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Chapter 1

INTRODUCTION TO THE MODELS-3 FRAMEWORK AND THE COMMUNITY MULTISCALE AIR QUALITY MODEL (CMAQ)

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ABSTRACT

Models-3, a flexible software framework, and its Community Multiscale Air Quality (CMAQ) modeling system form a powerful third generation air quality modeling and assessment tool designed to support air quality modeling applications ranging from regulatory issues to science inquiries on atmospheric science processes. The CMAQ system can address tropospheric ozone, acid deposition, visibility, fine particulate and other air pollutant issues in the context of "one" atmosphere perspective where complex interactions between atmospheric pollutants and regional and urban scales are confronted. This CMAQ Science Document contains chapters that address specific scientific and technical issues involved in the development and application of Models-3/CMAQ system; collectively, it provides the scientific basis and point of reference for the state of the science captured in the June 1998 initial release of the CMAQ. This chapter provides an overview and context of each contributing chapter to the CMAQ system.

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1.0 INTRODUCTION TO THE MODELS-3 FRAMEWORK AND THE COMMUNITY MULTISCALE AIR QUALITY MODEL (CMAQ)

Air quality simulation models are important tools for regulatory, policy, and environmental research communities. In the United States, the Clean Air Act provides a societal mandate to assess and 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 to achieve these objectives. Optimal control strategies should be both environmentally protective and cost effective. Up to now, air quality model paradigms typically addressed individual pollutant issues separately. However, it is becoming increasingly evident that when pollutant issues are treated in isolation, the resulting control strategies may solve one set of problems but may lead to unexpected aggravation of other related pollutant issues. Pollutants in the atmosphere are subject to myriad transport processes and transformation pathways that control their composition and levels. Also, pollutant concentration fields are sensitive to the type and history of the atmospheric mixtures of different chemical compounds. Thus, modeled abatement strategies of pollutant precursors, such as volatile organic compounds (VOC) and NO_x, to reduce ozone levels may under a variety of conditions, cause an exacerbation of other air pollutants such as particulate matter or issues of acidic deposition.

The development of comprehensive air quality models started in the late seventies. The Urban Airshed Model (UAM) (Morris and Meyers, 1990) followed by the Regional Oxidant Model (ROM) (Lamb, 1983a, 1983b) 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 were addressed in the eighties with the development and evaluation of regional acid deposition models such as the Regional Acid Deposition Model (RADM) (Chang et al., 1987; Chang et al., 1990), the Acid Deposition and Oxidant Model (ADOM) (Venkatram et al., 1988), and the Sulfur Transport and Emissions Model (STEM) (Carmichael and Peters, 1984a, 1984b; Carmichael et al., 1991). Other major modeling systems included the Regional Lagrangian Modeling of Air Pollution model (RELMAP) (Eder et al., 1986), a Lagrangian framework system, and semi-empirical and statistical models. The genre of models of this period were designed to address specific air pollution issues such as ozone or acid deposition and to be applied under relatively prescriptive implementation guidance strategies. Thus, flexibility to deal with other issues, such as particulate matter or toxics, was very limited. Further, With the passage of the Clean Air Act Amendments of 1990 (CAAA-90), a wide range of additional issues were identified including visibility, fine and coarse particles, indirect exposure to toxic pollutants such as heavy metals, semi-volatile organic species, and nutrient deposition to water bodies. The direct response approach is to modify, adapt or extend current models to handle more complex implementations and issues but is both cumbersome and limiting.

