SCIENCE FEATURES IN MODELS-3 COMMUNITY MULTISCALE AIR QUALITY SYSTEM

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1. INTRODUCTION

Air quality simulation models are important tools for use by regulatory, policy and research communities. The Clean Air Act provides a societal mandate to assess and to manage air pollution levels to protect human health and the environment. The U.S. Environmental Protection Agency (USEPA) has established National Ambient Air Quality Standards (NAAQS), requiring the development of effective emissions control strategies for such pollutants as ozone, particulate matter and nitrogen species. National and regional policies are needed for reducing and managing the amount and type of emissions that cause acid, nutrient and toxic pollutant deposition to ecosystems at risk and for enhancing the visual quality of the environment. Air quality models are used to develop emission control strategies that achieve these objectives. Control strategies must be both environmentally protective and cost effective. However, for effectiveness, one must recognize that air pollution problems and strategies for their mitigation are very complex and the linkages between sources, meteorology and natural sources and landscapes are highly varied, complex and not very well understood. The goal of developing cost-effective control strategies is challenging and is best considered holistically. The effectiveness of any control strategy is very limiting when air pollution issues are handled in isolation. Emissions from chemical, manufacturing, and other industrial activities, power generation, transportation and waste treatment activities contribute to a variety of air pollution issues, including ozone, particulate matter (PM), acid, nutrient and toxic deposition, and visibility in complex ways, and at a variety of spatial and temporal scales. The residence times of pollutants in the atmosphere can extend to multi day, thus, transport consideration must be at least regional in scale. NAAQS requirements and other goals for a cleaner environment vary over a large range of time scales, from peak hourly to annual averages.

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Development of air quality simulation models started in the late seventies. The Urban Airshed Model (UAM) followed by the Regional Oxidant Model (ROM) provided Eulerian-based models for ozone, the former for urban and the latter for regional scale. Strategies for State Implementation Plans (SIPS) used ROM to provide boundary conditions for UAM simulations. Attention to acid deposition issues was addressed in the eighties with the development and evaluation of regional acid deposition models such as the Regional Acid Deposition Model (RADM), the Acid Deposition and Oxidant Model (ADOM), and the Sulfur Transport and Emissions Model (STEM). Other major modeling systems included the Regional Lagrangian Modeling of Air Pollution model (RELMAP), a Lagrangian framework system, and semi-empirical and statistical models. Models of this period were designed to address specific air pollution issues, such as ozone or acid deposition. Thus, flexibility to deal with other issues such as particulate matter or toxics was very limited. With the passage of the Clean Air Act Amendments of 1990 (CAAA-90), a wide range of additional issues was identified including visibility, and fine and coarse particles, as well as indirect exposure to toxic pollutants such as heavy metals, semi-volatile organic species, and nutrient deposition to water bodies. These latter issues will require multi-media models.

To meet the challenges posed by the CAAA-90, the USEPA embarked upon the development of an advanced modeling framework, Models-3, designed for holistic environmental modeling utilizing state of science representation of atmospheric processes in a high performance computing environment. Descriptions of Models-3 can be found in Novak et al. (1998) and Byun et al. (1998). The science components in Models-3 are called the Community Multiscale Air Quality (CMAQ) system. The Models-3/CMAQ system is designed as a multi-pollutant, multi-scale Eulerian framework air quality and atmospheric deposition modeling system. It contains state-of-science parameterizations of atmospheric processes affecting transport, transformation and deposition of such pollutants as ozone, particulate matter, airborne toxics, and acidic and nutrient pollutant species. With science in a continuing state of advancement and review, it is an important design feature that the Models-3 framework and CMAQ have the capability to integrate and test future formulations in an efficient manner, without needing to develop a completely new modeling system.

In June 1998, the first release version (CMAQ-98)

will become available. It will contain options representing different model descriptions of the major science processes. The science options available to the user include the gas phase chemistry mechanisms, RADM2 and CB-IV, a set of numerical solvers for the mechanisms, options for horizontal and vertical advection schemes, algorithms for fine and coarse particulate matter predictions, photolysis rates and a plume-in-grid approach. The purpose of this paper is to briefly list the key science processes in general and the specific modeling options included throughout CMAQ-98, including the emissions and meteorological processors and their interface processors. Also discussed are methods to determine and test the relative contribution of different atmospheric processes to the air quality predictions, important functions built into the CMAQ system.

