United States
Environmental Protection
Agency

Environmental Sciences Research
Laboratory
Research Triangle Park NC 27711

Research and Development

EPA-600/S3-84-085 Aug. 1984

EPA

Project Summary

A Regional-Scale (1000 km) Model of Photochemical Air Pollution: Part 2. Input Processor Network Design

Robert G. Lamb

Detailed specifications are given for a network of data processors and submodels that can generate the parameter fields required by the regional oxidant model formulated in a previous report (A Regional Scale Model (1000 km) of Photochemical Air Pollution: Part 1. Theoretical Formulation, EPA-600/3-83-035, May 1983). Operations performed by the processor network include simulation of the motion and depth of the surface, nighttime radiation inversion layer; simulation of the depth of the convective mixed and cloud layers; estimation of the synoptic scale vertical motion fields; generation of ensembles of layer averaged horizontal winds; calculations of vertical turbulence fluxes, pollutant deposition velocities, and parameters for a subgrid scale chemistry parameterization scheme; and many other functions. This network of processors and submodels in combination with the core model developed in the previous report represents the EPA's first generation regional oxidant model.

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

In a previous report (A Regional Scale Model (1000 km) of Photochemical Air Pollution: Part 1. Theoretical Formulation), and hereafter referred to as Part 1, a theoretical basis was developed for a model that can simulate all the physical and chemical phenomena that are believed to control the fate of photochemical air pollutants over large time and space domains. Among the phenomena that the model was designed to consider are:

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, e.g., 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, and perturbing horizontal flow
6. Mesoscale eddy effects on urban plume trajectories and growth rates
7. Terrain effects on horizontal flows, removal, and 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.

In this report, Part 2, detailed plans are given for transforming the theory of Part 1 into an operational model.

To be practicable, the model design must satisfy several constraints. First, it must allow continued incorporation of state-of-the-art techniques without the need to overhaul the computer code each time. Second, the architecture of the model must be amenable to internal partitioning to facilitate a division of labor in the model construction and trouble-shooting operations during model tests. Third, the design must be capable of performing simulations with maximal efficiency. The last requirement is particularly important due to the unique manner in which this model is applied. Specifically, for a given source distribution, the model is used to simulate the concentrations that would result from each atmospheric flow field in a finite ensemble of flows; the set of concentration fields that is produced by this process are used as the basis for estimating the probability distribution of concentration values. By contrast, conventional air pollution models consider only a single wind field and the resulting concentration predictions are regarded as the values that one would expect to observe under the meteorological and emissions conditions considered.

Procedure

The design constraints were met by structuring the model in a modular form. Each module contains mathematical descriptions of small groups of individual physical and chemical processes, and the modules are interconnected by a network of communication channels

The principal module, designated CORE, contains computer language analogues of the differential equations that describe the governing processes considered in the development of the model theory in Part 1. The CORE module is expressed in a very primitive mathematical form in the sense that its inputs are matrices and vectors whose elements are composites of variables among which are meteorological parameters, and chemical rate constants. Module CORE is linked to a module labeled CHEM, which contains the analogue of the chemical kinetics scheme. The communication between these two modules consists of two vectors, $\underset{\sim}{P}$ and $\underset{\sim}{Q}$, each of length N, where N is the total number of chemical species simulated. The nth element of $\underset{\sim}{P}$ is the net rate of production of species n due to source emissions and chemical reactions among all other species, and the nth element of $\underset{\sim}{Q}$ is the net rate of destruction of species n due to its chemical interaction with all other species. Thus, any chemical kinetics mechanism can be incorporated into the model as long as it is expressed in a form that is compatible with the vector interfaces that link CORE with the chemistry module CHEM.

The remainder of the inputs required by CORE are prepared by a module designated BMC (b-matrix compiler). This module performs essentially the same task that language compilers perform in computers. The BMC translates the parameter fields such as the thicknesses of each of the model's layers, interfacial volume fluxes, and horizontal winds into the matrix and vector elements that are required by the algorithms in CORE.

The input variables are supplied in turn by a series of interconnected processors, several of which are rather complex models themselves. These processors generate the wind fields, the interfacial surfaces that separate the layers, turbulence parameters, source emissions, and many other variables. Their inputs consist of information generated by other processors in the network and partially processed raw data.

The processor network consists of both permanent and interchangeable components. The permanent elements are CORE, which embodies the theory developed in Part 1, the BMC, and the communication channels. All other processors including the chemical kinetics module CHEM are interchangeable components of the network. Any or all of the interchangeable elements can be replaced by other modules as long as they are compatible with the communication channel interfaces.

The Project Report on which this Summary is based provides detailed specifications for each of the processors in the network. As new techniques become available for estimating meteorological, chemical, and pollutant deposition parameters, and as information is acquired on the accuracy of the procedures that form the basis of the current processor designs, the interchangeable components of the system will eventually be replaced by more refined methods in the course of developing a second-generation regional oxidant model.

Conclusions

The regional oxidant model theory developed in Part 1 has been implemented in the form of a network of discrete processors. All processors except the central CORE processor can be interchanged with other modules that perform similar tasks. With this design, state-of-the-art techniques can be incorporated into the model with minimal effort, errors can be isolated relatively quickly during troubleshooting operations, and a high level of computational efficiency can be achieved in multiple simulation studies in which only a few of the many input parameter fields vary from one simulation to another.

Detailed plans are given for each processor based in part on currently available techniques for estimating meteorological and chemical parameters and in part on newly formulated procedures. Among the latter is a method for estimating vertical material fluxes in cumulus clouds, a scheme for handling lateral boundary conditions in numerical solution of the shallow water equations, a procedure for initializing the concentrations of each of the simulated pollutant species, and a method for generating ensembles of wind fields. Quantitative analyses of the performance of individual processors and the full model itself will be presented in subsequent reports.

Robert G. Lamb *(also the EPA Project Officer, see below) is with Environmental Sciences Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC 27711.*

The complete report, entitled "A Regional-Scale (1000 KM) Model of Photochemical Air Pollution, Part 2. Input Processor Network Design," (Order No. PB 84-232 651; Cost: $25.00, subject to change) will be available only from:

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650

The EPA Project Officer can be contacted at:

Environmental Sciences Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

☆ U S GOVERNMENT PRINTING OFFICE, 1984 — 759-015/7784

United States
Environmental Protection
Agency

Center for Environmental Research
Information
Cincinnati OH 45268

Official Business
Penalty for Private Use $300