Seeking a more strategic approach to handle the increased modeling requirements of the CAAA-90, more comprehensive modeling approaches appear to be needed. With projections for the increasing rapid pace of the development of computational capabilities at the start of the nineties, the opportunity arose for a strategic review of modeling approaches leading to design of a system that would both meet and keep pace with the increasing requirements on air quality modeling, of incorporating advances in state-of-science descriptions of atmospheric processes, as well as eliminate impediments of the current genre of models. The scope of such a system must be able to process great and diverse information from complicated emissions mixtures and complex distributions of sources, to modeling the complexities of atmospheric processes that transport and transform these mixtures in a dynamic environment that operates on a large range of time scales covering minutes to days and weeks. The corresponding spatial scales are commensurately large, ranging from local to continental scales. On these temporal and spatial scales, emissions from chemical manufacturing and other industrial activities, power generation, transportation, and waste treatment activities contribute to a variety of air pollution issues including visibility, ozone, particulate matter (PM), and acid, nutrient and toxic deposition. The residence times of pollutants in the atmosphere can extend to multiple days, therefore transport must be considered on at least a regional scale. NAAQS requirements and other goals for a cleaner environment vary over a range of time scales, from peak hourly to annual averages. These challenges suggest that more comprehensive approaches to air quality modeling are needed, and that assessments and pollution mitigation are achieved more successfully when the problems are viewed in a “one atmosphere” context that considers multiple pollutant issues. Further discussion of the needs for the third-generation air quality modeling system can be found in Dennis et al. (1996) and Dennis (1998).

To meet both the challenges posed by the CAAA-90 and the need to address the complex relationships between pollutants, the USEPA embarked upon the Models-3 project and developed the Community Multiscale Air Quality (CMAQ) system, an advanced air quality modeling system that addressed air quality from this “one atmosphere” multi-pollutant perspective. Based on its conceptual design, the high performance computational Models-3 framework serves to manage and orchestrate air quality simulations, using the CMAQ modeling system. The Models-3 framework is an advanced computational platform that provides a sophisticated and powerful modeling environment for science and regulatory communities. The framework provides tools used to develop and analyze emission control options, integrate related science components into a state-of-the-art quality modeling system, and apply graphical and analytical tools for facilitating model applications and evaluation. Descriptions of the Models-3 architecture are provided in **Chapter 2** and in Novak et al. (1998). CMAQ is a multi-pollutant, multiscale air quality model that contains state-of-science techniques for simulating all atmospheric and land processes that affect the transport, transformation, and deposition of atmospheric pollutants and/or their precursors on both regional and urban scales. It is designed as a science-based modeling tool for handling all the major pollutant issues (including photochemical oxidants, particulate matter, acidic, and nutrient deposition) holistically.

More than six years of investment and commitment from Federal staff and from scientists and model developers from the environmental and information communities were expended to develop the Models-3 framework and the CMAQ air quality modeling system. Models-3 CMAQ was released to the public in June 1998. The science and model engineering concepts and progress of the project have been described in two peer-reviewed AWMA Transaction papers (Byun et al., 1995a; Coats et al., 1995) and others (Byun et al., 1995b, 1996, and 1998a; Ching et al., 1995). This release version of the Model-3 software is supported by the following documents under the overall heading "Third Generation Air Quality Modeling System":

- System Installation and Operations Manual. EPA/600/R-98/069a, National Exposure Research Laboratory, EPA, Research Triangle Park, NC
- Users Manual. EPA/600/R-98/069b, National Exposure Research Laboratory, Research Triangle Park, NC
- Tutorial. EPA/600/R-98/069c, National Exposure Research Laboratory, EPA, Research Triangle Park, NC
- Science Concepts of the Third Generation Air Quality Models: Project Report. In preparation. Edited by D.W. Byun and A. Hanna. National Exposure Research Laboratory, EPA, Research Triangle Park, NC
- Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System, Edited by D.W. Byun and J.K.S. Ching. National Exposure Research Laboratory, EPA, Research Triangle Park, NC (this document)

The project report "Science Concepts of the Third Generation Air Quality Models" summarizes the basic atmospheric science concepts and mathematical principles pertinent to the development of the third generation air quality modeling. This document discusses the key scientific features and options incorporated into the Models-3 CMAQ modeling system.

1.1 The Models-3 Emissions, Meteorology, and the CMAQ Modeling Systems

The structure of the Models-3/CMAQ system is shown in Figure 1-1. Orchestrated through the Models-3 system framework, the Community Multiscale Air Quality (CMAQ) modeling system incorporates output fields from emissions and meteorological modeling systems and several other data source through special interface processors into the CMAQ Chemical Transport Model (CCTM). CCTM then performs chemical transport modeling for multiple pollutants on multiple scales. With this structure, CMAQ retains a flexibility to substitute other emissions processing systems and meteorological models. One of the main objectives of this project was to provide an air quality modeling system with a "one atmosphere" modeling capability based mainly on the "first principles" description of the atmospheric system. CMAQ 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, the modeling structure of CMAQ is designed to integrate and to test future formulations in an efficient manner, without requiring the development of a completely new modeling system. Contents of the CMAQ in the

June 1998 release version of Models-3 are summarized in Ching et al. (1998) and Byun et al. (1998b).

