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Chapter 3

DEVELOPING METEOROLOGICAL FIELDS

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ABSTRACT

Meteorological data are important in many of the processes simulated in the Community Multiscale Air Quality (CMAQ) model included in the first release of the Models-3 framework. The meteorology model that has been selected and evaluated with CMAQ is the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5). All software in the Penn State/NCAR mesoscale modeling system has been dedicated to the public domain and is presently used for both research and operational purposes at many organizations worldwide. Improvements to MM5 within the meteorological community are ongoing, and these enhancements should be evaluated for their applicability to air quality modeling. Other meteorological models are being considered for compatibility with CMAQ but are not provided with the initial release. The application of MM5 with CMAQ is described in Chapter 3.

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3.0 DEVELOPING METEOROLOGICAL FIELDS

3.1 Credits and Disclaimers for Use of MM5

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3.2 Meteorology Model Pre-Processing

Before the meteorology model can be run, several smaller ("pre-processing") programs must be run to set up the domain for the simulation and to generate a set of initial and boundary conditions for the meteorology model. The pre-processing programs are briefly described in this section.

3.2.1 Defining the Simulation Domain (*TERRAIN*)

Domains for the meteorology simulations are defined by several primary parameters: number of grid points in each horizontal dimension, grid spacing, center latitude, center longitude, map projection (Mercator, Lambert conformal, or polar stereographic), and number of "nested" domains and their horizontal dimensions. (Some other user-specific parameters are also defined based on the primary parameters, as required.) These parameters are processed by a program that is executed only when a new domain location is required. This program, *TERRAIN*, makes use of high-resolution global terrain and land use data sets to create "static files" for the domain. The static files currently include values for each grid point for terrain height and land use specification (e.g., deciduous forest, desert, water). Future versions of *TERRAIN* may include additional diurnal, seasonal, and location-specific information. The *TERRAIN* program is thoroughly described by Guo and Chen (1994).

3.2.2 Processing the Meteorological Background Fields (*DATAGRID*)

After the simulation domain has been established, the program *DATAGRID* is run to process the meteorological background fields. *DATAGRID* generates first-guess fields for the model simulation by horizontally interpolating a larger-scale data set (global or regional coverage) to the simulation domain. *DATAGRID* interpolates the background fields to the simulation domain for times throughout the simulation period; these files are used ultimately to generate lateral boundary conditions for the coarse-domain simulations. (Nested domains obtain lateral boundary conditions from the coarse domain.) *DATAGRID* also processes the sea-surface temperature and snow files by interpolating the analyses to the simulation domain. Lastly, *DATAGRID* calculates map-scale factors and Coriolis parameters at each grid point to be used by MM5. The *DATAGRID* program is thoroughly described by Manning and Haagenson (1992).

3.2.3 Objective Analysis (*RAWINS*)

The program *RAWINS* performs an objective analysis by blending the first-guess fields generated by *DATAGRID* with upper-air and surface observations. There are four objective analysis techniques available in *RAWINS*. The following descriptions are taken largely from Dudhia et al. (1998).

- **The Cressman scheme** assigns a circular radius of influence to each observation. The weights associated with the observations decrease radially from the observation to the radius of influence. The first-guess (meteorological background) field at each grid point is adjusted by taking into account all observations that influence that grid point. (See Cressman, 1959.)

- **The Ellipse scheme** alters the Cressman circles for analyses of wind and relative humidity by elongating the circles along the wind flow. The eccentricity of the ellipses increases as wind speed increases. This scheme reduces to the Cressman scheme under light wind conditions. (See Benjamin and Seaman, 1985.)

- **The Banana scheme** alters the Cressman circles for analyses of wind and relative humidity by elongating the circles in the direction of the flow and curving the influence region along streamlines. The resulting influence region is banana-shaped. This scheme reduces to the ellipse scheme under straight-flow conditions, and it further reduces to the Cressman scheme under light wind conditions. (See Benjamin and Seaman, 1985.)

- **The Multiquadric Interpolation scheme** uses hyperboloid radial basis functions to perform objective analysis. This scheme takes much more time and memory than the Cressman-based schemes. This scheme must be used with caution in data-sparse regions and when more than 25% of the domain is water-covered. (See Nuss and Titley, 1994.)

