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Project Summary

Development of the Regional Oxidant Model Version 2.1

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This report describes improvements that were made to version 2.0 of the Regional Oxidant Model (ROM) in order to create version 2.1. The ROM is an Eulerian grid model that calculates hourly concentrations of ozone and other chemical species for episodes up to about a month long. The ROM's modeling domain, composed of grid cells that are approximately 19 km on a side, encompasses an area on the order of 1000 km by 1000 km. The physical processes that the ROM simulates include photochemistry, nocturnal jets and temperature inversions, spatially- and temporally-varying wind fields, terrain effects, dry deposition, and emissions of biogenic and anthropogenic ozone precursors. Major technical improvements include upgrading the Carbon Bond Mechanism to version 4.2, improving the biogenic emissions processing system (which now includes a canopy model), updating the wind fields processor, and expanding the use of buoy data for determining meteorological data fields over water. Also, ROM 2.1 can be adapted more easily than version 2.0 to various modeling domains in eastern North America. In addition, the computer software has been redesigned to facilitate ROM's eventual application by outside users.

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 separate report of the same title (see Project Report ordering information at back).

Introduction

Field studies have shown that ozone and its precursors can be transported more than 100 km from their point of origin. This indicates that the high ozone concentrations in many areas of the Northeast—particularly in areas of low emissions density—may be due in significant part to the influx of these species from outside sources. Thus, urban-scale models may be inadequate for evaluating ozone-reduction emissions scenarios because these models cannot accurately treat long-range transport of ozone and its precursors. The regional character of the ozone problem led the EPA to begin work on the first version of the Regional Oxidant Model (ROM) in the mid-1970s. The ROM is a sophisticated regional-scale model that predicts hourly ozone concentrations for episodes extending up to about a month in duration; each episode is modeled as a series of three-day executions. The model domain, divided into a set of grid cells approximately 19 km by 19 km each, encompasses an area on the order of 1000 km by 1000 km. For much of eastern North America, the ROM can model the regional variability of the chemical and physical processes that affect photochemically-produced ozone concentrations on a regional scale.

The ROM system is composed of a core model, which solves the sets of

equations that describe the above processes, and a series of over 30 processors that prepare the input data needed by the core model. ROM 1.0, the first version of the ROM, emerged in 1984 and was used for a limited set of applications for the Northeast Corridor Regional Modeling Project. ROM 2.0 became operational in 1987. To create it from ROM 1.0, several features were changed or added: (1) The Demerjian chemical mechanism was replaced with version 4.0 of the Carbon Bond Mechanism (CBM 4.0), which simulates some 70 reactions among 28 chemical species. (2) Biogenic hydrocarbon emissions were added to the list of emission types modeled; ROM 1.0 modeled only anthropogenic emissions. (3) The code was modified to allow atmospheric layer thicknesses to vary over space and time; in ROM 1.0, these thicknesses remained constant. (4) The ability to simulate the effects of nocturnal jets and nighttime inversions was added.

Application requirements for EPA's Regional Ozone Modeling for Northeast Transport (ROMNET) project have prompted us to upgrade ROM 2.0 to produce ROM 2.1. For the ROMNET application, we have expanded the model's domain in the northeastern U.S. from 60 by 42 cells to 64 by 52 cells in order to include major urban emitters in Ohio and Virginia. As a result, the design of ROM 2.1 allows the user to increase or reduce the numbers of columns and rows in the grid more easily than before. ROM 2.1 also can be adapted more easily to other modeling domains in eastern North America. Some of the other modifications include an updated biogenic hydrocarbon processor; an improved wind fields processor; an upgraded Carbon Bond Mechanism (CBM 4.2) in the ROM's chemistry solver; expanded use of buoy data and the use of mobile-source emissions data; and changes that allow the ROM system to use computer resources more efficiently. We have also added features that should allow future outside users to apply the ROM more easily when it is released to them.