2. SCIENCE AND MODELING FEATURES OF CMAQ

In this section, the science components and related features of the CMAQ-98 system is briefly described. The multi-scale capabilities of Models-3/CMAQ are handled by a set of nested domains, each with successively finer resolution. The selection of grid resolution, domain size and area of interest is dependent on the application, and on computational resources. A configuration of three levels of nests with grid resolutions of 36-12-4 km will be provided in CMAQ-98. With such a configuration, the 36km grid resolution resolves the regional scale concentration fields and provides boundary conditions for an intermediate scale at 12 km resolutions to set up the transition to the 4km scale to handle features on urban scales.

2.1. CMAQ Preprocessors:

2.1.1 Meteorology

The CMAQ's generalized coordinate system accommodates meteorological data produced by any comprehensive meteorology model. Initial implementation uses the Fifth Generation PSU/NCAR Mesoscale Model (MM5), (Grell et al., 1993). The configuration for preliminary evaluation includes non-hydrostatic dynamics, four-dimensional data-assimilation (FDDA) of winds, temperature, and humidity, the Kain-Fritsch convective parameterization scheme, and the high resolution boundary layer. A set of four nested grids (108/36/12/4)km is used to achieve urban scale resolution which is consistent with continental scale dynamics.

In addition to the standard community version of MM5, a more sophisticated land-surface model has been developed and coupled to the MM5 to improve simulation of surface fluxes, surface temperature and humidity, and planetary boundary-layer (PBL) development (Pleim and Xiu, 1995). The surface scheme includes explicit simulation of soil moisture and vegetative evapotranspiration. The CMAQ has been designed to take advantage of the additional surface and PBL parameters produced by this scheme including bulk stomatal resistance which is then used to compute chemical dry deposition velocities. The surface model is being added to the community MM5 and will be available as an option in future releases from NCAR.

CMAQ uses an interface processor to link the meteorology and the chemistry-transport model (CTM) called MCIP. As part of its functionality, MCIP contains a generalized coordinate capability. It also contains algorithms for treating dry deposition.

2.1.2 Emissions

CMAQ-98 will use an emission processing system called Models-3 Emissions Processing and Projection System (MEPPS). The MEPPS is a crucial part of the Models-3 modeling framework. The MEPPS will processes emission inventory data, performs future projections (including control scenarios run using the Models-3 study planner) as well as pre-processing of data for use by the Models-3 CMAQ model. The MEPPS' input Data PROcessor (MEDPRO) will be capable of importing, performing QA and converting emission data, including but not limited to the 1985 National Acid Precipitation Assessment Program Inventory, 1990 Interim National Inventory, and 1990 National Emissions Trends Inventory. MEPPS estimates mobile sources using the Mobile 5a model, and biogenic emissions using the BEIS-2 model. Point and county level area source emissions data are taken from inventories. Emission data are tracked and reported by source category code. Spatial gridding is performed using Arc/Info GIS software. Meteorological data from MM5 via MCIP are used in modeling mobile sources and biogenic emissions. CMAQ-98 MEPPS will have the capability to provide speciated emissions needed for using CB-IV and RADM2 chemistry mechanisms or user-defined modifications. Future versions will be able to support other mechanisms.

2.1.3 Boundary and Initial Conditions

CMAQ-98 will establish the boundary conditions for the nests by first creating modeled fields at the coarse mode, either at the 108 or 36km resolution. Alternatively, future capabilities can incorporate observed data fields such as from remote sensors and satellite platforms. Initial conditions will be obtained from the end of spinup runs of several days.

2.2 The Chemistry-Transport Model (CTM).

The science core of the CMAQ system is the CTM. Science processors in CTM will include the following capabilities:

