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SCIENCE ALGORITHMS OF THE EPA MODELS-3 COMMUNITY MULTISCALE AIR QUALITY (CMAQ) MODELING SYSTEM

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FOREWORD

The Models-3 Community Multiscale Air Quality (CMAQ) modeling system has been developed under the leadership of the Atmospheric Modeling Division of the EPA National Exposure Research Laboratory in Research Triangle Park, NC. This new generation of modeling software was under development for seven years and was made available in June 1998 without charge for use by air quality regulators, policy makers, industry, and scientists to address multiscale, multi-pollutant air quality concerns.

Models-3/CMAQ has a unique framework and science design that enables scientists and regulators to build their own modeling system to suit their needs. Users can access pre-installed modeling systems provided by the EPA or can incorporate their own modeling systems to work within the existing framework software.

This direct user involvement is key to the concept of a community modeling and analysis system. This approach to model development, application, and analysis leverages the community's complementary talents and resources to set new standards for rapid incorporation of better science into air quality model applications. The resulting comprehensive system forms the foundation upon which the community, including governments, industry, academia, and other stakeholders, can collaborate in the examination of issues and the subsequent development of strategies that meet society challenges of environmental protection.

The release of Models-3/CMAQ is one of the many steps which we hope will unite the community under the common goal of advancing our knowledge and abilities to tackle critical problems of the future in far more effective ways than have been attempted in the past. Scientifically sound modeling systems, developed and supported by the community, are one method of achieving this goal.

The June 1998 release of the Models-3/CMAQ computer code was accompanied by a User Manual [EPA-600/R-98/069(b)] to serve as a reference on how to use the software system. This Science Document is the counterpart to the User Manual in that it presents the peer reviewed scientific bases for the Models-3/CMAQ modeling systems. This document also includes components such as interface processors, process analysis routines, and the present and planned evaluation program.

F. A. Schiermeier
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The development of the science components of the Models-3 Community Multiscale Air Quality (CMAQ) system represents a major undertaking by a large team of dedicated atmospheric scientists and a relatively long term effort beginning in the early 1990s, and covers a wide area of subject material as embodied in each of the contributing chapters. Most of the EPA Models-3 CMAQ Science Team are from the Atmospheric Modeling Division (AMD) in the EPA Office of Research And Development's National Exposure Research Laboratory (NERL). With several exceptions the contributing authors from this Division are on detail from the Air Resources Laboratory of the National Oceanic and Atmospheric Administration (NOAA). The NOAA-AMD effort is supported through Interagency Agreement (DW13937252) with the EPA. The authors of each of the chapters of this document would like to collectively express their gratitude to the other members of the NOAA Division. In particular we acknowledge the encouragement and support of the Director of the Atmospheric Modeling Division, Francis Schiermeier. We are indebted to Dr. Robin Dennis for his vision and role in ensuring the implementation of holistic-one-atmosphere approach into CMAQ. We also recognize the technical help from our colleagues Tom Pierce, Steven Howard, Alfreida Torian, and Gary Walter.

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- Transport Algorithms for Air Quality Simulation Models (CR-822059, MCNC), PI: Talat Odman;
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EXECUTIVE SUMMARY

THIS SCIENCE DOCUMENT PRESENTS THE PROCESSORS AND ALGORITHMS THAT EMBODY THE INITIAL RELEASE OF THE MODELS-3 COMMUNITY MULTISCALE AIR QUALITY (CMAQ) MODELING SYSTEM. CMAQ IS A MULTIPLE POLLUTANT MODEL THAT CONTAINS NEW SCIENTIFIC APPROACHES TO AIR QUALITY MODELING, WHICH REPRESENT THE CURRENT STATE OF SCIENCE. This CMAQ Science Document is a living document that will be updated as the state of the science progresses. The CMAQ Science Document provides a basis and point of reference for the state of the science captured in the June1998 initial release of Models-3. Current and future efforts to improve the Models-3 modeling system(s) will depart from the scientific reference points presented in this document.

Models-3 is a flexible software system that provides a user-interface framework for CMAQ air quality modeling applications and tools for analysis, management of model input/output, and visualization of data. The Models-3 framework relies on two modeling systems to provide the meteorological and emissions data needed for air quality modeling. With this data, the Models-3 CMAQ modeling system can be used for urban and regional scale air quality simulation of tropospheric ozone, acid deposition, visibility, and particulate matter ($PM_{2.5}$ and PM_{10}). The meteorological and emissions modeling systems that are provided with the current release of Models-3 will be described in this document. However, CMAQ is designed as an open system where alternative models can be used to generate the data.