In addition, *RAWINS* performs some data quality control checks and buddy checks with user-defined thresholds. The objective analysis is performed for a user-defined number of pressure surfaces (generally mandatory levels plus some additional surfaces). *RAWINS* is also used to prepare the analyses for the analysis nudging in the simulation model. The *RAWINS* program is thoroughly described by Manning and Haagenson (1992).

3.2.4 Setting the Initial and Boundary Conditions (*INTERP*)

The "standard" *INTERP* program sets the initial and boundary conditions for the meteorology simulation. The analyses from *RAWINS* are interpolated to MM5's staggered grid configuration and from their native vertical coordinate (pressure) to MM5's vertical coordinate (a terrain-following, pressure-based "sigma" coordinate). In addition, the state variables are converted as necessary, e.g., relative humidity to specific humidity. The analyses from one time (generally the first time analyzed by *RAWINS*) are interpolated by *INTERP* to provide MM5's initial conditions, while analyses from all times are interpolated to generate MM5's lateral boundary conditions.

INTERP can also be used for "one-way nesting," where the MM5 output from one model run is interpolated to provide initial and boundary conditions for the nested run. This is a "non-standard" use of the *INTERP* program, but it is commonly used to support air quality modeling.

3.3 The Meteorology Model (MM5)

The following subsections include brief summaries of the science and options that are available in MM5. Thorough descriptions of the standard MM5 options are found in Grell et al. (1994) and Dudhia et al. (1998). The source code for an early release of MM5 is documented in Haagenson et al. (1994). The Models-3 package does not include NCAR's most current release of MM5. MM5 user options have been tailored and expanded in the Models-3 release to support air quality modeling. Some of these options have not yet been accepted into the official version that is maintained by NCAR. Caution should be exercised when deviating from the version of MM5 that is included with Models-3. Refer to Section 3.5 for a summary of changes to MM5 for CMAQ.

3.3.1 Brief History

MM5 is the Fifth-Generation Penn State/NCAR Mesoscale Model. It has evolved from the model used by Anthes in the early 1970s, described by Anthes and Warner (1978). The improvements in MM5 over the previous version (MM4) include the option for non-hydrostatic physics, as well as more sophisticated explicit moisture, boundary layer processes, radiation, convective parameterization, among other improvements. Dudhia (1993) documented the major changes from MM4 to MM5. Starting with MM5 Version 2 (MM5v2), the software has been restructured to run on various hardware platforms in addition to the Cray, with emphasis placed on workstation-based MM5 simulations. The Cray version of MM5 provided on the Models-3 installation tape has been tested on the EPA's Cray C90. A workstation-based version of MM5 may be used with subsequent releases of Models-3.

3.3.2 Horizontal and Vertical Grid

The coordinate system for MM5 is (x, y, sigma-p). The x and y dimensions are a regular lattice of equally spaced points (delta-x = delta-y = horizontal grid spacing, in kilometers) forming rows and columns. Sigma is a terrain-following vertical coordinate that is a function of the pressure at the point on the grid (in hydrostatic runs) or the reference state pressure (in non-hydrostatic runs), the surface pressure at the grid point, and the pressure at the top of the model. Sigma varies from 1 at the surface to 0 at the top of the model. The influence of the terrain on the sigma structure diminishes with height, such that the sigma surfaces near the top of the model are nearly parallel.

The horizontal grid in MM5 has an Arakawa-B staggering of the velocity vectors with respect to the scalars (Arakawa and Lamb, 1977). The momentum variables (u- and v-components of wind and the Coriolis force) are on "dot" points, while all other variables (e.g., mass and moisture variables) are on "cross" points. The dot points form the regular lattice for the simulation domain, while the cross points are offset by 0.5 grid point in both the x and y directions. Note that the interpolation of the variables to the staggered grid is done automatically within the *INTERP* program.

3.3.3 Prognostic Equations

MM5 is based on primitive physical equations of momentum, thermodynamics, and moisture. The state variables are temperature, specific humidity, grid-relative wind components, and pressure.