Currently, the Models-3 Emission Projection and Processing System (MEPPS) produces the emissions and the Fifth Generation Penn State University/ National Center for Atmospheric Research Mesoscale Model (MM5) provides the meteorological fields needed for the CCTM. They are considered to meet the present application needs for diverse air pollution problems in urban and regional scales. However, given the CMAQ paradigm, and other considerations, the emissions processing and meteorological modeling systems can be replaced with alternative processors.

Each of these three modeling systems are described briefly below, where associated chapters of this document are highlighted to provide directions to more in-depth discussions of these topics:

- The PSU/NCAR MM5 meteorological modeling system (Grell et al., 1994) generates the meteorological fields for CMAQ. MM5 is a complex, state-of-the-science community model, which is maintained by NCAR. MM5 is well-documented by its primary developers in technical notes and referenced journal articles. **Chapter 3** briefly describes the scientific aspects of MM5, including grid definitions, model physics, nesting and four-dimensional data assimilation.

- The MEPPS emission modeling system is based on the Geocoded Emission Modeling and Projection System (GEMAP) (Wilkinson et al., 1994) now known as the Emission Modeling System-95 (EMS-95). MEPPS processes emission inventory data, performs future projections (including control scenarios), and pre-processes data for use in the CMAQ model (**Chapter 4**). It provides speciated emissions consistent with CB-IV or RADM2 chemistry mechanisms.

- The CMAQ chemical transport modeling system (CCTM) is then used to perform model simulations for multiple pollutants and multiple scales with these input data (**Chapters 6, 7, 8, 9, 10 and 11**). The fundamental concepts used for the one-atmosphere dynamic modeling is described in **Chapter 5**. The techniques used for the management of CMAQ's source code are discussed in **Chapter 18**.

  The CMAQ modeling system also includes interface processors that process input data for the emission and meteorological modeling systems, and other processors that calculate photolysis rates, and develop initial and boundary conditions (**Chapters 4, 12, 13, and 14**). CMAQ also has an internal program control processor which is discussed in **Chapter 15**.

  Using the analysis routines provided in Models-3, the CMAQ output can be processed to provide process analysis information (**Chapter 16**) and/or analyzed further to provide aggregated statistical information (**Chapter 17**).

An important design requirements for CMAQ is that it addresses multiple scales and pollutants, which requires that governing equations and computational algorithms among the different systems should be consistent and compatible across the multiple scales. However, modeling assumptions used in various modeling systems may not be valid across all scales. For example, the atmospheric dynamics description in a meteorological model may have been optimized for application of certain scale or limited range of scales (e.g., global vs mesoscale vs complex terrain to urban). It is incumbent upon the user community to ensure the model component formulations are applicable to the range of scales upon which CMAQ is applied. The current version of MM5 and the CCTM is designed for regional to urban scales. Furthermore, when using nesting procedures to scale down from regional to urban scales and for avoiding feedback between the scales, one way nesting is recommended. In addition to the challenges of creating a multiscale air quality model, CMAQ's multi-pollutant capability cannot be achieved if the emissions modeling system does not provide appropriate precursor or pollutant emissions to the chemical transport model (CTM). The development of Models-3 and CMAQ overcome these hurdles by providing the flexibility to modify specific requirements (e.g., chemical mechanisms, model inputs, etc.), a generic coordinate system that ensures consistency across spatial scales, and user interfaces that can integrate alternative emissions or meteorological modeling systems.

1.2 CMAQ Interface Processors

The CMAQ modeling system includes interface processors to incorporate the outputs of the meteorology and emissions processors and to prepare the requisite input information for initial and boundary conditions and photolysis rates to the CCTM. Figure 1-1 illustrates the relationship and purpose of each of the CMAQ processors (and requisite interfaces) and their relation to the chemical transport modeling system. The arrows show the flow of data through the modeling system. Two additional functional features of the CMAQ system are included, one for process analysis, which is primarily for model diagnostic analyses, and a second one that is an aggregation methodology for estimating longer term averaged fields. Each of these processors is described briefly below, and the associated chapter numbers are also listed to note where detailed discussions can be found on the topics.

