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Project Summary

A Regional-Scale (1000 km) Model of Photochemical Air Pollution: Part 3. Tests of the Numerical Algorithms

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The Regional Oxidant Model developed in two previous reports is applied to a series of test problems whose exact solutions are known. The predicted concentrations are compared with the true values to obtain a measure of the accuracy of the numerical algorithms that comprise the model's governing equations. Some of the problems test only the model's chemical kinetics algorithm, others test the kinetics and transport/diffusion algorithms jointly, and a few test all three of the model's basic algorithms together—kinetics, transport/diffusion, and vertical fluxes.

It is found that the kinetics algorithm produces exact solutions of the chemical rate equations over the full range of species concentrations that are likely to be encountered in applications. A modified version of the algorithm yields concentration estimates that are within ±5% of the correct values in one-half to one-third of the computer time needed for exact solutions.

In simulations of the advection of clouds of chemically reactive compounds, the kinetics and transport/diffusion algorithms jointly reproduce the correct shapes and motions of clouds, and they predict the peak concentration in the clouds to within 10% of the true value over 48-h simulation periods.

In applications to continuous finite line sources in steady, spatially variable flows, the combined algorithms reproduced plumes with negligible spreading due to pseudo diffusion. In the case of ozone, the predicted plume centerline concentration was within 5% of the true value in a plume five grid cells wide and within 15% of the true value in a plume two grid cells wide. Corresponding errors in the predicted CO concentrations were about 50% larger. In general, it was found that ozone is among the species most accurately simulated, while compounds such as nitrous acid, nitric acid, alkyl nitrate, and related nitrogen-containing species are the most poorly simulated. The predicted concentrations of free radical species are of intermediate accuracy. Evidence was also found that errors in plume concentration can be amplified when a plume crosses a second source. The zone of enhanced error tends to be confined to the vicinity of the second source.

This Project Summary was developed by EPA's Atmospheric 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

In two previous reports (A Regional Scale (1000 km) Model of Photochemical Air Pollution: Part 1. Theoretical Formulation, EPA-600/3-83-035, May 1983; and Part 2. Input Processor Network Design, EPA-600/3-84-085, August 1984), a model was developed for simulating the

fate of photochemical air pollutants over large time and space domains. The theoretical basis of this model is a set of differential equations that describe the chemical and physical processes that control the fate of substances in the atmosphere. Since the general forms of the solutions of these equations are not known, an operational model must be based on analogues of these equations that are amenable to computer solution. These analogues are referred to as numerical algorithms. Therefore, for the model to produce accurate concentration predictions, the solutions of the numerical algorithms must be accurate facsimiles of the corresponding solutions of the differential equations. In this study, we investigate whether the algorithms that form the basis of the Regional Oxidant Model (ROM) satisfy this condition. We consider this task to be a necessary prerequisite to any attempt to infer the model's predictive capability through comparisons of predicted and observed concentrations.

Procedure

The ROM's predictive equations are composed of three basic numerical algorithms: chemical kinetics, transport/diffusion, and vertical fluxes. To obtain quantitative measurements of the performance of these algorithms both individually and jointly, we apply the ROM to a series of hypothetical problems whose exact solutions are known. For example, to test the chemical kinetics algorithm alone, we apply the ROM to a situation in which the atmosphere is at rest; there is no diffusion, vertical fluxes, material deposition, or sources. In this case the full set of equations reduces to a system of nonlinear first-order ordinary differential equations whose exact solutions can be calculated by using the well-tested Gear routine. By examining situations characterized by various combinations of initial concentrations, we can determine whether the accuracy of the algorithm is constant over the range of species concentrations that the model will be called upon to treat in actual applications.

Similarly, to test the chemical kinetics and transport/diffusion algorithms jointly, we apply the model to a situation in which the horizontal flow speed is finite, but horizontal diffusion, vertical fluxes, and deposition are all zero. In this instance, a translation of coordinate systems to a moving frame reduces the full set of equations to the same set of ordinary differential equations described above. In this case, the accuracy of the combined kinetics and transport/diffusion algorithms is judged by comparing the exact solutions with the values predicted by the model along the moving reference frame.

Tests of the vertical flux algorithms were reported in Part 1, Section 9 of the previous project reports[1]. We test it in combination with the chemical kinetics algorithm in this study only in the case in which the vertical flux is infinite. We believe that the performance exhibited in this single extreme case is indicative of joint performance of these two algorithms in general, because the vertical flux differential equations are of the same type as the chemical kinetics equations, but they are linear in form.

Although the combined set of conditions under which we test the model algorithms constitutes only a limited part of the parameter space in which the model would be applied in actual applications, these tests provide a minimum standard for judging the model's predictive capability. Indeed, if the model is unable to accurately simulate these rather elementary situations, there are no grounds for expecting it to perform well in general applications.

Conclusions

The chemical kinetics algorithm was found to provide exact solutions of the corresponding differential equations over a wide range of species concentrations. In fact, the algorithm's accuracy is unnecessarily high because none of the input data used in the model nor any of the model's other components are equally accurate. For this reason, we sacrificed some accuracy in exchange for higher computing speeds. The modified algorithm yields concentration estimates within ±5% of the true values in about one-tenth of the time required to calculate the exact solutions with the Gear routine.

Tests of the combined kinetics and transport/diffusion algorithms showed that plumes were underestimated by only 10% or less over a 48-h simulation period. Widening of the concentration distributions due to pseudo diffusion was negligible, and errors in the predicted shapes and transport speeds of clouds and plumes were nil. These results are particularly significant, since the transport/diffiusion algorithm used in the ROM is a type that does not maintain positive definite concentrations. When negative concentrations are generated, they are merely reset to zero or clamped, before the chemical kinetics algorithm operates on them.

Not all species were simulated equally well. Ozone is among the compounds most accurately predicted while nitrous and nitric acid were among those most poorly simulated. For any given species, the error level is inversely proportional to the width of the cloud or plume and there is a slight enhancement of the error in the concentrations of some species once they cross a second source. Overall, our tests showed that the algorithms on which the ROM is based are quite accurate descriptions of the physical and chemical processes that the model is intended to treat.

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The complete report, entitled "A Regional-Scale (1000 km) Model of Photochemical Air Pollution: Part 3—Tests of the Numerical Algorithms," (Order No. PB 85-203 818/AS; Cost: $23.50, subject to change) will be available only from:

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