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Project Summary

The Regional Oxidant Model (ROM) User's Guide

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The Regional Oxidant Model (ROM) determines hourly concentrations and fates of ozone and 34 other chemical species over a scale of 1000 km x 1000 km for ozone "episodes" of up to one month's duration. The model structure, based on phenomenological concepts, consists of 31/2-layers. The surfaces separating the layers respond to variations in space and time of the meteorological phenomena simulated in each layer. The model simulates many physical and chemical processes that affect the motion and distribution of chemical concentrations: among these are horizontal transport, photochemistry, nighttime wind shear and nocturnal jet, cumulus cloud effects and mesoscale vertical motion, terrain and mesoscale eddy effects, subgrid scale chemistry processes, natural sources of hydrocarbon, and dry deposition. The ROM is a complex model that requires users to have expertise in photochemical grid modeling. Meteorologists, engineers, and computer scientists familiar with this type of modeling will find this User's Guide relevant and helpful for running the ROM.

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

Introduction

The Regional Oxidant Model (ROM) is a three-dimensional photochemical Eulerian grid model designed to simulate concentrations of ozone and related species. ROM is a 3 1/2-layer model with a horizontal resolution of approximately 19 km; each grid cell has dimensions of 1/6° latitude by 1/4° longitude. The typical horizontal extent of the modeling domain is 1000 km. The model is designed to simulate hourly regional concentrations of ozone during largely stagnant summertime conditions that are associated with elevated smog episodes. ROM is also intended to simulate the effect of alternative emission control strategies that might be used to mitigate harmful levels of ozone pollution.

Development of the ROM began in the middle 1970's. Research versions of the model were tested and modified during the 1980's. The model described in this user's guide (version 2.1) became operational in late 1989 and has been extensively used in applications by the EPA.

The model simulates many physical and chemical processes that affect the motion and distribution of chemical concentrations. These processes include horizontal transport using a refined objective analysis scheme, photochemistry using the Carbon Bond 4 mechanism, cumulus cloud effects and mesoscale vertical motion, nighttime wind shear and nocturnal jets, terrain and mesoscale eddy effects, subgrid scale chemistry processes, bio-

genic emissions of hydrocarbons, and dry deposition.

The purpose of this user's guide is to provide potential users with sufficient information to execute the ROM on a combination VAX and IBM computer system. Readers are referred to other publications to obtain details on the model's technical background. Because of the model's complexity, the user's guide is divided into three parts. Part 1 discusses the preprocessors, which manipulate the raw data. Part 2 contains information on the many processors that are used to generate four data files for input to the core model. Part 3 discusses operation of the core model on the IBM computer.

ROM Preprocessors (Part 1)

This portion of the user's guide discusses the programs that are used to convert raw data into a format acceptable for use in the processor network. Raw data that are handled by the preprocessors include the following:

(1) meteorological data from buoys,
(2) surface meteorological data (both U.S. and Canada),
(3) upper-air meteorological data (both U.S. and Canada),
(4) anthropogenic emissions,
(5) biogenic emissions,
(6) ozone boundary conditions,
(7) chemistry initial conditions, and
(8) line source information.

Much of the initial quality assurance of the data is performed during preprocessing. Other operations that are performed include merging and sorting the databases and converting them into appropriate formats. All preprocessor programs, except for the ozone boundary-condition procedure, are FORTRAN programs that reside on the VAX computer. The ozone boundary-condition procedure is an ad hoc process that is performed using a spreadsheet program on a desktop computer.

ROM Processor Network (Part 2)

Figure 1 shows the ROM 2.1 processor network. Processing occurs in several stages. The initial data files are entered into processors in Stage 0 and processing continues through Stage 8. The processor network transforms the raw data into four core mode input files: ICON (initial-concentration data); BCON (boundary-condition concentration data); BTRK [diffusivity and backtrack (advection transport) information]; and BMAT (parameterization for vertical fluxes, meteorological parameters necessary for chemistry rate constant adjustments, and parameterized emissions source strengths).

All of the processors have been written in FORTRAN-77 and have been executed on EPA's cluster of VAX computers. Data processing for a typical three-day simulation of the northeastern U.S. requires 12 hours of CPU on a VAX 8650.

Core Model (Part 3)

Unlike other components of the ROM modeling system, the core model resides on an IBM 3090 computer. The core model takes data from the four files generated by the processor network (ICON, BCON, BTRK, and BMAT) and computes concentrations of ozone and 34 other chemical species.

There are two principal components of the core model: BIGGAM and LILGAM. BIGGAM solves the horizontal transport for each grid cell in 30-minute time steps. LILGAM solves the chemistry in time steps that are allowed to vary according to the "stiffness" of the solution. Vertical mass fluxes, including emissions injection, are also accounted for in LILGAM. The primary output of the core model is a large concentration file consisting of gridded 30-minute average concentrations for all chemical species. A typical three-day simulation of the core model for the northeastern U.S. uses 9.5 hours of CPU on an IBM 3090.