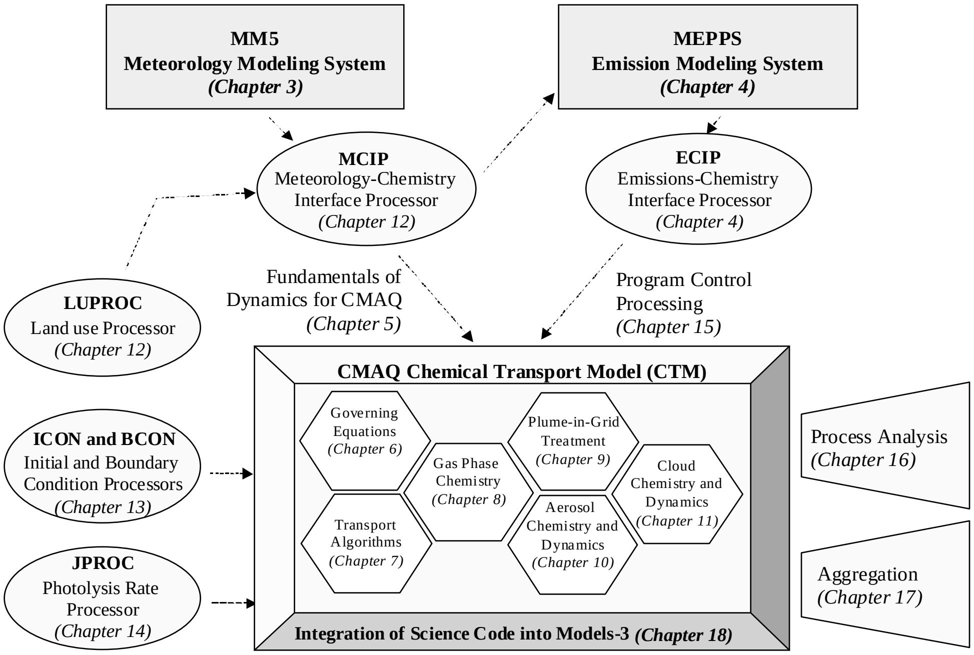

Figure 1-1. Emissions and Meteorological modeling systems and the CMAQ Chemical Transport Model and Interface Processor

- The Emission-Chemistry Interface Processor (ECIP) translates data from the MEPPS emission model for use in the CCTM. ECIP generates hourly three-dimensional emission data for CMAQ from the separate source type files produced by MEPPS, which include mobile, area, and point sources (**Chapter 4**). ECIP calculates the plume rise and initial vertical plume spread of point source emissions to determine the vertical level(s) of CCTM into which point source emissions should be introduced. Since meteorological conditions affect both point source plume rise and biogenic emissions, meteorological data from MCIP is also used in ECIP.

- The Meteorology-Chemistry Interface Processor (MCIP) translates and processes model outputs from the meteorology model for the CCTM (**Chapter 12**). MCIP interpolates the meteorological data if needed, converts between coordinate systems, computes cloud parameters, and computes surface and planetary boundary layer (PBL) parameters for the CCTM. MCIP uses landuse information from the landuse processor (LUPROC) to calculate the PBL and surface parameters.

- Initial Conditions and Boundary Conditions (ICON and BCON) provide concentration fields for individual chemical species for the beginning of a simulation and for the grids surrounding the modeling domain, respectively. The ICON and BCON processors (**Chapter 13**) use data provided from previous three-dimensional model simulations or from clean-troposphere vertical profiles. Both the vertical profiles and modeled concentration fields have a specific chemical mechanisms associated with them, which are a function of how these files were originally generated.

- The photolysis processor (JPROC) calculates temporally varying photolysis rates (**Chapter 14**). JPROC requires vertical ozone profiles, temperature profiles, a profile of the aerosol number density, and the earth's surface albedo to produce the photolysis rates for the CCTM. JPROC uses this information in radiative transfer models to calculate the actinic flux needed for calculating photolysis rates. JPROC generates a lookup table of photo-dissociation reaction rates.

