Operational Guidance for the Community Multiscale Air Quality (CMAQ) Modeling System

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Disclaimer

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Foreword

The Community Multiscale Air Quality (CMAQ) modeling system is being developed and maintained under the leadership of the EPA National Exposure Research Laboratory in Research Triangle Park, NC. CMAQ represents over two decades of research in atmospheric modeling and has been in active development since the early 1990's. The first release of CMAQ was made available in 1998 without charge for use by air quality scientists, policy makers, and stakeholder groups to address multiscale, multipollutant air quality concerns. All subsequent CMAQ releases, past, current, and future, will adhere to this same level of code accessibility and scope.

Introduction

Under the authority of the Clean Air Act, the U.S. Environmental Protection Agency (EPA) has established National Ambient Air Quality Standards (NAAQS) (U.S. EPA, 2008). These standards are designed to protect human health and the environment from high levels of criteria pollutants, such as ozone and particulate matter. Meeting the NAAQS often requires the use of controls on sources of air pollutants. The complex nature of air pollution scenarios requires control strategies to be effective for a variety of air pollutants, geographic regions, and scales. As part of the effort to decrease ambient concentrations of criteria pollutants, the EPA has approved air quality simulation models for use at regional, state, and local scales within the United States. The models have been applied to estimate the ability of various control strategies to improve air quality and ensure cost-effective results.

So-called first-generation air quality models simulated air quality using simple chemistry at local scales, and Gaussian plume formulation was the basis for prediction. Second-generation models covered a broader

range of scales (local, urban, regional) and pollutants, addressing each scale with a separate model that often focused on a single pollutant or issue (e.g., ozone, acid deposition). It became apparent, however, that single-pollutant models were not sufficient. Depending on the release characteristics, the pollutants in question, and the surrounding meteorological conditions at the time of pollutant release, modeling scenarios can range from a localized, short-term phenomenon to a longterm regional event. Because some emission sources contribute to the ambient levels of more than one pollutant and can affect an entire region on various time scales, an integrated modeling approach capable of handling multiple air pollutants and spatiotemporal scales was needed to isolate control strategies that improve overall air quality in a costeffective manner. New air quality issues identified by the Clean Air Act Amendments of 1990 (such as visibility, fine and coarse particles, and indirect exposure to toxic pollutants) made an integrated modeling approach that could address multiple pollutants even more essential. Third-generation models were needed that could treat multiple pollutants simultaneously and at scales up to continental or larger. Future efforts toward fourth-generation systems will extend linkages and process feedback to include air, water, land, and biota to provide a more holistic approach to simulating transport and fate of chemicals and nutrients throughout an ecosystem

The EPA Community Multiscale Air Quality (CMAQ) modeling system is a third-generation air quality model. It is available online at CMAQ Model Website. CMAQ is designed for applications ranging from regulatory and policy analysis to understanding the complex interactions of atmospheric chemistry and physics. It is a three-dimensional Eulerian (i.e., gridded) atmospheric chemistry and transport modeling system that simulates ozone, particulate matter (PM), toxic airborne pollutants, visibility, and acidic and nutrient pollutant species throughout the troposphere.

Designed as a "one-atmosphere" model, CMAQ can address the complex couplings among several air quality issues simultaneously across spatial scales ranging from local to hemispheric. The CMAQ source code is transparent and modular to facilitate the model's extensibility through community development by all members of the air quality modeling community.

Model Background and Goals

Air quality models integrate our understandings of the complex processes that affect the concentrations of pollutants in the atmosphere. Establishing the relationships among meteorology, chemical transformations, emissions of chemical species, and removal processes in the context of atmospheric pollutants is the fundamental goal of an air quality model (Seinfeld and Pandis, 1998). In contrast to statistical air quality models that use historical trends in observed atmospheric conditions to predict air pollution, CMAQ uses coupled mathematical representations of actual chemical and physical processes to simulate air quality. The model is based upon the underlying concept of preserving mass through a series of contiguous three-dimensional (3-D) grid cells covering a fixed model grid. A model grid is an x-y-z array that is fixed in space and covers a particular domain, i.e., a geographic area of interest. CMAQ therefore belongs to the Eulerian class of mathematical models that calculate a mass balance within each grid cell by solving the transport across each cell boundary and chemical transformations within each cell during a given time period. As a framework for simulating the interactions of multiple complex atmospheric processes, CMAQ thus requires two primary types of inputs: meteorological information, and emission rates from sources of emissions that affect air quality.