Overview of the Regional Oxidant Model

The ROM is an Eulerian, episodic grid model that simulates the hourly concentrations of chemical species in a rectangular domain that is on the order of 1000 km on a side. The domain is represented by a grid of cells that are approximately 19 km on a side; the coordinate system that delineates the columns and rows of cells is based on the latitude-longitude system, so cell size varies somewhat over the domain. Columns are the north-south components of the grid (marked off in degrees longitude) and rows are the east-west components (marked off in degrees latitude). To date, the model has been adapted for three different regions: the Northeast Regional Oxidant Study (NEROS) region, consisting of 60 columns by 42 rows (2520 cells per atmospheric layer); the Southeast Regional Oxidant Study (SEROS) region (60 columns by 42 rows); and the Regional Ozone Modeling for Northeast Transport (ROMNET) region (64 columns by 52 rows, or 3328 cells per layer). Figure 1 shows the ROMNET region.

The ROM has three and one-half vertical layers—termed layers 0, 1, 2, and 3—whose thicknesses vary dynamically in space and time in response to meteorological phenomena. We say there are three and one-half layers rather than four because in layers 1, 2, and 3 the concentrations of chemical species are treated prognostically, while in layer 0 they are treated diagnostically.

For each model layer, the ROM system combines observational data and theoretical formulations of the governing chemical and physical processes to produce predicted species concentrations. The main component of the system, the core model, is a set of algorithms that calculate the solutions to computer-solvable analogues of the differential equations that describe the governing processes. The core model outputs concentrations for all species for every cell in every layer, for each model time step. The basic model time step, called the advection time step, is one-half hour. Within each advection time step, the vertical fluxes and chemical kinetics are modeled using smaller time steps. A single core model run can simulate episodes up to 72 hours (144 advection time steps) in length; this limit is imposed because of file-size restrictions. Episodes of longer than three days are run as a series of 72-hour executions; simulations usually are limited to the length of an ozone episode (approximately two weeks).

The core model requires five types of input data: air quality, meteorology, emissions, land use, and topography. We acquire these rawdata from various sources and process them through data extraction and quality assurance routines. This process produces data that are then prepared for the core model by a network of over 30 processors, which range in function from simple data reformatting routines to programs that generate the complex wind fields that drive the atmospheric transport. The processors are organized into nine distinct stages that reflect the sequence of program execution. Processors at the same stage may execute simultaneously, but each processor must wait to execute until all the lower-stage processors in its data path have finished running.

Most of the processors in the network produce either processor files (PFs) or model files (MFs). PFs, generally written by lower-stage processors, contain data used by higher-stage processors. MFs also provide input to some higher-stage processors, but they primarily contain the parameter fields that are transformed into the data elements required by the core model governing equations. The processor network ultimately produces several large data files for the core model, which contain initial-condition and boundary-condition concentrations as well as the data used to model all physical and chemical processes affecting species concentrations in a given episode. These files combined contain tens of millions of core model input values; simulating one day, for example, requires nearly 100 billion computations with these millions of values.

Figure 2 is a schematic of the ROM system. By structuring the ROM in this modular fashion, we can change the method used to generate values of a particular independent variable without having to overhaul the entire ROM system. Thus, to create ROM 2.1 from ROM 2.0, we have been able to modify and improve some components without having to rewrite the code for all the others. Figure 3 shows the resulting ROM 2.1 processor network. It consists of three interrelated parts: the initial-condition and boundary-condition (IC/BC) processors, the meteorology processors, which process topography and land use data in addition to meteorology data; and the emissions processors. The network transforms the raw data input files into the four core model input files shown on the right: ICON (initial-condition 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 emission source strengths). Table 1 summarizes the functions of all the processors in the ROM 2.1 network.