In the prognostic equations, the state variables are mass-weighted with a modified surface pressure. MM5 can be run as either a hydrostatic or non-hydrostatic model. In the hydrostatic model, the state variables are explicitly forecast. In the non-hydrostatic model (Dudhia, 1993), pressure, temperature, and density are defined in terms of a reference state and perturbations from the reference state. MM5 is not mass-conserving in the non-hydrostatic mode. The vertical (sigma) coordinate is defined as a function of pressure. The model's prognostic equations are thoroughly discussed in Grell et al. (1994) and Dudhia et al. (1998).

3.3.3.1 Time Differencing

The hydrostatic and non-hydrostatic versions of MM5 use different time differencing schemes to filter the fast waves from the prognostic solutions in the model. In the non-hydrostatic model, a semi-implicit scheme based on Klemp and Wilhelmson (1978) is used to control the acoustic waves in the model solution. In the hydrostatic model, a split-explicit scheme based on Madala (1981) is used to control gravity waves in the model solution. The time differencing in MM5 is discussed at length in Grell et al. (1994) and Dudhia et al. (1998).

3.3.3.2 Lateral Boundary Conditions

There are five options for lateral boundary conditions in MM5: fixed, relaxation, time dependent, time and inflow/outflow dependent, and sponge. The lateral boundaries in MM5 consist of either the outer five grid points (relaxation and sponge options) or the outer grid point (all other options) on the horizontal perimeter of the simulation domain. (The outer four grid points are used for boundary conditions for "cross" point variables for the relaxation and sponge options.) The lateral boundary conditions for the coarse domain are derived from the background fields processed in *DATAGRID* and *INTERP*. When the one-way nest option is selected, the lateral boundary conditions for nested domains are interpolated from the simulation on the parent domain.

3.3.4 Model Physics

Several model physics options in MM5 are briefly noted below. The model physics options are further discussed and compared in Dudhia et al. (1998). The descriptions of the model physics options are largely taken from Dudhia et al. (1998), and other pertinent references are noted.

3.3.4.1 Radiation

There are five atmospheric radiation cooling schemes available in MM5.

- **The "None" option** applies no mean radiative tendency to the atmospheric temperature. This scheme is unrealistic for long-term simulations.

- **The Simple Cooling scheme** sets the atmospheric cooling rate strictly as a function of temperature. There is no cloud interaction or diurnal cycle.

- **The Surface Radiation scheme** is used with the "none" and "simple cooling" schemes. This scheme includes a diurnally varying shortwave and longwave flux at the surface for use in the ground energy budget. These fluxes are calculated based on atmospheric column-integrated water vapor and low/middle/high cloud fraction estimated from relative humidity.

- **The Dudhia Longwave and Shortwave Radiation scheme** is sophisticated enough to account for longwave and shortwave interactions with explicit cloud and clean air. This scheme includes surface radiation fluxes and atmospheric temperature tendencies. This scheme requires longer CPU time, but not much memory. (See Dudhia, 1989.)

- **The CCM2 Radiation scheme** includes multiple spectral bands in shortwave and longwave, but the clouds are treated simply as functions of relative humidity. This scheme is suitable for larger grid scales and probably more accurate for long time integration (e.g., climate modeling). It also provides radiative fluxes at the surface. (See Hack et al., 1993.)

3.3.4.2 Convective Parameterization

There are currently six convective parameterization schemes in MM5. There is also the option for no convective parameterization and an independent option for shallow convection. The convective parameterization schemes have been designed for use at various simulation scales, and they are not entirely interchangeable. For example, each scheme uses different assumptions for convective coverage on the sub-grid-scale and for the convective trigger function. The convective parameterization schemes also differ greatly in CPU usage and memory requirements.

- **The Anthes-Kuo scheme** is based on moisture convergence and is mostly applicable to larger grid scales (i.e., greater than 30 km). This scheme tends to produce more convective rainfall and less resolved-scale precipitation. This scheme uses a specified heating profile where moistening is dependent on relative humidity. (See Anthes, 1977.)

- **The Fritsch-Chappel scheme** is based on relaxation to a profile due to updraft, downdraft, and subsidence region properties. The convective mass flux removes 50% of the available buoyant energy in the relaxation time. There is a fixed entrainment rate. This scheme is suitable for 20-30 km scales due to the single cloud assumption and local subsidence. (See Fritsch and Chappel, 1980.)