Each of these CMAQ interface processors incorporates raw data into CMAQ and performs functions such as calculating parameters and interpolating or converting data. 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 raw input data, so that alternative data sets with varying resolutions or measurement units can be used.

1.3 The CMAQ Chemical Transport Model (CCTM)

The CCTM simulates the relevant and major atmospheric chemistry, transport and deposition processes involved throughout the modeling domains. The fundamental basis for CMAQ's one-atmosphere dynamics modeling is discussed in **Chapter 5**. Governing equations and model structure, including definitions of CMAQ's science process modules, are discussed in **Chapter 6**. 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. Through the Models-3 framework, CMAQ simulations can be developed using these different options without modifying source code. A general overview of these science process options is provided below along with a reference to the chapter(s) of this document where more scientific detail can be found.

- Advection and Diffusion (**Chapter 7**): Several advection methods are implemented in the CMAQ; these include a scheme by Bott (1989), a piecewise parabolic method (PPM) (Collela and Woodward, 1984), and the Yamartino-Blackman cubic algorithm. Options for computing subgrid vertical transport include eddy diffusion, and the Asymmetric Convective Model (ACM) (Pleim and Chang, 1992) applicable to convective conditions. Horizontal diffusion is modeled using a constant eddy diffusion coefficient. Numerical methods differ in the handling of advection of concentration fields.

- Gas Phase Chemistry (**Chapter 8**): CMAQ includes both the RADM2 and CB4 gas-phase chemical mechanisms. The CMAQ version of CB4 includes the most recent representation of isoprene chemistry and two additional variants of the RADM2 mechanism also contain the newer isoprene chemistry at two levels of detail. In addition, CMAQ provides the capability to edit these mechanisms or to import a completely new mechanism by means of a generalized chemical mechanism processor. CMAQ also accounts for the formation of secondary aerosols and the reactions of pollutants in the aqueous phase, and aqueous reactions are simulated by means of the aqueous chemical mechanism incorporated in RADM. All CMAQ gas-phase mechanisms are linked to these processes to provide the capability to simulate multi-phase interactions.

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.

- Plume-in-Grid (PinG) Modeling (**Chapter 9**): CMAQ includes algorithms to treat subgrid scale physical and chemical processes impacting pollutant species in plumes released from selected Major Elevated Point Source Emitters (MEPSEs). The PinG modules simulate plume rise and growth, and the relevant dynamic and chemical reaction processes of subgrid plumes. PinG can be used for the simulations at 36 km and 12 km resolutions, PinG is not invoked at 4 km resolutions and the MEPSE emissions are directly released into the CTM 3-D grid cells.

- Particle Modeling and Visibility (**Chapter 10**): One of the major advancements in CMAQ is the modeling of fine and coarse mode particles, with the use of the fine particle model described in Binkowski and Shankar (1995). CMAQ predicts hourly gridded concentrations of fine particle mass whose size is equal to or less that 2.5 microns in diameter ($PM_{2.5}$), speciated to sulfate, nitrate, ammonium, organics and aerosol water. Secondary sulfate is produced when hydroxyl radicals react with sulfur dioxide to produce sulfuric acid that either condenses to existing particles or nucleates to form new particles. CMAQ model output includes number densities for both fine and coarse modes. The modeling of aerosols in CMAQ also provides the capability to handle visibility, which is another CMAQ output. 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.

- Cloud processes (**Chapter 11 and 12**): Proper descriptions of 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 they indirectly affect concentrations by altering radiative transmittances which affect photolysis rates and biogenic fluxes. CMAQ models deep convective clouds (Walcek and Taylor, 1986) and shallow clouds using the algorithms as implemented in RADM (Dennis et al., 1993) for 36 and 12 km resolutions. At 4 km resolution, the clouds are generally resolved, and explicit type cloud dominates.

- Photolysis Rates (**Chapter 14**): The photochemistry of air pollutants is initiated by photodissociation of smog precursors, which are driven by solar radiation. The amount of solar radiation is dependent on sun angle (time of day), season, latitude, and land surface characteristics, and is greatly affected by atmospheric scatterers and absorbers. Photolytic rates are also wavelength- and temperature-dependent. Within CCTM, temporally resolved 3-D gridded photolysis rates are interpolated from a lookup table generated by JPROC processor and corrected for cloud coverage.