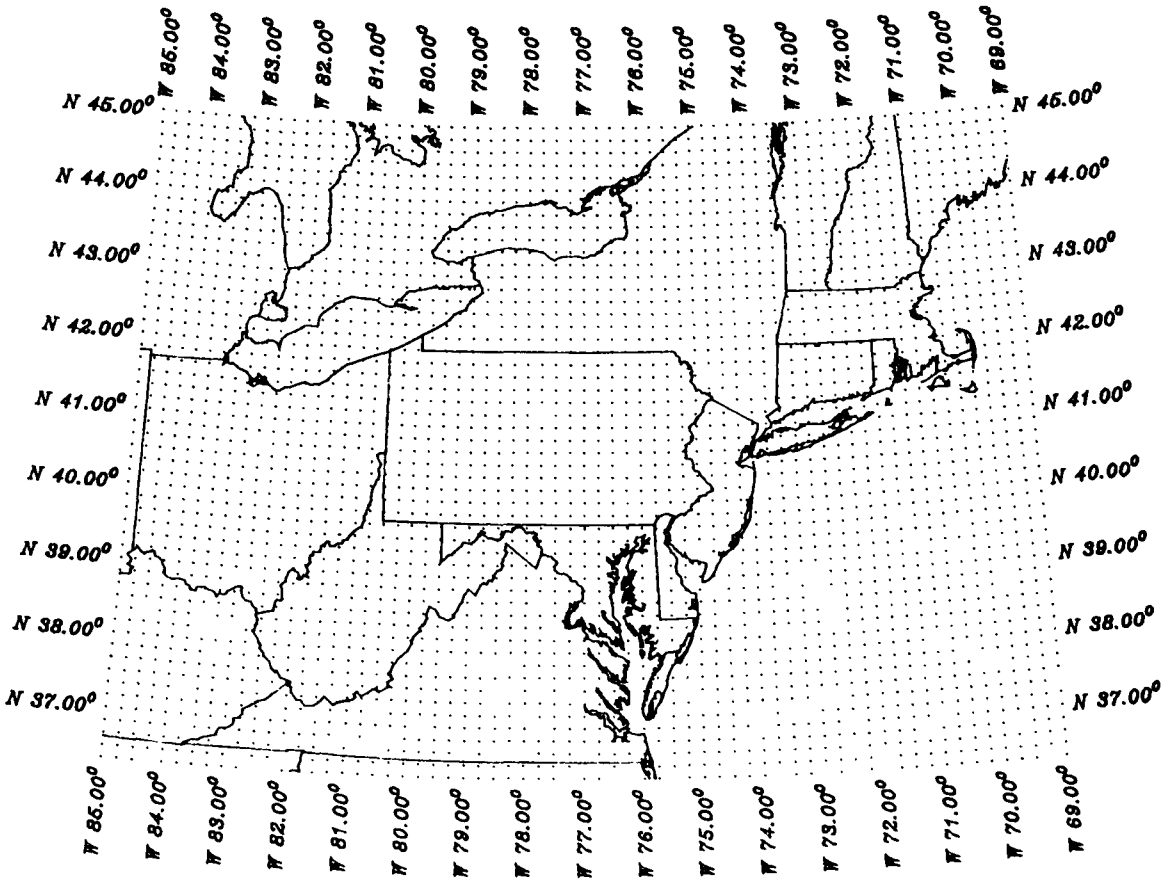

Figure 1 *The gridded ROMNET region (64 columns by 52 rows); dots represent grid cell corners.*

The modular structure is also advantageous because it facilitates implementing quality assurance (QA) procedures. All programs in the system are operated and maintained in strict conformance with a set of QA procedures that involve both machine and human checks of the computer code, the input and output data streams of each submodule, and the overall behavior of the model.

The ROM system has been programmed using the American National Standards Institute (ANSI) FORTRAN-77 full language specification, except for the Biogenic Emissions Inventory System (BEIS), an emissions processing system written in SAS®. Development of the system began on the EPA's Sperry UNIVAC® 1100 mainframe computer. It was then shifted to a VAX™ 11/780 minicomputer in May 1983. Currently, we are running the core model on the EPA-NCC's IBM® 3090 and the processor network on the EPA-NCC VAX cluster, consisting of two VAX 8650s and one VAX 11/785. Running the model system requires a significant amount of CPU time; for example, for one three-day execution the ROM 2.0 core model required about 6 h of IBM 3090 CPU time and the ROM 2.0 processor network used about 12 h of VAX 8600 CPU time.

Summary of the Differences Between ROM 2.0 and ROM 2.1

This section briefly lists the major differences between the 2.0 and 2.1 versions of the ROM.