This CMAQ Science Document contains chapters that address specific scientific and technical issues involved in the development and application of the Models-3 CMAQ modeling system. The principal researchers for each model component or function authored the coinciding chapter in this document. They serve as the points of contact for scientific questions regarding their CMAQ air quality model components. For instructions on using the Models-3 framework and using the MM5, MEPPS, and CMAQ modeling systems, refer to the Models-3 *User Manual* (EPA/600/R-98/069b, National Exposure Research Laboratory, Research Triangle Park, NC) and *Tutorial* (EPA/600/R-98/069c, National Exposure Research Laboratory, Research Triangle Park, NC).

An overview of the MEPPS emissions, MM5 meteorology, and CMAQ air quality modeling systems is provided in Chapter 1. Chapter 2 then introduces the Models-3 framework and structure and explains how the framework's user-interface is used with the MEPPS and CMAQ modeling systems. More detailed discussions on the modeling systems are then discussed separately in the following chapters. The amount of detail and the length of these discussions vary depending on whether this information has already been provided elsewhere. Some chapters provide a synopsis of the scientific components and refer to previously published material on the subject, while other chapters provide extensive detail on new scientific techniques that are not currently described in other publications.

MM5 Meteorological data are essential for many processes simulated in the CMAQ chemical transport model including transport, chemistry, and cloud processes. The Fifth-Generation Penn State/NCAR Mesoscale Model (MM5) is the only meteorology model compatible with the initial release of Models-3. MM5 is a complex, state-of-the-science community model, and it is maintained by NCAR. MM5 is well documented by its primary developers in technical notes and refereed journal articles. Chapter 3 briefly describes the scientific aspects of MM5, including grid definitions, model physics, nesting, and four dimensional data assimilation. These descriptions generally direct the user to more complete documentation about particular aspects of MM5. To promote the flexibility of CMAQ, additional meteorology models will be compatible with Models-3 future releases.

MEPPS Chapter 4 provides a description of the Models-3 Emission Processing and Projection System (MEPPS) structure, its scientific approach, and the assumptions used in modeling and processing emission data in the Models-3 framework. The chapter also discusses data flow and quality control used with emission inventory and meteorological input data for MEPPS. The description of the main Emission Processor addresses the basis of spatial and temporal allocation procedures, and the methods and assumptions used in modeling mobile and biogenic emissions and in the "lumping" of individual chemical species are also presented. This chapter also explains the procedures used by the Models-3 Emission Projection Processor to estimate emission data for use in modeling future air quality scenarios.

THE CMAQ CHEMICAL TRANSPORT MODEL (CCTM)

Fundamentals of One-Atmosphere Dynamics for Multiscale Air Quality Modeling Chapter 5 provides information essential to the proper use of meteorological data in air quality modeling systems. The chapter introduces a robust and fully compressible set of governing equations for the atmosphere, which provides an integral view of atmospheric modeling. The limitations of several simplifying assumptions on atmospheric dynamics are presented, as are concepts of on-line and off-line coupling of meteorological and air quality models. In addition, this chapter describes a procedure for conserving the mixing ratio of trace species even in the case of meteorological data that are not mass consistent. In summary, Chapter 5 attempts to bridge the information gap between dynamic meteorologists and air quality modelers by highlighting the implication of using different meteorological coordinates and dynamic assumptions for air quality simulations.

Governing Equations and Computational Structure In Chapter 6, the governing diffusion equation is derived in a generalized coordinate system, which is suitable for multiscale atmospheric applications. CMAQ's use of generalized coordinates for its governing equations provides the flexibility to span multiple scales and to incorporate meteorological data on different coordinates. The CMAQ system's modularity concepts and fractional time-step formulation, and CCTM's key science processes are described. Chapter 6 also presents the dynamic formulations of several popular Eulerian air quality models as emulated by the governing diffusion equations in the generalized coordinate system.

Numerical Transport Algorithms The transport processes in the atmosphere primarily consist of advection and diffusion. In Chapter 7, CMAQ's numerical algorithms for advection and vertical and horizontal diffusion are discussed. To provide the CMAQ system with multiscale capability, the transport processes, both advection and diffusion, are formulated in conservation (i.e., flux) forms for the generalized coordinate system. Therefore, CMAQ's numerical transport algorithms will function under a wide variety of dynamical situations and concentration distribution characteristics. Users are encouraged to experiment with their own algorithms to test different numerical schemes for air quality simulations.

