U.S. EPA Models-3/CMAQ – Status and Applications

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Extended Abstract:

An advanced third-generation air quality modeling system has been developed by the Atmospheric Modeling Division of the U.S. EPA. The air quality simulation model at the heart of the system is known as the Community Multiscale Air Quality (CMAQ) Model. It is comprehensive in scope and allows for the simulation of ozone and photochemical oxidants, acid deposition, and fine and coarse particles at spatial scales ranging from urban to regional. The model is contained within a computational framework, Models-3 (for 3rd generation), that enables users to interact with the modeling system through a high-level graphical user interface and also facilitates data transmission among the components of the system and provides for analysis, graphics, and visualization capabilities for model simulation results. The modeling system is available from the U.S. EPA (see web site: www.epa.gov/asmdnerl/models3/), and is currently being evaluated for photochemical oxidants and fine particles using field study databases from the eastern United States from 1990 and 1995. The CMAQ is also being extended to include the modeling of selected air toxics, including atmospheric mercury and atrazine (a pesticide).

Models-3 is a sophisticated computational framework for air quality modeling systems. It has been designed and programmed using object-oriented principles (in C++ language). At the highest level, Models-3 presents a graphical user interface (GUI) to the model user. Components presented include the Program and Dataset Managers, for registering programs and datasets; Science Manager and Model Builder for defining science process components and building an executable model, Study Planner for defining and running the required preprocessors and models, Strategy manager for defining emission control strategies and processing emissions, and Tools Manager which is the gateway to the analysis and visualization tools. Models-3 assists the user in setting up new model domains and applications, accessing and tracking data files, and controlling the flow of data and model runs. Component models may be run on the same computer platform as Models-3, or on remote computers where communications links are maintained to the Models-3 server. A configuration currently used at the U.S. EPA has the Models-3 server maintained on a SUN workstation with CMAQ model runs initiated on remote CRAY supercomputers linked to the workstation through fast telecommunication lines.

The most recent release of the Models-3 framework is compatible with SUN workstations running the Solaris2.6 operating system. Another version of the framework, capable of being

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operated on a Windows-NT computer, will become available for beta-testing in late 1999. The fully operational version of the Windows-NT Models-3 framework is expected by summer 2000. In addition to these two platforms, a third port of Models-3 is currently underway to a SGI workstation (beta-version available in early 2000). The Tools Manager currently contains the IBM-DX Explorer graphics and analysis software, and the Vis5D and PAVE visualization packages. Users and Tutorial Manuals are provided with the Models-3 package.

The CMAQ model is a set of Fortran language science codes that include the CMAQ chemical transport (air quality) model (CCTM) and its upstream driver models and processors. These codes are generally portable to any computer platform with available Fortran compilers. (Fortran-77 is the current coding standard; CMAQ-2000 release will begin to use Fortran-90 constructs.) A complete set of CMAQ science documentation is available.[2] A meteorological model is required to provide hourly gridded meteorological fields to the emissions and chemical transport model. Currently the NCAR/Penn State MM5 model is used for that purpose; other meteorological models will be adapted in the future. The meteorological model is run outside of the Models-3 framework and the data that it generates are then brought into Models-3 for use by the downstream models. The MM5 is a freely-available community mesoscale model supported and released by the National Center for Atmospheric Research in Boulder, Colorado. The version that we have adapted for CMAQ use is MM5-v2.10, with a few of our own CMAQ-specific modifications. It is a non-hydrostatic model, and we are using it in one-way nested mode to feed meteorological data to the one-way nested CCTM. Four-dimensional data assimilation is a key feature used to correct errors that typically accumulate over time during the meteorological model run.

The Meteorology-Chemistry Interface Processor (MCIP) assimilates the data generated by the meteorological model and performs a dynamically consistent merging of layers if the number of CCTM layers is smaller than that of MM5. It also computes dry deposition parameters based on an algorithm of M. Wesely for the CCTM. Presently, the MCIP also rediagnoses certain planetary boundary layer parameters, including boundary layer depth, although in the 2000 version of the model these parameters will be passed through directly from the MM5 to the CCTM. The fields produced from the MCIP are then provided to the emissions model and to the CCTM.

The Models-3 Emissions Processor and Projection System (MEPPS) processes base-year emissions, both anthropogenic and biogenic, in chemically speciated, hourly allocated, and gridded form for the chemical transport model. The projection portion of the system estimates emissions for a future year, based on the effects of growth and control programs. The MEPPS is an exception to the other science codes in that it is based mainly on SAS programming code and not Fortran, as well as making use of GIS techniques for allocating the source emissions to model

[2] Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. EPA-600/R-99/030, March 1999, U.S. EPA, Research Triangle Park (also available from Models-3 web site: www.epa.gov/asmdnerl/models3/)

grid cells. Chemically speciated emissions profiles are cataloged by Source Classification Codes (SCC) representing most industrial, transportation, and manufacturing activities. At present MEPPS supports the organic compound classes from two chemical mechanisms, RADM-2 and CB-4. As other chemical mechanisms are added to the CCTM, the emissions system will also be extended to include the proper emissions categories corresponding to the specific chemical mechanism. As part of MEPPS, mobile source emission factors are calculated using the MOBILE5a model. The PART5 model calculates mobile source fine particle emission factors. The BEIS2 is used to estimate hourly biogenic emissions of VOCs and NO. Emissions estimates are made for the appropriate CCTM domain sizes and grid resolutions. The MEPPS-2000 version may contain the MOBILE6 and/or BEIS3 emissions models if they are operationally ready in time. The Emissions-Chemistry Interface Processor (ECIP) takes the emissions outputs from MEPPS and transforms them into CCTM-ready emissions fields, as well as calculating the plume rise from major point source stacks.