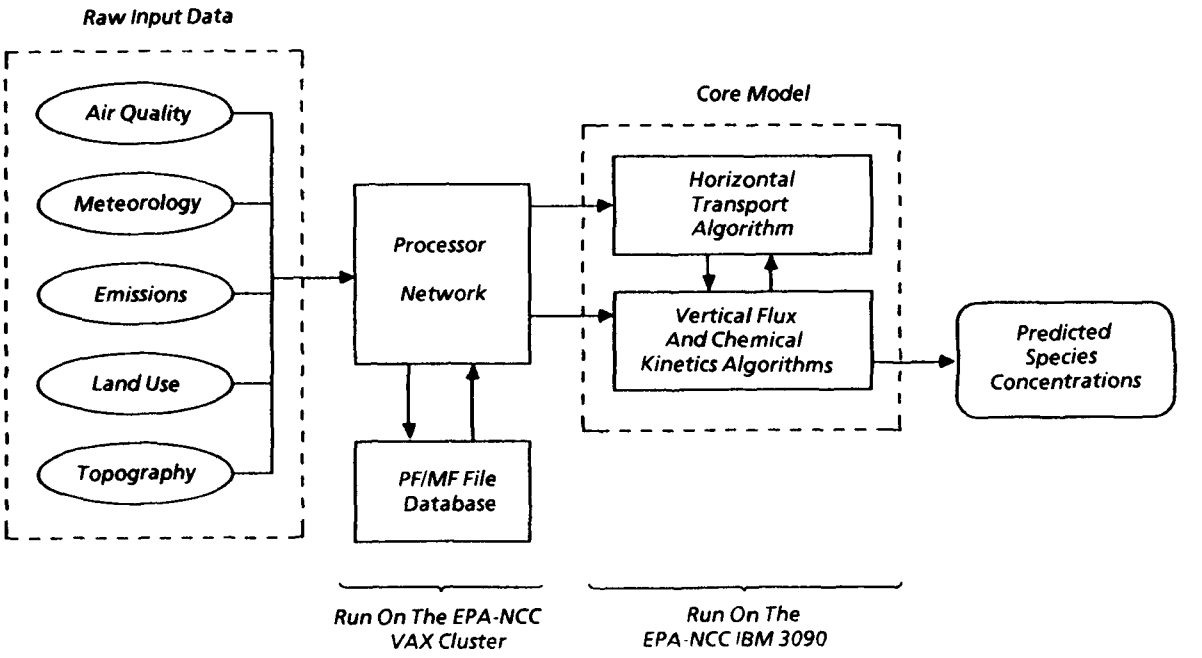

Figure 2. *General structure of the ROM system, from input data through final output concentrations.*