Gas Phase Chemistry Chapter 8 examines the way gas-phase chemistry is treated in CMAQ. The CMAQ system currently includes two base chemical mechanisms, RADM2 and CB4, while the incorporation of a third, the SAPRC97 mechanism, is planned for the future. Chapter 8 describes each of these chemical mechanisms as well as the manner in which the first two are linked to the aqueous chemistry and aerosol formation processes. The chapter also discusses procedures for entering new chemical mechanisms in the CMAQ system, the representation of reaction kinetics, the numerical modeling of gas-phase chemistry, and the two numerical solvers included in CMAQ, SMVGEAR and a variant of the QSSA method.

Plume-in-Grid Chapter 9 introduces the plume-in-grid (PinG) technique developed for CMAQ. PinG is designed to treat more realistically the dynamic and chemical processes impacting selected major point source pollutant plumes in CMAQ. The Plume Dynamics Model (PDM) simulates plume rise, horizontal and vertical plume growth, and transport of each plume section during the subgrid scale phase. The PinG module simulates the relevant physical and chemical processes during a subgrid scale phase. This technique is in contrast to the traditional Eulerian grid modeling method of instantly mixing the point source emissions into an entire grid cell volume. Chapter 9 describes the technical approach and model formulation of the relevant processes, and discusses the capabilities and limitations of the initial version of the PinG approach.

The Aerosol Module One of CMAQ's key strengths is that it is a multi-pollutant model that fully addresses the criteria pollutants PM and ozone. Chapter 10 discusses the aerosol module of CMAQ, which is designed to be an efficient and economical depiction of aerosol dynamics in the atmosphere. This chapter discusses the techniques for distributing particulates in three modes: coagulation, particle growth by the addition of new mass, and particle formation. The aerosol module considers both $PM_{2.5}$ and PM_{10} and includes estimates of the primary emissions of elemental and organic carbon, dust, and other species not further specified. Secondary species considered are sulfate, nitrate, ammonium, water and organic from precursors of anthropogenic and biogenic origin.

Cloud Chemistry and Dynamics Chapter 11 discusses the role and functions of clouds in CMAQ. Clouds are involved in aqueous chemical reactions, vertical mixing of pollutants, and removal of aerosols by wet deposition, all of which affect the

concentration of air pollutants. CMAQ's cloud module performs several functions related to cloud physics and chemistry, and it models three types of clouds: sub-grid convective precipitating clouds, sub-grid non-precipitating clouds, and grid-resolved clouds. The cloud module vertically redistributes pollutants for the sub-grid clouds, calculates in-cloud and precipitation scavenging, performs aqueous chemistry, and accumulates wet deposition amounts.

CMAQ INTERFACE PROCESSORS PREPARE INPUT DATA FROM SOURCES INCLUDING THE EMISSION AND METEOROLOGICAL MODELING SYSTEMS FOR USE IN THE CMAQ CTM. EACH OF THESE PROCESSORS, EACH OF WHICH HAVE SPECIFIC FUNCTIONS, ARE DESCRIBED IN THE CHAPTERS MENTIONED BELOW.

The interface processors that handle input data from the emissions and meteorological models are essential because CMAQ is an open system in which meteorological and emissions data are calculated separately (i.e., "off-line"), rather than during the chemical transport model simulation. These interface processors also add extra quality control, so that inconsistencies between input data and the CCTM are minimized.

ECIP In addition to describing the Models-3 MEPPS emission modeling system, Chapter 4 discusses the Emission-Chemistry Interface Processor (ECIP). ECIP serves as the key link between the MEPPS system and CCTM. ECIP's primary function is to generate hourly 3-D emission data files for CCTM from the individual emission file types produced by the MEPPS. The key inputs for ECIP are the area emissions file, the stack parameter and emission files for the point sources generated in MEPPS, and a set of meteorological data files generated by the Meteorology-Chemistry Interface Processor (MCIP) for the CCTM domain. All major point sources are subject to plume-rise and initial vertical dispersion processes before being allocated to a particular vertical model layer.