Work is on-going to replace portions of the MEPPS emissions processor with the Fortran-based Sparse Matrix Operator Kernel Emissions (SMOKE) processor. The SMOKE processor is not only more advantageous because of the Fortran based portable code, but also because it is an order of magnitude more efficient to run. The initial (Beta) implementation will occur in 1999, with the first operational version within Models-3 completed in late 2000, subject to funding constraints. The operational version will have associated full user documentation and quality control modules.

As part of the SMOKE implementation in Models-3, enhancements are being made to handle reactivity controls and projections. Reactivity control packets, by SCC source category or by specific source, will allow for changing the VOC profile from an emissions process, including substituting a compound of lower reactivity for a higher reactivity compound. The implementation will also allow for a phase-in period for market penetration of substituted compounds when making future-year emissions projections. A new reactivity control matrix is added to the SMOKE processing along with the existing base emissions, speciation, and gridding matrices. SMOKE is also being adapted to increase flexibility to add new pollutants as needed to the emissions processing.

The CCTM is the principal air quality simulation portion of the modeling system. It assimilates the meteorological and emissions data processed as described above, as well as appropriate sets of initial and boundary conditions, and estimates ambient concentrations of modeled pollutant species. The CCTM currently models relevant chemical species participating in ambient photochemical oxidant and aerosol chemistry, and acid deposition. The model has been constructed in a modular and generalized manner to facilitate its pairing with a variety of meteorological models and its inclusion of various process modules for representing a specific numerical solution or science process. The 2000 version will also add an initial air toxics capability for mercury and atrazine (a pesticide).

The gas-phase chemical kinetic mechanisms now supported within the CCTM are the

RADM-2 and CB-4. The SAPRC-99 mechanism is currently being added. Bill Stockwell (DRI) has expressed an interest in working with the Models-3/CMAQ system and possibly adding the RACM mechanism, a successor to RADM-2. In addition, a new approach to kinetic mechanisms, the "morphecule" mechanism (developed by H. Jeffries and colleagues) is being tested now in box models and will be ready for initial testing in CMAQ during 2001-2002. The mechanism reader, a feature of the Models-3 framework, facilitates the inclusion of mechanism changes or new mechanisms in the CMAQ. There are two numerical chemistry solvers available in the CCTM. The first is a general form quasi-steady state approximation (QSSA). It is a predictor-corrector method that makes no steady-state assumptions, and thus can be applied to most chemical mechanisms. The other solver choice is the sparse-matrix vectorized Gear solution (SMVGEAR) which is only applicable to vector computer platforms. This solver is considered as the most accurate of available numerical chemical solutions. We will also be working over the coming year to implement a version of the Hertel numerical solver, a very efficient solver, but whose implementation will be specific to particular chemical mechanisms. Photolysis rates are selected during model simulation from a multi-dimensional look-up table, and they are attenuated based on cloud amount and depth. An optional process analysis and integrated reaction rate module calculates the incremental contribution to process rates from all major modeled processes, and performs a diagnostic analysis of all major chemical pathways. Aqueous chemistry is performed as part of the cloud package in the CCTM, and has been adapted from the earlier Regional Acid Deposition Model.

The chemistry and physics of fine and coarse particles are also simulated within the CCTM. A modal approach is used to describe the size distribution of particles, with three modes: the Aitken mode (<0.1 µm diameter particles), the accumulation mode (0.1-2.5 µm diameter particles), and the coarse mode (>2.5 µm diameter particles). For the fine particles, those in the two size modes less than 2.5 µm, there are 8 chemical species categories for each mode: sulfate, nitrate, ammonium, primary anthropogenic organics, secondary anthropogenic organics, biogenic organics, elemental carbon, and miscellaneous primary (mostly crustal materials). The fine particles also participate in the aqueous chemistry and are dry deposited as well. The particles in the coarse mode do not participate in the chemistry, but are transported, diffused, and dry deposited.

The current U.S. EPA applications of the Models-3/CMAQ modeling system are to nested domains in the eastern U.S., centered on the Northeast including the Washington-New York corridor, as well as on the Nashville, TN area. We are modeling periods during the summer of 1995 at which time several major field campaigns for photo-oxidants took place in these areas. We will be diagnostically evaluating the model for its ability to simulate the key constituents of photo-oxidant and fine particle chemistry. We are also modeling the first six months of 1990 in which we will be assessing the CMAQ's ability to characterize acid deposition and secondary particles against field data from that period from the eastern U.S.

We are seeking to build a community of air quality modelers around the Models-3/CMAQ platform who are interested in applying, evaluating, and extending the CMAQ and its

associated models, and in helping to support and maintain the Models-3 computer framework to facilitate use of the CMAQ and other models. Over the next several years we will be working with the academic, policy, and other communities to implement the modeling system and begin implementing the community model concept for air quality. The first of a series of annual Models-3 Workshops is being planned for the spring of 2000.