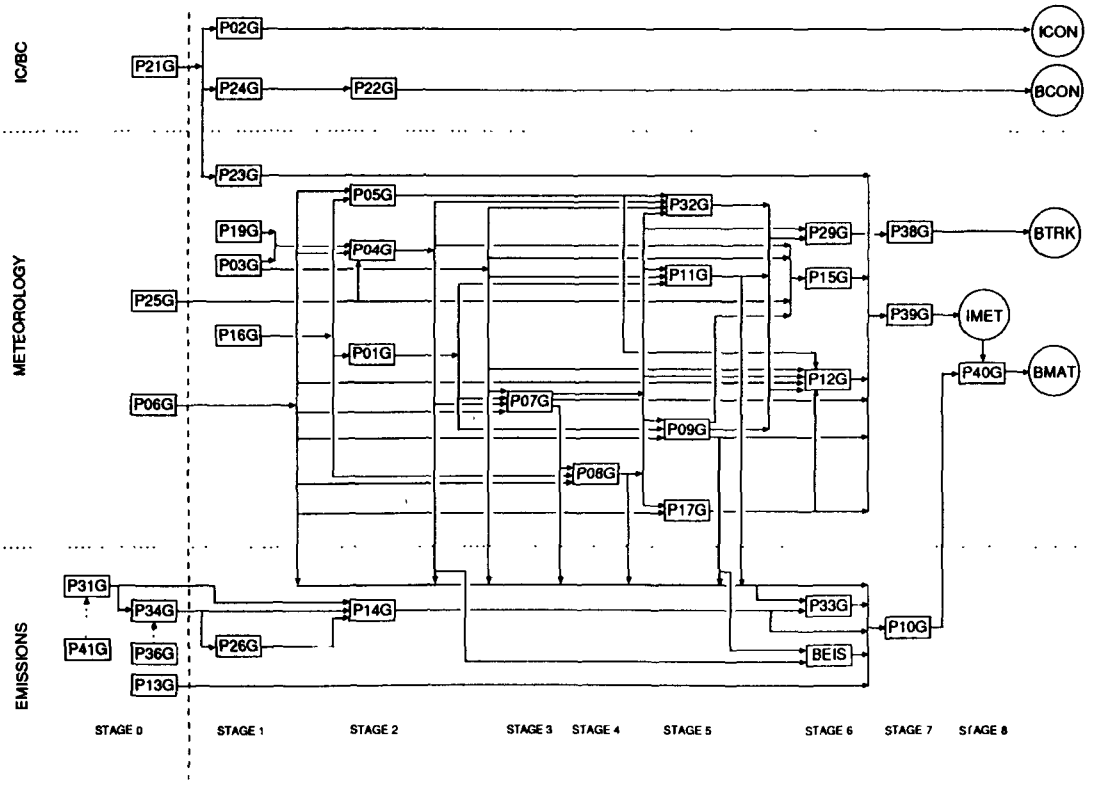

Figure 3. *Structure and output files of the ROM 2.1 input processor network.*

Table 1. *Functional Descriptions of the ROM 2.1 Input Processors*

Processor	Stage	Function in ROM 2.1
P01G	2	Interpolates profiles of upper-air meteorological parameters at intervals of 50 m from hourly rawinsonde vertical profiles
P02G	1	Writes to the file ICON the gridded initial-condition concentrations for each layer and species simulated by the core model, using P21G's clean-air concentrations as initial-condition concentrations
P03G	1	Prepares surface meteorology data (e.g., mixing ratio, virtual temperature, and wind speed) for use in higher-stage processors
P04G	2	Computes gridded surface roughness, and hourly gridded Monin-Obukhov length, surface heat flux, friction velocity, surface temperature, surface relative humidity, and surface wind speed
P05G	2	Uses surface observations to compute hourly gridded values for the fraction of sky covered by cumulus clouds, and also calculates cumulus cloud-top heights
P06G	0	Computes the smoothed terrain elevation for each 10' lat. by 15' long. ROM domain grid cell, and also for a larger domain that extends three grid cells beyond the ROM domain. In addition, it computes average terrain elevations in a finer-resolution domain (cells 5' lat. by 5' long.) for the terrain penetration calculation. Finally, it computes the north-south and east-west components of the terrain elevation gradient (slope)
P07G	3	Computes hourly gridded wind fields in the cold layer, hourly gridded terrain penetration fractions, hourly gridded cold layer growth rates, and hourly gridded thicknesses for layers 0 and 1
P08G	4	Computers hourly gridded cell thicknesses for layers 2 and 3, and various parameters used to specify volume fluxes between these two layers
P09G	5	Computes hourly gridded atmospheric density, temperature, cloud cover, solar zenith angle, and water vapor concentration
P10G	7	Computes hourly gridded emissions source functions in layers 0, 1, and 2 for combined anthropogenic and biogenic sources, and also computes the plume volume fraction in layer 0
P11G	5	Computes hourly gridded horizontal winds for each layer, using rawinsonde vertical profiles and surface-station wind observations
P12G	6	Computes hourly gridded volume fluxes through all model layer boundaries, and cumulus cloud vertical flux parameters
P13G	0	Computes the total length of all line emissions sources (highways and railroads) within each grid cell
P14G	2	Prepares files containing hourly emissions values and stack descriptions for all major point sources, and combined hourly gridded emissions values for minor point sources, area sources, and mobile sources
P15G	6	Computes hourly gridded effective deposition velocities for a set of representative species
P16G	1	Interpolates between rawinsonde observations to produce hourly upper-air profiles at 25-mb resolution
P17G	5	Computes hourly gridded elevations (above MSL) for the tops of layers 0, 1, 2, and 3, and local time derivatives of these elevations
P19G	1	Computes hourly gridded values of fractional sky coverage at the terrain surface for all cloud types combined
P21G	0	Computes daytime and nighttime tropospheric background (clean-air) concentrations in each layer for each chemical species
P22G	2	Computes and writes to the file BCON the gridded boundary-condition concentrations for each species, layer, and advection time step simulated by the core model, for the north, south, east, and west boundaries
P23G	1	Computes hourly gridded upper-boundary-condition concentrations (C-infinity) for a set of representative species
P24G	1	Equilibrates background concentrations of all modeled chemical species with averaged observed ozone concentrations on the north, south, east, and west boundaries, for both daytime and nighttime conditions in each layer
P25G	0	Computes the fraction of each grid cell in each land use category recognized by the model
P26G	1	Computes hourly gridded mobile-source VOC, NO_x, and CO emissions parameters, adjusted for daily average temperature
P29G	6	Computes hourly gridded 30-min backtrack (advection) cell locations and horizontal diffusivities for each layer simulated by the core model
P31G	0	Allocates annual point-source emissions data between a weekday-emissions file, a Saturday-emissions file, and a Sunday-emissions file
P32G	5	Calculates hourly gridded horizontal eddy diffusivities for layers 1, 2, and 3, and also produces parameter fields needed to compute interfacial volume fluxes across layer boundaries
P33G	6	Generates hourly gridded locations and strengths of constant-source emitters for a tracer emissions species
P34G	0	Converts all point-, area-, and mobile-source data files from GMT to LST
P36G	0	Applies NO_x and VOC emission controls at the county level for area- and mobile-source emissions data