2.2.1 Chemistry.

CMAQ includes both the RADM2 and the CB-IV gas phase mechanisms. In addition the CMAQ provides the capability to edit the RADM2 and the CB-IV mechanisms or to import a completely new chemical mechanism by means of a generalized chemical mechanism reader. This reader is external to the CTM, and can significantly simplify the task of altering the chemical representation in a CTM. However, any change to the

fundamental representation of the organic species in these two mechanisms will correspondingly require substantial changes to MEPPS. The CMAQ also accounts for the formation of secondary aerosols and the reactions of pollutants in the aqueous phase. Secondary aerosol formation is parameterized on the basis of important gas-phase reaction rates and aqueous reactions are simulated by means of the aqueous chemical mechanism incorporated in RADM. Both the CB-IV and RADM2 gas-phase mechanisms are linked to these processes, however, providing the capability to simulate multi-phase interactions using either gas-phase mechanism. Finally, two chemistry solvers are available -- the Sparse Matrix Vectorized Gear (SMVGEAR) algorithm developed by Jacobson and Turco (1994) and the Quasi-Steady State Approximation (QSSA) method used in the Regional Oxidant Model. SMVGEAR is generally recognized as the more accurate of the two, but it is much slower than QSSA on non-vector computers.

2.2.2 Cloud processes:

Modeling clouds are essential in air quality modeling due to their critical role in atmospheric pollutant transport and chemistry processes. Clouds have both direct and indirect effects on the pollutant concentrations: they directly modify concentrations via aqueous chemical reactions, vertical mixing, and wet deposition removal processes, and indirectly affect concentrations by altering radiative transmittances which affect photolysis rates and biogenic fluxes. CMAQ-98 will model deep and shallow clouds using the RADM-type (Walcek-Taylor) algorithms for 36 and 12 km; an explicit type cloud scheme is being tested for the 4 km simulations.

2.2.3 Diffusion and Advection

Options for computing subgrid vertical transport include eddy diffusion, and the Asymmetric Convective Model (ACM) (Pleim and Chang, 1992), the latter applicable to convective conditions. Horizontal diffusion is limited to use of a constant eddy diffusion coefficient. Numerical methods differ in the handling of advection of concentration fields. Several methods are implemented in the CMAQ; these include the method by Smolarkewicz (1983), a scheme by Bott (1989), and a piecewise parabolic method (PPM) (Collela and Woodward, 1984). The Smolarkiewicz technique is mass conservative, and it is based on the first order upstream method. The Bott scheme CPU costs are comparable to Smolarkiewicz's, negative concentration values are limited, and it is highly accurate and mass conservative. The PPM subgrid distributions of advective quantities are represented by a parabola in each grid. PPM provides local fit to data, is monotonic, and contains special steepening procedures where sharp gradients exist.

2.2.4 Particle Modeling and Visibility:

One of the major advancements in CMAQ is the modeling of fine and coarse mode particles. The fine fraction model described in Binkowski and Shankar (1995) is incorporated into CMAQ-98. CMAQ will predict hourly gridded concentration of fine particle mass whose size is equal to or less that 2.5 microns, speciated to sulfate, nitrate, ammonium, organics and aerosol water. Secondary sulfate is produced by chemical reactions of hydroxyl radicals with sulfur dioxide producing sulfuric acid that either condenses to existing particles or nucleates to form new particles. Anthropogenic and biogenic hydrocarbon precursors also react with hydroxyl radicals, and with ozone and nitrates to produce condensible material. Aerosol water is equilibrated with relative humidity and the ammonium to sulfur molar ratios. The fine range is modeled with two log-normal size distributions; the coarse fraction uses one log-normal distribution. Nuclei and Aitken particles are modeled in the smaller of the two fine particle modes. The second mode is called the accumulation mode. At the point of overlap, particles from the nuclei mode are shifted to the accumulation mode when the Aitken-mode growth rate exceeds that of the accumulation mode. CMAQ model outputs also include number densities for both fine modes and for the coarse modes. CMAQ-98 will provide methods for computing particle nucleation, aerosol dry deposition, and cloud processes including the oxidation of Sulfur(IV) to Sulfur(VI) by hydrogen peroxide. Primary particles enter from MEPPS.

The modeling of aerosols in CMAQ provides the capability to handle other environmental issues including visibility and semi-volatile air toxics. Visibility (in Deciview units) is output for each grid and model time step. The visibility formulation in CMAQ-98 is based on integrating the Mie scattering over the distribution of the predicted particles. In another potential application, CMAQ can provide the basis for modeling the atmospheric transport and deposition of semi-volatile organic compounds (SVOC) with parameterizations for their rates of condensation to and/or volatilization from the modeled particles.

