NEW FEATURES OF THE 2005 RELEASE

1. Overview

The Community Multiscale Air Quality (CMAQ) model has been updated to version 4.5 for the 2005 release. The CMAQv4.5 model has been improved in its scientific representation of several important processes including, convective clouds, aerosol dry deposition, aerosol thermodynamics, and mass conservation, and its capabilities have been expanded to include many hazardous air pollutants (HAPs), chlorine chemistry, and sea salt aerosols. The new release also includes two new diagnostic tools: sulfur tracking and carbon source apportionment. This document provides a brief description of the updates and new features. For more details on code modifications and execution guidance, refer to README files that accompany the model release.

2. Physical processes

2.1 Mass Conservation

A new mass continuity scheme, similar to that used in the air quality forecasting version of CMAQ, has been implemented for the 2005 release. This scheme is globally mass-conserving and uses the piecewise parabolic method (PPM) (Colella and Woodward, 1984) advection scheme for horizontal advection, deriving a vertical velocity component at each grid cell that satisfies the mass continuity equation using the driving meteorology model's air density. The mixing ratio correction step, used in previous CMAQ versions, is not needed with this method. Note that, the former advection scheme, with the same horizontal advection but also using PPM for the vertical velocity component, is still available, along with the mixing ratio correction step.

2.2 Convective Cloud model

The CMAQ convective cloud model (RADM-cloud) has deficiencies that result in excessive transport from upper model layers down to the below-cloud layers, and artificial restrictions on cloud fraction due to its 1 hour time step. New modifications to the subgrid vertical mixing scheme correct these problems. Many basic features of the CMAQ cloud model, such as diagnosis of cloud base and top, cloud fraction estimation from precipitation rate, and the entrainment closure assumptions, have not been changed (see Chang et al., 1987, for details). The analytical mixing scheme has been replaced with a new mixing scheme based on the Asymmetrical Convective Model (ACM) that was originally developed for PBL mixing (Pleim and Chang 1992). The ACM simulates a detraining convective plume by non-local transport from the source layer directly to each model layer within the convective layer. An important difference from the RADM-cloud scheme is that the downward mixing in ACM is by gradual layer-by-layer compensatory subsidence. While the PBL version of the ACM has a vertically invariant upward non-local mixing rate, in the cloud application the mixing rate varies with height according to the ratio of liquid water content to the adiabatic liquid water content.

The RADM-cloud scheme restricts cloud coverage whenever the modeled mass flux over the 1 hour time step exceeds the available below cloud mass. This artificial restriction of cloud coverage is eliminated in ACM-cloud by setting a mixing time step according to mass flux constraints and iterating up to the lifetime of the cloud (1 hour).

2.3 Aerosol Dry deposition

There are three updates to the aerosol dry deposition algorithm. 1. The impaction term has been replaced with a new form. 2. The impaction process has been restored to the coarse mode. 3. The equation for combining turbulent deposition fluxes and gravitational settling has been replaced.

The original impaction term is a function of Stokes number following Slinn (1982) for smooth surfaces. Many, including Slinn, have observed that this form of the impaction term changes too abruptly as aerosol size decreases resulting in dry deposition velocities in the accumulation mode that are too small. The new model is based on a form of the impaction term suggested by Giorgi (1986). After simplification this form could be integrated over the log-normal size distribution of each mode. Using this new modally integrated impaction term, deposition velocities are greater in the accumulation mode.

The aerosol dry deposition velocity equation has been updated to the form suggested by Venkatram and Pleim (1999). This change results in small differences in aerosol dry deposition velocity.

2.4 Minimum eddy diffusivity

The minimum value for eddy diffusivity has an important impact on nighttime concentrations. Traditionally this parameter has been set to a high value ($K_{zmin} = 1.0$ m^2/s). Meteorology models generally use lower values, typically raging from $0.1 – 0.5$ m^2/s. Minimum K_z values in this range often result in unrealistically high concentrations of primary species in areas of high emissions. On the other hand, the higher minimum K_z value produces overpredictions of ozone at night in the more rural areas due to reduced titration. The new version specifies the minimum K_z according to the fractional area of urban land use:

$$K_{zmin} = 0.5\ (1\text{-}F_{urban}) + 2.0\ F_{urban}$$

where F_{urban} is the fraction of urban area in the grid cell (0.0 - 1.0). The higher value of K_{zmin} in urban areas is meant to reflect less nocturnal stability resulting from urban heat island effects.