Table 1. (Continued)

Processor	Stage	Function in ROM 2.1
P38G	7	Reads the backtrack and diffusivity hourly gridded MF files and computes the BTRK file parameters for each advection t step simulated by the core model
P39G	7	Reads all meteorology hourly gridded MF files except the backtrack and diffusivity files read by P38G and computes the intermediate meteorology (IMET) file parameters for each advection time step simulated by the core model
P40G	8	Reads the intermediate meteorology (IMET) file and the emissions sources hourly gridded MF files and computes the BI parameters for each advection time step simulated by the core model
P41G	0	Applies NO_x and VOC emission controls to point-source emissions data, at a state, county, point, or individual-boiler lev
BEIS*	6	Prepares hourly gridded biogenic emission rates for isoprene, paraffin, olefin, high molecular weight aldehydes (RCHO, R>H), nonreactive hydrocarbons, NO and NO_2, based on a canopy model

*All processors (PnnG) are written in FORTRAN, but the Biogenic Emissions Inventory System (BEIS) is written in SAS. Because of the differen the BEIS is not given a PnnG name.

Changes Made to the Core Model and Its Input Files

ROM Chemistry Solver Changes

The first two changes listed below have increased the computation time for a core model run by about 54%, for a NEROS domain three-day execution on the IBM 3090.

- We implemented a more recent version of the Carbon Bond Mechanism, CBM 4.2; ROM 2.0 used CBM 4.0. CBM 4.2 includes a different chemical species list, a different list of chemical reactions and their rate constants, and it uses an additional variable, water vapor concentration, to adjust some of the reaction rate constants.
- Partly as a result of implementing CBM 4.2, we have altered the FRAX mechanism, which chooses the lengths of the model's chemistry time steps and controls the degree of solution accuracy for the chemical kinetics equations. Overall, the changes cause the model to choose shorter time steps more often than in ROM 2.0, resulting in increased computation time. However, we have offset this increase by changing the minimum allowable time step length from 10 s to 20 s.
- We have added methanol to the list of model species (in addition to the other species list changes caused by implementing CBM 4.2), so that ROM 2.1 can be used to evaluate ozone-reduction strategies involving choices between automotive fuels.

Core Model I/O Modifications to Improve Efficiency

- We have split the ROM 2.0 B-matrix (BMAT) file into two files. BTRK and the new BMAT. The BTRK file contains the backtrack and diffusivity information used by the core model's BIGGAM module; the new BMAT file contains the parameterization for vertical fluxes, the meteorological parameters necessary for chemistry rate constant adjustment, and parameterized emissions source strengths, all needed by the core model's LILGAM module. We also designed the new BMAT file to be a multiple BMAT file that can be distributed over many disks.
- We eliminated the row-windowing feature, which was included in ROM 2.0 because of memory limits on older computers.