2.2.5 Plume-in-Grid (PinG) modeling:

CMAQ-98 will include algorithms to provide a more realistic treatment of the subgrid scale physical and chemical processes impacting pollutant species in plumes released from selected Major Elevated Point Source Emitters (MEPSEs). The key PinG components developed to treat the relevant processes at the proper spatial and temporal scales for pollutant plumes include a Plume Dynamics Model (PDM) processor, which simulates plume rise, vertical/horizontal growth, and plume position and a Lagrangian Reactive Plume Module (LRPM), which simulates the relevant dynamic and chemical reaction processes of subgrid plumes until certain criteria are met triggering the handover of plume material to intercepted grid cells. PinG will be used for the 36km and the 12 km simulations while at 4 km resolutions, PinG is not invoked as the MEPSE emissions are directly released into the CTM 3-D grid cells. A detailed description of the PinG features is given in Gillani et al. (1998).

2.2.6 Photolysis Modeling:

The photochemistry of pollution is initiated by photo

dissociation of smog precursors driven by solar radiation. The amount of radiation available for photochemistry is clearly dependent on sun angle (time of day), season, latitude, and land surface characteristics, and greatly affected by atmospheric scatterers and absorbers, as well as cloud fields. Additionally, photolytic rates are wavelength and temperature dependent, thus, making their calculation very complex, and requiring great accuracy. An advanced photolysis rate model will be installed in CMAQ-98, with capabilities to predict temporally resolved 3-D gridded photolyses rates using input data from the MM5-FDDA and other available sources. It will have flexibility in the specification of wavelength bands, extraterrestrial irradiances, vertical profiles of ozone and aerosols, cloud distribution and adsorption cross section and quantum yield data. The model will have the capability of computing photolysis rates for any chemical mechanism with a user specified absorption cross section and quantum yields data. CMAQ-98 defaults have been set up for CB-IV and RADM2 mechanisms. Studies have shown great sensitivities to the modeled cloud fields, and clearly photolysis rates will be limited by the accuracy of the modeled cloud fields.

2.3. Process Analysis

Process analysis involves examining the effects that different physical and chemical atmospheric processes have on pollutant concentrations. It is accomplished in a model by quantifying the contributions of individual processes to the overall change in a species concentration. This information explains how individual model predictions come about and reveals the relative importance of each process. It can be used diagnostically to identify potential sources of error in either the model formulation or the model input data. Further, it is particularly useful for gaining understanding of the effects of making changes to the model or to its inputs. CMAQ-98 provides the capability to perform process analyses using two different pieces of information: Integrated Process Rates (IPRs) and Integrated Reaction Rates (IRRs).

The IPRs are obtained during a model simulation by computing and saving the change in concentration of each species caused by physical processes including advection, diffusion, emissions, etc. IPRs are also calculated for chemical reaction, aerosol production, and aqueous chemistry, but values provide no information on the particulars occurring within each process (i.e., they only give the *net* effect of each process). These IPRs can be output for each species at varying times to show how the effects of each process vary both in time and in space. Thus, they are particularly useful for identifying unexpectedly low or high process contributions which could be indicative of model errors.

The IRR analysis deals with the details of the chemical transformations. CMAQ-98 currently provides the capability to conduct IRR analyses for gas-phase chemical species only, but extensions to aqueous chemistry and aerosol formation are planned. For gas-phase chemistry, the CTM has been instrumented to compute not only the concentration of each species, but also to compute the integral of the individual chemical reaction rates. The computation and output of the IRRs are synchronized with the standard concentration field calculations and outputs to permit one to study details of the atmospheric transformations and their effects on pollutant concentrations. IRR analyses have been primarily applied to aid in the understanding of ozone formation (Jeffries and Tonnesen, 1994). For example, IRRs have been used to quantify such chemical characteristics as OH and NO chain lengths, the amount of new radical production and termination, the amount of ozone produced by and the yield of radical species from each VOC species. These quantities have typically been used to understand the reasons for differences in model predictions obtained with different chemical mechanisms.