2.5 Dynamic vertical layers -

Like the previously released implementation of dynamic horizontal domain specification, where the horizontal extents (columns and rows) and horizontal grid-spacing are set at run time by reference to the GRID_NAME variable in a GRIDDESC

file, this release features an implementation of dynamic vertical layers specification. The run script now contains a LAYER_FILE variable that points to a 3-D input file (typically the MET_CRO_3D file), which allows the user to set the layer definition at run time according to that file's I/O-API header.

3. Aerosols

3.1 Sea Salt

The new aerosol module is called AERO4. The difference between AERO4 and AERO3 is that AERO4 includes consideration of sea salt aerosols. Emissions of sea salt from the open ocean are calculated as a function of wind speed and relative humidity, following the parameterizations of Gong (2003) and Zhang et al. (2005), respectively. These emissions are speciated into sodium, chloride, and sulfate, and are distributed by size to the accumulation and coarse modes by fitting the emission parameterization to a bimodal distribution. Note that sea-salt emissions are calculated within the CMAQ model and do not require special pre-processing in SMOKE. Equilibrium between the accumulation mode (which now contains sodium and chloride) and the gas phase (which now contains hydrochloric acid) is calculated within the ISORROPIA thermodynamic module. As in previous CMAQ releases, mass transfer is not simulated between the coarse mode and the gas phase. These sea-salt processes can be activated by selecting the AERO4 module and deactivated by using AERO3.

3.2 PM2.5 Size Cut.

A new subroutine has been added to the aerosol module to calculate the volume fraction of each mode that is composed of particles smaller than 2.5um aerodynamic diameter, following the methodology of Jiang et al. (2005). These new variables (PM25AT, PM25AC, and PM25CO) have been added to the aerosol diagnostic file and facilitate a more rigorous calculation of PM2.5 that is more comparable to measurements than the summation of Aitken and accumulation modes.

3.3 Modifications to the ISORROPIA thermodynamic Module

The ISORROPIA code has been updated in CMAQv4.5 to Version 1.5 (Oct. 2003), with a few modifications as noted in the in-line code documentation. The most significant difference is the inclusion of updated Zdanovskii-Stokes-Robinson (ZSR) correlation parameters, which are used to determine the aerosol liquid water content. Use of these updated parameters smoothes out the discontinuities in CMAQv4.4 reported by Bhave et al. (2004a), although other numerical instabilities still exist in the ISORROPIA module. In addition, a bug has been corrected in which the index to the Kusik-Meissner binary activity coefficient lookup tables (ipos) was computed incorrectly for high ionic strengths.

3.4 Aerosol module bug fixes.

The aerosol emission processor has been modified to correctly convert the H_2SO_4 emissions into particulate sulfate. A bug in the mode-merging section of the subroutine AEROPROC was fixed, eliminating the most extreme cases of "mode crossover" (instances where the Aitken mode diameter grew larger than the accumulation mode). The sulfate concentration used as input to ISORROPIA was modified to include the pre-existing sulfate plus the sulfate produced by gas-phase oxidation in the previous time step. As a result, the inorganic aerosol components printed to the CONC file are in thermodynamic equilibrium with the gas phase at the end of each time step. An inconsistency in the minimum standard deviation parameter between the AERODEPV subroutine and the AERO_INFO module was resolved.

4. Chemical processes

4.1 Toxics

Four mechanisms for gas chemistry have been added to simulate the atmospheric fate and transport for a subset of Hazardous Air Pollutants (HAPs). They are modifications of either the CB-IV (Gery et. al. 1989, and Gipson and Young 1999) or the SAPRC-99 (Carter 2000a) mechanisms. The new mechanisms have the base names, CB4TX1P and SAPRC99TX2P. Mechanisms with the same base name differ by including aerosols or not including aerosols. All new mechanisms include aqueous chemistry. These four mechanisms have twenty-four or twenty-five new species, depending on the base mechanism.