1.4 Analysis of CMAQ Output

Air quality modeling simulations arise from modeling of complex atmospheric processes. It is important to assure and to understand the model results. Sensitivity tests are needed to detect problems in model formulations and to determine if the model is credible for assessing emission control strategies. A very powerful sensitivity analysis tool called process analysis is provided with CMAQ. Also, an aggregation technique is provided with CMAQ. Aggregation can be used to estimate seasonal or annual concentrations for pollutants from CMAQ simulations which are usually performed for shorter time periods due to time and computational limitations.

1.4.1 Process Analysis (Chapter 16)

Sensitivity analyses are needed to detect errors and uncertainties introduced into a model by the parameterization schemes and the input data. Results must also be analyzed to ensure that realistic values are obtained for the right reasons rather than through compensating errors among the science processes. Process Analysis techniques quantify the contributions of individual physical and chemical atmospheric processes to the overall change in a pollutant's concentration, revealing the relative importance of each process. Process analysis is particularly useful for understanding the effects from model or input changes. CMAQ 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 the change in concentration of each species caused by physical processes (e.g., advection, diffusion, emissions), chemical reaction, aerosol production, and aqueous chemistry. Values provide only the *net* effect of each process. IPRs are particularly useful for identifying unexpectedly low or high process contributions which could be indicative of model errors.

- The IRR analysis involves the details of the chemical transformations. For gas-phase chemistry, the CCTM has been designed to compute not only the concentration of each species, but also the integral of the individual chemical reaction rates. IRR analyses have typically been used to understand the reasons for differences in model predictions obtained with different chemical mechanisms.

1.4.2 Aggregation (Chapter 17)

In support of studies mandated by the CAAA-90, CMAQ can be used to estimate deposition and air pollutant concentrations associated with specific levels of emissions. Assessment studies require estimates of ozone, acidic deposition, particulate matter as well as visibility, on seasonal and annual time frames. A statistical procedure called the “aggregation” has been developed and is provided for the CMAQ to derive the required seasonal and annual estimates. This methodology is an efficient technique and can be used instead of executing multiple CMAQ model runs for the intended period of averaging.

A typical CMAQ simulation provides hourly air quality fields for regional to urban scales for multi-day episodes, typically up to five days in duration. The new $PM_{2.5}$ standard includes an annual average value, so utilization of CMAQ for $PM_{2.5}$ will require the use aggregation techniques in order to estimate annual average $PM_{2.5}$ values. One such technique, initially developed for RADM wet deposition applications, was recently modified and successfully applied to $PM_{2.5}$ by Eder and LeDuc (1996). The approach utilizes visibility data as a surrogate for $PM_{2.5}$, and it 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 $PM_{2.5}$ samplers is deployed; also, aggregation approaches for mesoscale domains will need to be developed perhaps utilizing the method by Eder and LeDuc (1994).

1.5 Management of CMAQ Science Information Objects and Codes in Models-3

The CMAQ source code is managed through the Models-3 framework to make the CMAQ modeling system more efficient and easier to use by applying a program control processor, management and integration of source code, and implementing a modularity concept. These techniques also help users customize CMAQ for their own modeling applications without source code modifications.

1.5.1 Program Control Processors (Chapter 15)

Certain science information, such as grid and layer definitions and dimensions, chemical mechanisms, species list, model configurations, and episode (case) specification, is used repeatedly across the several process components in Models-3 CMAQ modeling system. Program control processors are a set of programs embedded in the Models-3 framework to handle these science information components and their codes. Program Control Processing (PCP) refers to setting up internal arrays, mappings of species names in the input processors, defining global parameters, and establishing linkages among processors in the CMAQ system. PCP allows users to define globally shared information on model components, and it uses that information to generate the global FORTRAN include files required for building a model in CMAQ.