2.4. CMAQ Code Integration:

The codes for CMAQ system integrated into the Models-3 framework are in FORTRAN. The integration procedure was facilitated by following a small set of design, coding and implementation standards that include: (1) modularity, which employs the concept of interchangeable modules within process classes, allowing easy exchange of time-splitting, science process solvers such as Bott and PPM; (2) a standard subroutine interface at the module level. (Each science module is conceived as operating on the gas and aerosol species concentrations within the domain grid space for its specified time period (model synchronization time step) in sequence throughout the modeling scenario.); (3) restriction of coding practices, which conceal data dependencies, hinder maintenance and foster hidden bugs, e.g., eliminating common blocks, at least across modules; and (4) the Models-3 I/O-API (ref 9), which contains standardized file I/O functions and a modeler-friendly interface built on top of self-describing netCDF (ref 10) files that are portable across most, if not all Unix platforms.

The CMAQ codes have been generalized to accommodate a range of different computational coordinate systems. The essential solution in making the code sufficiently general is to relegate the problem to the MCIP which produces data in the correct coordinate form for CMAQ. Once a user has selected the modules and options, building that version of a CMAQ is made relatively easy. The selected domain and chemistry information is encapsulated in parameter or data statements that are automatically written to FORTRAN include files, which in turn, are linked into the code during the build process to produce the CMAQ executable. Execution of this CMAQ requires the correct linkage with the meteorological and emissions interface processor data to ensure the correct generalized coordinate implementation.

3. DISCUSSION

A typical simulation of Models-3/CMAQ provides hourly air quality fields for regional to urban scales for multi-day episodes, typically of up to five days in duration. The new PM-fine standard will be based on annual averages; thus, utilization of CMAQ in this application will require aggregation

techniques. One such technique, initially developed for RADM wet deposition applications, was recently modified and successfully applied to fine particulate matter by Eder and LeDuc (1996). This approach, which utilizes visibility data as a surrogate for fine PM, will be applied to CMAQ on a continental scale (i.e., contiguous United States, southern Canada and northern Mexico). Future efforts will be needed to validate this approach when a network of fine particulate samplers is deployed; also, aggregation approaches for mesoscale domains will need to be developed perhaps utilizing the method by Eder et al., (1994).

The design basis for the CMAQ is its ability to adapt to science advances in atmospheric process modeling. Thus there will be a continuing need for evaluating the performance and the veracity of the process modules as the CMAQ advances its science basis. The model evaluation activity for the CMAQ will be staged with the initial efforts to show relative performance against the RADM, which itself has undergone extensive model evaluation efforts. Diagnostic evaluation will continue using-data bases from different regional studies such as the 1995 Southern Oxidant Study conducted in the vicinity of Nashville, TN and the NARSTO-NE study.

CMAQ can be configured for a wide range of applications from science studies and investigations to regulatory applications. An evaluated CMAQ can provide the benchmark from which more operational configurations can be referenced. It is anticipated that as science advances are provided to CMAQ, future configurations of a more operational nature can be periodically rebenched as appropriate.

Finally, we encourage full participation by the scientific and modeling communities to engage in the growth and use of Models-3/CMAQ. Models-3/CMAQ has flexibility for incorporating scientific and modeling advances in its air quality science process modules, for testing of alternative science descriptions of processes, and for extending its current capability to handle multimedia environmental issues. Additionally, the community of users should be vigilant in performing evaluations and testing against improved databases and measurement technology to insure model comparability to the real world.

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15. SUPPLEMENTARY NOTES

16. ABSTRACT

Models-3 is framework for environmental modeling utilizing state of science representation of atmospheric processes in a high performance computing environment. The Community-based Multi scale Air Quality (CMAQ) system is Models-3 air quality modeling system. Models-3/CMAQ model is designed as a multi-pollutant Eulerian grid regional to urban scale air quality and atmospheric deposition modeling system. It contains state-of-science parameterizations and algorithms of the relevant and contributing atmospheric processes affecting transport, transformation and deposition of sources contributing to such pollutant issues as ozone, particulate matter, airborne toxics and deposition of acidic and nutrient pollutant species. The release version of Models-3/CMAQ will feature science options available to the user including the gas phase chemistry mechanisms, RADM2, and CB-IV a set of chemistry solvers, options for horizontal and vertical advection schemes, algorithms for fine and coarse particulate matter, photolysis rates and a plume-in-grid approach. These current science options are discussed in the context of the overall structure of Models-3/CMAQ model which includes an emission and meteorological preprocessors linked to the CMAQ by interface processors. Also discussed are the methods to determine and test the relative contribution of different atmospheric processes to the air quality predictions, important functions built into the CMAQ system.

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