A maximum of seven new species add reactions to the original mechanisms shown in the mechanism definition file. For CB4TX1P mechanisms, two species separate original species representing formaldehyde-like and acetaldehyde-like compounds into explicit and surrogate representations. Surrogates lump Volatile Organic Compounds that are heavier aldehydes or have aldehyde-like properties. Thus, formaldehyde and acetaldehyde are now explicit species. For the SAPRC99TX2P mechanisms, this change was made only for acetaldehyde because the original SAPRC-99 explicitly represents formaldehyde. Two other species represent 1,3-butadiene and acrolein. They add reactions for the loss of 1,3-butadiene and the loss and production of acrolein. These reactions were based on Liu et. al (1999) and Grosjean et. al (1994) for CB4TX1P and based on Carter (2000b) for SAPRCTX2P. Three of the seven species are reactive tracers for formaldehyde, acetaldehyde, and acrolein emissions.

The remaining new species do not add reactions and cannot affect radical, ozone and aerosol concentrations but do undergo losses from atmospheric chemistry. Their losses are exponential based on photochemical rate constants and concentrations determined after integrating over time the reactions shown in the mechanism definition file.

Solvers for the new mechanisms include all that are current available in CMAQ (SMV Gear, Rosenbrock and EBI). Note that separate EBI solvers exist for the CB4TX1P and SAPRC99TX2P mechanisms.

In addition to their photochemistry, new species undergo transport and deposition. All undergo wet deposition based on the precipitation rate and their Henry's Law constant. All representations of formaldehyde and acetaldehyde undergo dry deposition. Remaining new species have zero dry deposition velocities based on analogies to similar hydrocarbon species and their volatilities.

4.2 Chlorine

A chlorine chemical mechanism has been added to the CMAQ model based on Tanaka et al. (2003). The original chlorine mechanism proposed by Tanaka et al. (2003) contains 13 reactions. However, two of those reactions involves 1,3 butadiene and its reaction product. Since the base CB-IV mechanism does not contain 1,3 butadience, these two reactions were eliminated and the remaining 11 reactions were combined with the CB-IV mechanism and incorporated into the CMAQ model. An EBI solver has also been developed for the combined mechanism (chlorine + CB-IV mechanism). The current chlorine chemistry can not be used in conjunction with the SAPRC-99 mechanism.
In-house tests were conducted using chlorine emissions for two cases (Sarwar and Gipson, 2005). In one case, CMAQ was run with molecular chlorine emissions from the 1999 National Emissions Inventory for Hazardous Air Pollutants, in the other case, the molecular chlorine was supplemented with HOCl emissions estimated from swimming pools and cooling towers. Initial test results indicate that when molecular chlorine emissions were included in the model, the only significant impact occurred near the Great Salt Lake. When both molecular chlorine and hypochlorous acid emissions were included in the model, the impacts were evident in several areas, including the Great Salt Lake and the Houston area.

5. New diagnostic tools

5.1 Carbon source apportionment.

New codes and mechanism include files in this release provide users the option to track the contributions of elemental carbon and primary organic carbon from up to 10 different source categories or source regions. A detailed description of this model option is provided by Bhave et al. (2004b).

5.2 Sulfur tracking

CMAQv4.5 includes an optional diagnostic model configuration that provides detailed information on the modeled sulfur budget. This model version, referred to as the CMAQ Sulfate Tracking Model, tracks sulfate production from the gas-phase and the five aqueous-phase chemical reactions, as well as contributions from direct emissions and initial and boundary conditions. Each of the tracked species is advected, diffused, processed through clouds, and deposited (both wet and dry) individually. The CMAQ sulfate tracking model is a valuable tool in examining the nonlinearities in the production of sulfate. Note that, currently the Sulfate Tracking Model only operates on the aero3

(AE3) and cloud_radm modules. We plan to extend the sulfate tracking capability to the aero4 and cloud_acm modules in the next release.

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