1.5.2 CMAQ Code Integration (Chapter 18)

CMAQ's modularity facilitates efficient coordination of development work and management of the science codes. Chapter 18 describes the modularity concepts, code management method, and integration schemes of CMAQ science code with the Models-3 framework. Integrating the CMAQ code into the Models-3 framework is achieved by following a set of design, coding, and implementation standards that include:

- A standard subroutine interface at the module level
- The restriction of coding practices to avoid practices that can conceal data dependencies, hinder maintenance and foster hidden bugs
- The Models-3 Input/Output Applications Programming Interface (I/O API) (http://www.iceis.mcnc.org/EDSS/ioapi/index.html/), which contains standardized file I/O functions. The I/O API is an interface built on top of self-describing netCDF (http://www.unidata.ucar.edu/packages/netcdf/) files that are portable across most Unix platforms.

1.6 Post Release Studies and Near-Future Plans

1.6.1 CMAQ Evaluation Study

It is important to conduct extensive evaluation of the CMAQ. Subsequent to the initial release of the Models-3/CMAQ, the development team is engaged in a substantial program of evaluation. The scope of the effort includes analyses of the performance and veracity of each individual process module as well as the integrated air quality system. Findings from this evaluation can be incorporated into future releases of the CMAQ modeling system. The degree and rigor of this evaluation provides the basis for understanding the strengths or weaknesses of the current state-of-science in CMAQ. The evaluation of the initial release version of CMAQ is underway for three nested grids with 36, 12, and 4 km grid resolutions. With these results, CMAQ's performance can be evaluated on both the regional and urban scales. This model evaluation activity for CMAQ will be staged with the initial efforts to show relative performance against the RADM model, which has undergone extensive model evaluation efforts. Diagnostic evaluation will continue using databases from different regional studies such as the 1995 Southern Oxidant Study conducted in the vicinity of Nashville, TN and the 1995 NARSTO-NE study.

1.6.2 Testing Operational Configurations

CMAQ can be configured for a wide range of applications from science studies and investigations to regulatory applications. While the scientific community can take advantage of the CMAQ open system and flexibility to create alternative applications of CMAQ for research and development purposes, regulatory applications depend upon a standardized, evaluated form of CMAQ. The CMAQ evaluation program will provide the scientific benchmark needed for this. As science advances in CMAQ, future configurations of a more operational nature can also be periodically re-benched as appropriate. As understanding of atmospheric processes improves, it is a natural tendency for models to become more complex and have increased computational demands. Efforts are underway to improve model computational efficiencies to compensate for this.

1.6.3 Extensions and Science Additions

Two major extensions are planned for the CMAQ modeling

- A version of the SAPRC-97 gas phase mechanism will be incorporated into CMAQ, in addition to the current CB-IV and RADM2 mechanisms available. The initial configuration of SAPRC will be in a fixed parameter mode, with a preset number of organic species. Another possible future implementation of SAPRC will allow the user to select from about 100 organic surrogate species in the semi-explicit SAPRC mechanism to construct a user-defined, smaller SAPRC mechanism. Another approach for representing gas-phase chemistry in CMAQ is also being developed. It will use a limited number reactive entities termed “morphecules” to include in the chemical reactions while using a much larger number of chemical species (singly or lumped) called allomorphs to provide extra chemical detail. This latter approach provides a means for including a much more detailed representation of atmospheric chemistry than conventional chemical mechanisms without significantly increasing computational burden, albeit at the expense of additional computer memory.

- A new emissions processor will be implemented which is called the Sparse Matrix Operator Kernel Emissions modeling system (SMOKE) (http://envpro.ncsc.org/products/). The linear operations used in emission processing can be represented as multiplications by matrices. Since most entries in these matrices are zeros, the SMOKE model formulates emissions modeling in terms of sparse matrix operations that require considerably less time to perform than current systems. Efficiency is enhanced even further when considering variations in emissions projections from base case scenarios by temporally modeling once per episode, calculating gridding matrices only once per grid, and calculating speciation matrices only once per chemical mechanism.

Development and testing of several science options is underway for incorporation into future releases of the CMAQ. These include an advanced surface-PBL linked system (Pleim and Xiu, 1995), optional meteorological processors such as the Regional Atmospheric Modeling System, RAMS, and an advanced 4-D Photolysis Rates Processor.