MCIP Chapter 12 describes MCIP, which links meteorological models, such as MM5, with the CCTM system to provide the complete set of meteorological data needed for air quality simulation. To support CCTM's multiscale generalized coordinate implementation, MCIP provides appropriate dynamic meteorological parameters to allow mass-consistent air quality computations. MCIP deals with issues related to data format translation, conversion of parameter units, diagnostic estimations of parameters not provided, extraction of data for appropriate window domains, and reconstruction of meteorological data on different grid and layer structures. MCIP also relies on the **Landuse Processor** (LUPROC) to provide landuse and vegetation information to define surface characteristics to compute dry deposition and other PBL parameters. LUPROC extracts information about landuse in the CMAQ domain from a landuse database and converts it into the fractional landuse data used in MCIP.

Initial and Boundary Conditions Initial conditions provide a simulation's starting point, while boundary conditions define influences from outside the domain.

Chapter 13 describes the two interface processors that generate the concentration fields for the initial and boundary conditions for CCTM. The chapter describes how the initial condition (ICON) and boundary condition (BCON) processors can be used to generate the concentration fields from either predefined default vertical profiles or from other CMAQ simulation results when model nesting is being performed. This chapter also discusses generating initial and boundary concentrations for special tracer species and procedures for horizontal and vertical interpolation and conversions between chemical mechanisms.

Photolysis Rate Processor Many chemical reactions in the atmosphere are initiated by the photodissociation of numerous trace gases, including NO_2, O_3, and HCHO. Chapter 14 describes the photolysis rate processor (JPROC) that produces the photolysis rates used in the CMAQ chemical transport simulation. JPROC predicts photolysis rates for various altitudes, latitudes, and zenith angles. Currently, the radiative transfer algorithm assumes clear-sky conditions (i.e., no clouds present), and CCTM then attenuates for cloudiness.

As described above, each of the CMAQ interface processors incorporate raw data for CMAQ and perform functions such as calculating parameters and interpolating or converting data. The functions of the interface processors also include capabilities to handle raw data with various resolutions or measurement units. Raw input data is currently specified in the source code for JPROC, LUPROC, ICON, and BCON; however, the interface processors in future releases of CMAQ will be modified to handle a more generalized set of input data.

PROGRAM CONTROL PROCESSORS, A SET OF PROGRAMS EMBEDDED IN THE MODELS-3 FRAMEWORK, HANDLE SCIENCE INFORMATION OBJECTS SUCH AS GRID AND LAYER SPECIFICATIONS, CHEMICAL MECHANISMS, AND MODEL CONFIGURATIONS FOR REPEATED USE ACROSS SEVERAL PROCESS COMPONENTS OF CMAQ.

Program Control Processing (PCP) Chapter 15 explains how PCP is used within Models-3 to set up internal arrays, map species names, define global parameters, and establish linkages among processors in the Models-3 CMAQ system. Specifications needed for the CCTM simulation (e.g., grid and coordinate conditions and chemical species names) are entered into the Models-3 system once by the graphical user interfaces, and an object-oriented database accessible by all model components is established. PCP utilizes this information in the object database and automatically generates the required global FORTRAN include files. As a part of PCP, Models-3 CMAQ system employs a generalized chemistry mechanism processor (MP), also called the "mechanism reader." It greatly simplifies the task of implementing or altering gas-phase chemistry mechanisms and provides the capability of easily and safely using different mechanisms in the CMAQ system.

Integration of Science Codes into Models-3 One of the major objectives of the Models-3 project was to develop a flexible, comprehensive air quality modeling system with a modular coding structure that allows easy replacement of science process components. Chapter 18 describes the modularity concepts, code management method, and integration schemes of CMAQ science code with the Models-3 framework. The CMAQ FORTRAN code was integrated into the Models-3 framework with the following set of design, coding, and implementation standards: (1) modularity to allow easy exchange of science process solvers, (2) a standard subroutine interface at the module level, (3) restriction of coding practices, (4) the Models-3 I/O API (http://www.iceis.mcnc.org/EDSS/ioapi/index.html/), which contains standardized file I/O functions and a modeler-friendly interface built on top of self-describing netCDF (http://www.unidata.ucar.edu/packages/netcdf/) files that are portable across most Unix platforms.

MODELS-3 ALSO PROVIDES ANALYSIS ROUTINES FOR USE WITH CMAQ OUTPUT, WHICH CAN BE USED TO PROVIDE PROCESS ANALYSIS RESULTS AND STATISTICAL AGGREGATION TECHNIQUES.

Process Analysis Chapter 16 describes the implementation of process analysis techniques in the CMAQ modeling system. These techniques can be used in CMAQ to provide insights into how model predictions are obtained, which is particularly useful when modeling nonlinear systems like atmospheric photochemistry. Two techniques are available in the CMAQ system, integrated process rate (IPR) analysis and integrated reaction rate (IRR) analysis. IPR analysis can be used to determine the relative contributions of individual physical and chemical processes, and IRR analysis can help elucidate important chemical pathways and identify key chemical characteristics.