With weather conditions contributing the primary physical driving forces

in the atmosphere (such as the changes in temperature, winds, cloud formation, and precipitation rates), representative gridded meteorology forms the basis of all 3-D air quality model simulations. The Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Model (MM5) (Grell et al., 1994) and the Weather Research and Forecasting (WRF) model – Advanced Research WRF (WRF-ARW) (Skamarock et al., 2005) are two meteorological models that are compatible with CMAQ. The meteorology inputs dictate the following CMAQ configuration parameters:

- Horizontal grid coordinate system (e.g., latitude-longitude) and map projection (e.g., Lambert Conformal Conic)
- Horizontal grid resolution (i.e., the size of the cells composing the grid)
- Maximum spatial coverage (horizontal geographic extent, i.e., the domain) of the grid
- Maximum vertical grid extent (model top)
- Temporal extent (the starting and ending dates and times and the meteorology update frequency)

To obtain inputs on emissions, CMAQ relies on an emissions model to estimate the magnitude, location, and temporal variability of pollution sources. Open-source models such as the Sparse Matrix Operator Kernel Emissions (SMOKE) model (IE, 2008) SMOKE Website are available for computing emissions inputs to CMAQ from emissions inventories. These emissions inputs must be on the same horizontal and vertical spatial scales and cover the same time period as are used in the air quality model simulation. The emissions inputs to CMAQ must also represent volatile organic compound (VOC) emissions using a chemical parameterization supported by CMAQ; currently supported photochemical mechanisms are recent versions of the Carbon Bond mechanism, the Statewide Air Pollution Research Center (SAPRC)

mechanism, and the Regional Atmospheric Chemistry Mechanism (RACM). Additional details about the gas-phase chemistry in CMAQ are provided in the OGD section on CMAQ Chemistry and Transport Modules and in Byun and Ching (1999), Byun and Schere (2006). Those two sources also describe the primary aerosol emissions species that are supported by CMAQ ("aerosol" refers to particulate matter [tiny solid or liquid particles] suspended in the atmosphere.).

Note: CMAQ Output File Format

CMAQ uses a modified version of the netCDF file format. Although

CMAQ output is described as being in the netCDF format, it is

actually a hybrid format of the I/O API and the netCDF.

CMAQ was designed from the start as a community model. "Community modeling" is the concept that air quality model development should be a collective effort by a broad community of developers. By adopting a standardized modeling architecture, the air quality modeling community can focus its efforts on creating software enhancements and new science modules. CMAQ's modular structure facilitates customization and open-source development by the community. Using the Input/Output Applications Programming Interface (I/O API) library to control the internal and external data flows to the model, and the network Common Data Form (netCDF) library to control the input and output file formats, CMAQ is based around a transparent and platformindependent code infrastructure that promotes extensibility. The modularity of CMAQ also leads to multiple science configuration options (i.e., how various processes are represented) that model users can choose from when setting up new simulations. The trade-off for this flexibility is complexity in the model configuration; the model user is faced with hundreds of different configuration combinations when designing new simulations. To avoid confusing new CMAQ users, this document provides guidance on a basic configuration to use for getting

started with the model. For experienced air quality model users, the multiple configuration combinations available provide a high level of flexibility for optimizing model performance for different air quality model applications.

CMAQ is designed to meet the needs of the multiple groups contained within the air quality modeling community: research and regulatory modelers, algorithm and science module developers, air quality forecasters, and planners and policy makers. While each of these groups has distinct individual requirements for CMAQ, they also share a common need for an efficient, transparent, and scientifically credible tool to simulate air pollution formation and transport. To address these individual and common needs, CMAQ development and maintenance have the following goals:

- 1. Scientific Integrity. Ensure that the model remains state-of-thescience through subjecting it to regular peer reviews
- Community Development. Utilize a design that encourages innovations and enhancements by all members of the air quality modeling community
- 3. *Multiscale Modeling*. Provide adequate technical formulations to address air quality issues on multiple spatial scales, from urban to hemispheric
- 4. One-Atmosphere Design. Provide robust and integrated science for modeling multiple, coupled air quality issues in a single simulation
- Modularity. Maintain flexibility to add new, or select from existing, science modules to optimize model performance for specific applications
- 6. *Transparency*. Utilize programming practices that promote understanding of the model formulation at the source-code level
- 7. Computational Efficiency. Provide scientifically acceptable results without compromising the speed at which the results are generated

8. *Open-Source Design*. Enable no-cost distribution and application by the modeling community

CMAQ OGD List Tables and Figures

CMAQ OGD Acronyms

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