- **The Arakawa-Schubert scheme** is a multi-cloud scheme that is otherwise similar to the Grell scheme (described below). This scheme is based on a cloud population, and it allows for entrainment into updrafts and the existence of downdrafts. This scheme is suitable for larger grid scales (i.e., greater than 30 km). This scheme can be computationally expensive compared to the other available schemes. (See Arakawa and Schubert, 1974.)

- **The Kain-Fritsch scheme** is similar to the Fritsch-Chappel scheme, but it uses a sophisticated cloud-mixing scheme to determine entrainment and detrainment. This scheme also removes all available buoyant energy in the relaxation time. (See Kain and Fritsch, 1990, 1993.)

- **The Betts-Miller scheme** is based on relaxation adjustment to a reference post-convective thermodynamic profile over a given period. This scheme is suitable for scales larger than 30 km. However, there is no explicit downdraft, so this scheme may not be suitable for severe convection. (See Betts, 1986; Betts and Miller, 1986, 1993; and Janjic, 1994.)

- **The Grell scheme** is based on rate of destabilization or quasi-equilibrium. This is a single-cloud scheme with updraft and downdraft fluxes and compensating motion that determines the heating and moistening profiles. This scheme is useful for smaller grid scales (e.g., 10-30 km), and it tends to allow a balance between the resolved scale rainfall and the convective rainfall. (See Grell et al., 1991; and Grell, 1993.)

- **The "no convective parameterization" option** (e.g., explicitly resolved convection on the grid scale) is also available. This option is generally used for simulations on domains with horizontal grid spacing smaller than 10 km.

- **The Shallow Convection scheme** is an independent option that handles non-precipitating clouds that are assumed to be uniform and to have strong entrainment, a small radius, and no downdrafts. This scheme is based on the Grell and Arakawa-Schubert schemes. There is also an equilibrium assumption between cloud strength and sub-grid boundary layer forcing.

3.3.4.3 Planetary Boundary Layer Processes

Four planetary boundary layer (PBL) parameterization schemes are available in MM5. These parameterizations are most different in the turbulent closure assumptions that are used. The PBL parameterization schemes also differ greatly in CPU usage.

- **The Bulk Formula scheme** is suitable for coarse vertical resolution in the PBL (i.e., greater than 250 m vertical grid sizes). This scheme includes two stability regimes.

- **The Blackadar scheme** is suitable for "high-resolution" PBL (e.g., five layers in the lowest kilometer and a surface layer less than 100 m thick). This scheme has four stability regimes; three stable and neutral regimes are handled with a first-order closure, while a free convective layer is treated with a non-local closure. (See Blackadar, 1979.)

- **The Burk-Thompson scheme** is suitable for coarse and high-resolution PBL. This scheme explicitly predicts turbulent kinetic energy for use in vertical mixing, based on a 1.5-order closure derived from the Mellor-Yamada formulas. (See Burk and Thompson, 1989.)

- **The Medium Range Forecast (MRF) model scheme** is suitable for high-resolution PBL. This scheme is computationally efficient. It is based on a Troen-Mahrt representation of the counter-gradient term and a first-order eddy diffusivity (K) profile in the well-mixed PBL. This scheme has been taken from the National Centers for Environmental Prediction's (NCEP's) MRF model. (See Hong and Pan, 1996.)

3.3.4.4 Surface Layer Processes

The surface layer processes with the Blackadar and MRF PBL schemes have been parameterized with fluxes of momentum, sensible heat, and latent heat, following Zhang and Anthes (1982). The energy balance equation is used to predict the changes in ground temperature using a single slab and a fixed-temperature substrate. The slab temperature is based on an energy budget, and the depth is assumed to represent the depth of the diurnal temperature variation (~10-20 cm). The 13 land use categories are used to seasonally define the physical properties at each grid point (e.g., albedo, available moisture, emissivity, roughness length, and thermal inertia).