Aggregation Chapter 17 discusses a statistical procedure called aggregation that is applied to CMAQ's outputs in order to derive the seasonal and annual estimates required by assessment studies. Assessment studies require CMAQ-based distributional estimates of ozone, acidic deposition, and $PM_{2.5}$, as well as visibility, on seasonal and annual time frames. Unfortunately, it is not financially feasible to execute CMAQ over such extended time periods. Therefore, in practice CMAQ must be executed for a finite number of episodes or "events," which are selected to represent a variety of meteorological classes. The aggregation technique is used to incorporate these episode simulations into annual and seasonal estimates.

THE MODEL-3 CMAQ MODELING SYSTEM IS BEING FORMALLY EVALUATED TO ASSESS THE PERFORMANCE OF CMAQ'S NEW DEVELOPMENTS IN AIR QUALITY MODELING. THE EVALUATION WILL PROVIDE THE BASIS FOR UNDERSTANDING THE STRENGTHS OR WEAKNESSES OF THE CURRENT STATE-OF-SCIENCE IN CMAQ. With an evaluation of CMAQ simulations of 36, 12, and 4 km grid resolution, CMAQ's performance can be evaluated on both the regional and urban scales. This evaluation

will include an initial comparison of relative performance against the RADM model and diagnostic evaluation against databases from regional studies such as the 1995 Southern Oxidant Study conducted in the vicinity of Nashville, TN and the 1995 NARSTO-NE study.

CMAQ can be configured for a wide range of applications, from scientific studies to regulatory applications. While the scientific community can take advantage of CMAQ's ability to create alternative applications for research and development purposes, regulatory applications depend upon a standardized, evaluated form of CMAQ for regulatory applications. The CMAQ evaluation program will provide the scientific benchmark needed for this.

FUTURE EXTENSIONS OF CMAQ INCLUDE NEAR-TERM EFFORTS TO PROVIDE A NEW CHEMICAL MECHANISM AND EMISSION MODELING SYSTEM.

The SAPRC-97 gas phase mechanism will soon be incorporated into CMAQ, in addition to the current CB-IV and RADM2 mechanisms available. The SAPRC mechanism will be incorporated with a fixed subset of the approximately 100 organic species contained in the semi-explicit version of the SAPRC mechanism.

The Sparse Matrix Operator Kernel Emissions modeling system (SMOKE) (http://envpro.ncsc.org/products/) will also be incorporated into CMAQ in the near-term. The SMOKE model formulates emissions modeling in terms of sparse matrix operations which require considerably less time to perform than current systems.

WE ENCOURAGE THE FULL PARTICIPATION AND INVOLVEMENT OF THE SCIENTIFIC AND MODELING COMMUNITIES IN THE GROWTH AND USE OF MODELS-3 CMAQ. THERE ARE MANY IDEAS AND PLANS FOR FUTURE DEVELOPMENTS OF CMAQ, INCLUDING TOXIC POLLUTANT MODELING AND LINKAGES TO OTHER MODELS.

Modeling atmospheric toxic pollutants A key opportunity for CMAQ is developing the capability to model toxic pollutants. Models of airborne toxic pollutants are essential for human exposure and risk assessments. They can also be used to assess the exchange of toxic compounds between the atmosphere and sensitive ecosystems. With the ability to simulate toxic pollutant processes in addition to the current photochemical oxidants and particulates, it is planned to transport the CMAQ model to a finer than urban scale to link with human exposure models.

New linkages with global models It is hoped that information from the urban and regional CMAQ applications and from global modeling applications can be bridged. CMAQ output, produced using state of the science techniques, can be used to benchmark or examine the parametric basis of process formulations in global models. In addition, global model output can be used to improve or enhance the initial and boundary conditions for regional and urban scale CMAQ simulations.

Modeling ecosystems Efforts to combine environmental modeling techniques to encompass an entire ecosystem is needed to address issues including (a) nutrient cycling through the atmosphere, water bodies, and soil and (b) acidic wet and dry deposition into sensitive ecosystems, including critical load analyses. With this ecosystem modeling approach, air quality issues can be studied in combination with other aspects of environmental health.

This is the Executive Summary of *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System,* edited by D. W. Byun and J. K. S. Ching, 1999.