Changes That Should Allow Future Outside Users to Apply the Core Model

- Eventually, we plan to release the core model to outside users so that they can perform their own emission control strategy evaluations. To assist these users, we have designed the ROM 2.1 processor network to produce one large file from stages 0 through 7 of the meteorology network, called the IMET file (see Figure 3). For each three-day episode outside users want to model, we will run the meteorology portion of the network and provide them with the resulting IMET file; the users will run the emissions portion of the processor network themselves to produce the final emissions MF files, and then combine these with our IMET file to produce their own BMAT file. We will also give them the other three files needed to run the core model (ICON, BCON, and BTRK) for each episode.

In addition to the changes listed in the three subsections above, we also improved the core model by (1) reversing the vertical-layer-then-column order of BIGGAM's computations, (2) improv reporting to the run-time log file, standardizing the code so that it is ea to read and to maintain, and (4) simpl ing and standardizing the structure of file headers that give information on contents of each core model file.

Changes Made to the Input Processor Network

ROM 2.0 Processors Deleted from the Network During the Upgrade

Overall, in converting from ROM 2.(ROM 2.1, we deleted the following ROM 2.0 processors from the netw **P18G** and **P20G**, which we have corporated as subroutines into the R 2.1 version of P11G; **P27G**, which been transformed into the ROM 2.1 I genic Emissions Inventory Syst (BEIS); **P28G** whose functions are p formed in ROM 2.1 by process P38G,P39G, and P40G; and **P3** whose functions are performed by ROM 2.1 processors P36G and P41G.

ROM 2.1 Processors Added to the Network During the Upgra

We also added seven new proces and the new BEIS to the network upgrading the ROM to version 2.1. Sc of these perform functions that were cluded in ROM 2.0 processors we h deleted from the network (see abo and some perform functions not inclu in ROM 2.0's processor network at Refer to Table 1 for descriptions of seven new processors: **P21G**, **P2 P36G**, **P38G**, **P39G**, **P40G**, and **P4** The other addition, **BEIS**, performs combined functions of ROM 2.0's BI and P27G. Because the BEIS is very ferent from the ROM 2.0 biogenic e

sions processing system, we have augmented the Table 1 BEIS information by listing other major differences below:

- In computing biogenic hydrocarbon emission rates, the BEIS uses broad vegetation classes instead of individual species.
- It includes a canopy model that allows it to compute more accurately the temperature and solar intensity profiles within a tree canopy.
- It calculates emission rates for isoprene, α-pinene, monoterpene, and unknown species (instead of for nine roughly-defined hydrocarbon classes), and then converts these into emission rates for the CBM 4.2 species isoprene, paraffin, olefin, high molecular weight aldehydes (RCHO, R > H), and nonreactive hydrocarbons.
- It calculates NO and NO_2 emission rates for grasslands; P27G in ROM 2.0 did not output these species at all.

ROM 2.0 Processors that are Included in the ROM 2.1 Network

Twenty-seven of the ROM 2.0 processors are also included in the ROM 2.1 processor network. Some are essentially unmodified, but all have been changed in minor or major ways. In addition to the changes listed below, the code for all processors has been standardized so that it is easier to read and to maintain. Also, we have completed enhancements to the network that allow us to model domains with dimensions other than 60 columns by 42 rows, and that allow us to apply the network more easily to different geographic regions.

We have modified the PF/MF database directory file, which controls the processors' access to the PFs and MFs, to reflect the changes we have made to the processor network for ROM 2.1. We have also upgraded the PF/MF database software by incorporating better error checking procedures.

In addition to upgrading processors, we have also created a set of raw data processing routines that preprocess the emissions data before they reach the emissions portion of the network. These routines reduce file sizes, and therefore computation time, by eliminating unnecessary parameters.

ROM 2.0 Processors that Did Not Change for ROM 2.1—

There were eight ROM 2.0 processors that we did not modify in converting to ROM 2.1, except in the general ways mentioned in the previous paragraph: **P01G**, **P06G**, **P13G**, **P17G**, **P19G**, **P25G**, **P29G** and **P32G**. Table 1 describes their functions.

