The NO, $O_3$, and meteorological data reported by the participants of the 1975 Northeast Oxidant Transport Study were analyzed and it was concluded that to describe the phenomena revealed by those data would require at the very least a three-level model: one level assigned to the surface layer, another layer assigned to the remainder of the daytime mixed layer, and an additional layer atop the mixed layer. The top level would be used in conjunction with the mixed layer to account for downward fluxes of stratospheric ozone as well as upward fluxes of ozone and its precursors into the subsidence inversion layer above. Material that entered this top layer could be transported by winds aloft to areas outside the modeling region; it could reenter the mixed layer by subsidence or entrainment; it could enter precipitating clouds and be rained out of the atmosphere; or it could undergo chemical transformation. Representing the subsidence inversion, where cumulus clouds often form under stagnant high pressure conditions, the top level of the model would be instrumental in simulating the chemical sink effects of heterogeneous (within cloud droplets) reactions among ozone, its precursors, and other natural and pollutant species. Including cloud effects in the model would be especially important in simulating $SO_2$ and sulfates. An extra "half layer" would be necessary adjacent to the ground to parameterize dry deposition and subgrid scale chemistry processes induced by point and line sources of pollutants.

Having three layers in a model is insufficient in itself to simulate the phenomena we have discussed above. The need is, rather for three "dynamic" layers that are free to expand and contract locally in response to changes in the phenomena being modeled. The model developed in this program possesses these properties. The surfaces that comprise the interfaces of adjacent layers are variable in both space and time in order that each layer can fully account for the changes that occur in its own domain of phenomena. Working in concert, the model's three and one-half layers can effect the simulation of all of the phenomena cited above.

To address the questions of what models are capable of predicting, how accurately they can predict given variables and how one would proceed to verify the validity of a model, we considered the basic problem of model formulation from the viewpoint of fundamental mathematical principles. The aim was to delineate in mathematical terms the nature of the statements that one can deduce about natural phenomena, such as air pollutant concentrations, given descriptions of the universal laws governing those phenomena and values of the parameters, in terms of discrete observations, involved in those laws.

## Conclusions

Special numerical techniques were developed to meet the rather unique needs of this model. One of these techniques is a high-order, explicit differencing scheme that suppresses errors in the advection and diffusion simulation that the nonlinear chemical processes would amplify. This scheme also permits the model domain to be handled in a piecewise fashion. Without this capability, awkward, inefficient computing procedures would be required to operate this large model on EPA's UNIVAC computer. Tests of this numerical method showed that its performance is superior in a number of important respects to that of existing alternative algorithms.

Another special numerical technique developed for this project is a scheme that allows the set of nonlinear differential equations that describe air pollution chemistry to be handled in their full form rather than in pseudosteady-state form. Coupling of the chemistry with the vertical fluxes of material among the model's three layers is accomplished with the aid of still another new algorithm that is computationally stable over virtually an infinite range of parameter values. Tests of these two numerical schemes showed that they provide an acceptable level of accuracy in much less computation time than alternative methods.

The mathematical analyses of predictability, model accuracy, and validation procedures showed that physical laws and discrete descriptions of atmospheric variables are insufficient to define uniquely such variables as pollutant concentration distributions. As a consequence, even if all data used in the model were precise and the mathematical equations that describe the governing physical laws could be solved exactly, a model still could not predict the concentration that would occur at a given place at a given time. Rather, it could prescribe only a range of values in which the observed value would fall. Thus, the utility of a model in a given application is determined by the width of this interval of possible values. An ongoing aspect of this research program is to quantify the predictability of pollutant concentrations as a function of averaging time, distance between the source and receptor, the pollutant species, meteorological conditions, and other relevant parameters. Results of this work will be presented in a future report.

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*The complete report, entitled "A Regional Scale (1000 km) Model of Photochemical Air Pollution: Part 1. Theoretical Formulation," (Order No. PB 83-207 688; Cost: $20.50, subject to change) will be available only from:*
*National Technical Information Service*
*5285 Port Royal Road*
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