Summary

This three-part user's guide provides the information necessary to execute version 2.1 of the Regional Oxidant Model (ROM). Potential users of the system should be forewarned that the modeling system is complex and requires extensive computer resources. The services of engineers, meteorologists, or computer scientists experienced in photochemical grid modeling are required. Although the code has been designed and executed on VAX and IBM computers, it should be adaptable to other computer systems.

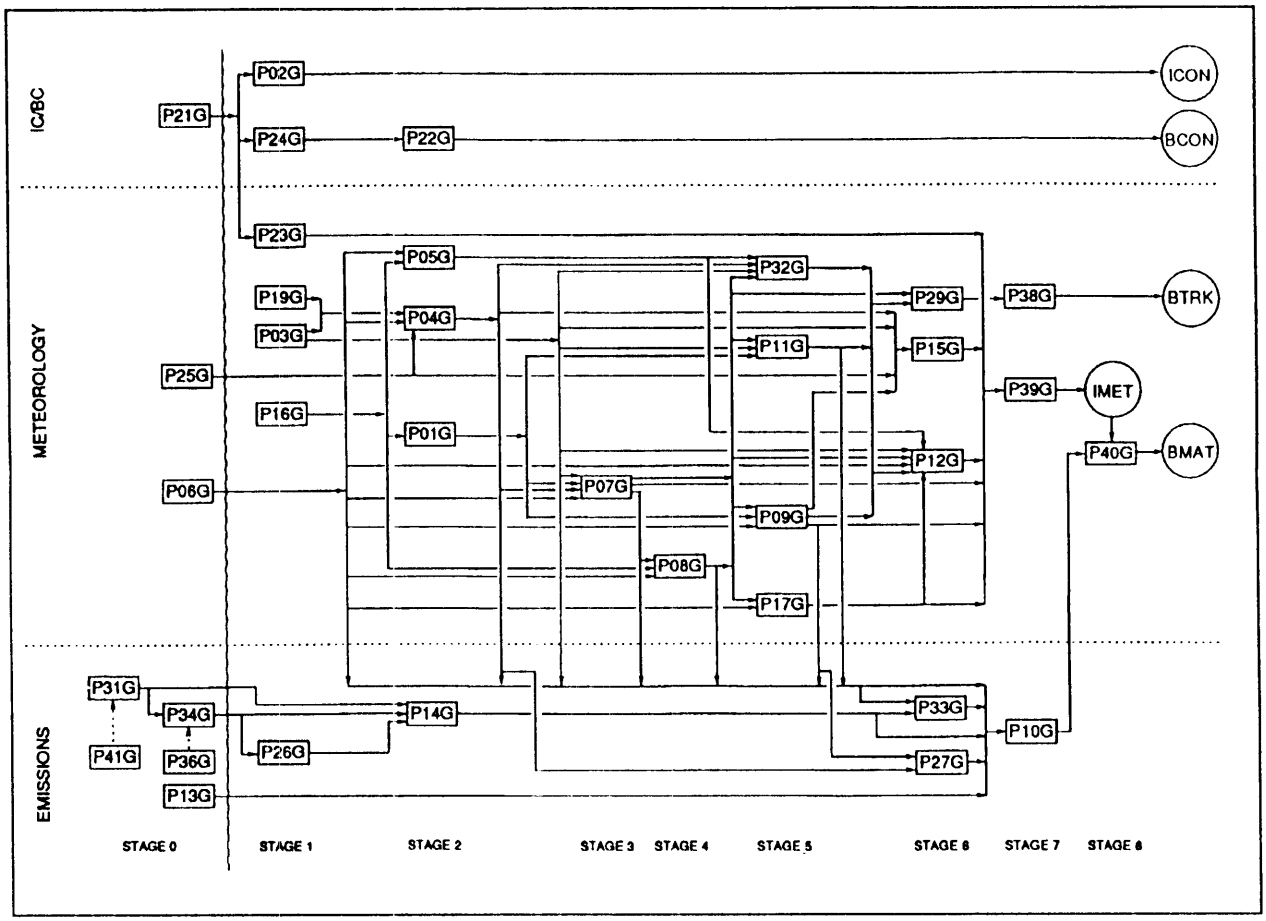

Figure 1. *Structure and final output files of the ROM 2.1 Processor Network.*

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The complete report, entitled "The Regional Oxidant Model (ROM) User's Guide,"
Part 1. The ROM Preprocessors (Order No. PB91-171 926/AS; Cost: $39.00, subject to change)
Part 2. The ROM Processor Network (Order No. PB91-171 934/AS; Cost: $45.00, subject to change)
Part 3. The Core Model (Order No. PB91-171 942/AS; Cost: $31.00, and the Complete Set. (Order No. PB 91-171 918/AS; Cost: $98.00, subject to change) will be available only from:

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