ROM 2.0 Processors Altered for ROM 2.1—

We made minor or major modifications to 19 of the ROM 2.0 processors during the upgrade to ROM 2.1, in addition to the general changes we made to all processors. The items listed below are all differences between ROM 2.0 and ROM 2.1 versions of the processors.

- **P02G** processes the CBM 4.2 species instead of the CBM 4.0 species, and also writes the ICON file header in the new format required by the ROM 2.1 core model.
- **P03G** can now estimate the occurrence of nighttime inversions on a local (grid cell by grid cell) basis.
- **P04G** now writes hourly gridded files of surface temperature, surface relative humidity, and surface wind speed. We have also added new procedures that use buoy data to estimate meteorological parameters.
- **P05G** can accept surface meteorology station identification codes in either WBAN or call-letter format.
- We eliminated a coding error in **P07G** that caused the magnitudes of the computed cold-layer winds to be in error by about 20%.
- **P08G** no longer computes gridded layer 1, 2, and 3 divergence fields used in wind fields processing; we transferred this function to P11G. Also, P08G now grids the top of layer 2 with respect to ground level instead of sea level. Also, if the top of layer 2 in the morning is higher than 800 m, it is reset to 800 m exactly. Finally, P08G can accept surface meteorology station identification codes in either WBAN or call-letter format.
- **P09G** uses an improved gridding method, and also outputs water vapor concentration values.
- **P10G** makes better use of terrain penetration factors to compute cell volumes and source strengths, and also includes methanol in the list of species it can process. In addition, we eliminated the option to include hazardous waste TSDF input data.
- We made substantial changes to **P11G**:
  - —P11G now uses a height-dependent weighting scheme to compute averages for layers 2 and 3 from rawinsonde profiles.
  - —It includes scaling factors in shear transformations in order to model the variations in both wind speed and direction with altitude.
  - —It now computes divergence fields for layers 1, 2, and 3; P08G performed this function in ROM 2.0. Also, the algorithm for layer 1 divergences now incorporates surface data, in addition to the vertical-profile rawinsonde data used by the older P08G version of the algorithm.
  - —We have incorporated the ROM 2.0 processors P18G and P20G into P11G as subroutines.
  - —We corrected three errors in the ROM 2.0 version; overall, these corrections resulted in winds having less of a westerly component and having somewhat higher energy.
- Because we changed the gridded inversion indicator file read by **P12G**, we had to change the processor's mechanism for deciding which of two volume flux schemes to use. Also, we substantially improved and optimized P12G's code so that it runs noticeably faster than before.
- **P14G** now allows mobile-source and area-source data to be input as separate files; it also includes methanol in the list of species it can process.
- **P15G** includes improved parameterizations for species-dependent deposition resistances, and models ten representative species instead of seven.
- To produce its upper-air profiles, **P16G** now uses an improved smoothing method that does not oversmooth the data. We have also eliminated the option to read in data for nonstandard rawinsonde launch times, and have modified P16G to accept surface meteorology station identification codes in either WBAN or call-letter format.
- **P22G** can now process the CBM 4.2 species. It also reads in four sets of boundary conditions instead of one, and writes the BCON file header in the new format required by the 2.1 core model.
- **P23G** now processes the CBM 4.2 species, and includes the GPRIME set of algorithms that is based on the CBM 4.2 ROM chemistry solver mechanism. In addition, P23G equilibrates background concentrations with an ozone level representative of the top boundary of the model. It also models 12 representative species instead of 13, and calculates the values for these 12 species a different way.
- Like P23G, **P24G** now processes the CBM 4.2 species and includes the GPRIME set of algorithms. It also produces four different sets of boundary conditions instead of just one.

- **P31G** no longer windows the annual point-source data for a particular season, and it no longer writes the data file containing the major point-source stack parameters; the new raw emissions data preprocessing routines perform both these functions. Also, P31G now includes methanol in the list of species it can process.
- **P33G** can now process the species methanol.
- **P34G** now includes mobile-source emissions in its time-shifting process, and it includes methanol in the list of species it can process.

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The complete report, entitled "Development of the Regional Oxidant Model Version 2.1," (Order No. PB 89-194 252/AS; Cost: $15.95, subject to change) will be available only from:

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