1.7 Opportunities and Encouragement for Long Term Extensions and Science Community Involvement

The Models-3/CMAQ concept is based on an open system design, we encourage the full participation and involvement of the scientific and modeling communities in the growth and use of Models-3 CMAQ. As described in this document, the Models-3 CMAQ system has flexibility for incorporating scientific and modeling advances into CMAQ processors, for testing of alternative modeling techniques for science processes, and for extending its current capability to handle multimedia environmental issues. Additionally, the community of users should be vigilant in performing evaluations against improved databases and measurement technology to assess the realism of model performance and to measure the strengths and weaknesses of the current state of the-science as presented in the CMAQ modeling system. Some suggestions for extensions and community involvement are provided below, but certainly not limited to:

(1) <u>Modeling airborne and deposition of atmospheric toxic pollutants:</u> A key opportunity for CMAQ is the development of a modeling capability for toxic pollutants into the CMAQ chemical transport modeling system. Models of airborne toxic pollutant provide an important tool for understanding the transport and chemical pathways that are concerns to human exposure assessments and for risk assessments and its management. It also provides a powerful means to assess the exchange of toxic compounds between the atmosphere and sensitive ecosystems. However, developing such models is challenging. Air toxics arise from a wide variety of sources, which may have a wide range of chemical lifetimes and reactivity. Consequently, their toxicological impacts as well as their time-space distributions may be highly variable. These complex mixtures of reactive compounds can exhibit wide range and variability in physical properties and exist at various gas, liquid or particulate ambient metastates. Modeling paradigms might evolve from introducing gas-particulate partitioning of the semi-volatile species (Ching et al., 1997) to more fundamental modeling with detailed chemical mechanisms.

(2) <u>Development of modeling capability to link with human exposure models:</u> 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. International efforts to determine and understand the etiology of adverse human effects of air pollutants, especially those that or associated with fine particles is underway. Modeled concentrations of air pollutant constituents at neighborhood scales when coupled with the limited numbers of sampling provide a powerful basis for driving human exposure models. With this necessary data, human exposure models provide a basis for the causality studies and for risk assessment research. Models have not yet been developed to predict the spatial and temporal distributions of the various causal pollutant classes under current consideration at the neighborhood scale. The downscaling requirements represent a great challenge to the scientific basis in current meteorological processors.

(3) <u>Advanced data assimilation capability:</u> As air quality modeling efforts extend to finer horizontal resolutions and time scales, it becomes increasingly important to make use of higher frequency asynoptic meteorological data such as satellite, radar wind profilers and NEXRAD. There is a need to develop and extend data assimilation techniques to these meteorological data sources. Improved methods for introducing cloud information into the CMAQ should also be investigated. Such fields have significant impact on chemical photolysis rates, the atmospheric and surface energy budgets, the stability and dispersive power of the boundary layer, and aqueous chemistry.

(4) Development of an air quality predictive mode: With further development of the emissions and meteorological modeling systems, plans include developing a predictive capability in the CMAQ modeling system. CMAQ is currently developed in retrospective mode for performing assessments and for implementation of the National Ambient Air Quality Standards (NAAQS). In principle, CMAQ may be extended to a forecast mode in order to provide air quality advisories for pollutants such as ozone and visibility and for operational support for issues such as smoke and PM/haze from prescribed fires. These capabilities will require the development and testing of day-specific emissions inventories and a real time data processing system for the meteorological mode.

(5) Up and downscale links to global scale models: New linkages with other areas of modeling, including scale and media, are envisioned. It is hoped that information from the urban and regional CMAQ applications and from global modeling applications can be bridged. Because CMAQ offers the state of science to simulate atmospheric process as realistically as possible at time scales commensurate with reality, CMAQ output can be used to benchmark or examine the parametric basis of process formulations in global models. From a downscale perspective, global model output can be used to improve or enhance the initial and boundary conditions in CMAQ regional and urban scale simulations.

(6) Ecosystem modeling: Efforts to combine environmental modeling techniques to encompass an entire ecosystem is needed to address issues including: (a) nutrient cycle modeling, which includes pathways 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. For example, nitrogen deposition can cause adverse nutrient loadings to ecosystems that can result in a reduction of water quality due to adverse biological responses. Further, toxic deposition can lead to adverse indirect human exposure from bioaccumulation through the food chain.

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