A five-layer soil temperature model (Dudhia, 1996) is also available as an option in MM5. In this model, the soil temperature is predicted at layers of approximate depths of 1, 2, 4, 8, and 16 cm, with a fixed substrate below using a vertical diffusion equation. This scheme vertically resolves the diurnal temperature variation, allowing for more rapid response of surface temperature. This model can only be used in conjunction with the Blackadar and MRF PBL schemes.

In a subsequent release of CMAQ, the Pleim-Xiu land-surface scheme (Pleim and Xiu, 1995) may be included in MM5. The Pleim-Xiu scheme has been developed to address surface processes that can significantly impact air quality modeling, including evapotranspiration and soil moisture. Notable in the Pleim-Xiu scheme is the more careful treatment of the surface characteristics (particularly vegetation parameters) that are currently assigned to grid points based on land use specification, as well as a more detailed land use and soil type classification database.

3.3.4.5 Resolvable-Scale Microphysics Schemes

There are six resolvable-scale (explicit grid-scale) microphysics schemes in MM5. There is also an option for a "dry" model run. The microphysics schemes have been designed with varying degrees of complexity for different applications of the model. In addition, there are new prognostic output variables that are generated by the more sophisticated schemes. These microphysics schemes also differ greatly in CPU usage and memory requirements.

- **The Dry scheme** has no moisture prediction. Water vapor is set to zero. This scheme is generally used for sensitivity studies.
- **The Stable Precipitation scheme** generates non-convective precipitation. Large-scale saturation is removed and rained out immediately. There is no evaporation of rain or explicit cloud prediction.
- **The Warm Rain scheme** uses microphysical processes for explicit predictions of cloud and rainwater fields. This scheme does not consider ice phase processes. (See Hsie and Anthes, 1984.)
- **The Simple Ice scheme** adds ice phase processes to the warm rain scheme without adding memory. This scheme does not have supercooled water, and snow is immediately melted below the freezing level. (See Dudhia, 1989.)
- **The Mixed-Phase scheme** adds supercooled water to the simple ice scheme, and slow melting of snow is allowed. Additional memory was added to accommodate the ice and snow. This scheme does not include graupel or riming processes. (See Reisner et al., 1993, 1998.)
- **The Mixed-Phase with Graupel scheme** adds graupel and ice number concentration prediction equations to the mixed-phase scheme. This scheme is suitable for cloud-resolving scales. (See Reisner et al., 1998.)
- **The NASA/Goddard Microphysics scheme** explicitly predicts ice, snow, graupel, and hail. This scheme is suitable for cloud-resolving scales. (See Tao and Simpson, 1993.)

3.3.5 Nesting

MM5 can simulate nested domains of finer resolutions within the primary simulation domain. In MM5, the software is configured to enable up to nine nests (ten domains) within a particular run. However, due to current hardware resources, the state of the science, numerical stability, and practicality, the number of domains in a simulation is generally limited to four or fewer.

Nesting can be accomplished by either a "one-way" or a "two-way" method. In one-way nesting, the coarse-resolution domain simulation is run independently of the nest. The coarse domain can then provide the initial and boundary conditions for its nest. In one-way nesting, each domain can be defined with independent terrain fields, and there are no feedbacks to the coarse domain from its nest. Note that the simulated meteorology at the same grid point in the coarse-resolution domain is likely to be different (if only slightly) from the nest in a one-way nest simulation.

Two-way interactive nesting (Zhang et al., 1986; Smolarkiewicz and Grell, 1992) allows for feedback to occur between the coarse-resolution domain and the nest throughout the simulation. The two domains are run simultaneously to enable this feedback, and terrain in the overlapping regions must be compatible to avoid mass inconsistencies and generation of numerical noise. The *TERRAIN* program automatically defines the terrain compatibility when the user specifies the two-way nesting interaction. When two-way nesting is used, the portion of the coarse-resolution domain that is simulated in the nest may reflect too much smaller-scale detail from the nest to be useful for the CMAQ simulations.

The nesting ratio between domains in MM5 is generally 3:1. (Some other mesoscale meteorology models allow for user-defined nest ratios.) For example, if the coarse domain is a 36-km resolution domain, its nest will be a 12-km resolution domain. This is strictly true for a two-way nest, but is largely held as a standard for the one-way nests in MM5. The nest ratio restricts the number of grid points in each dimension of the nest domains to a multiple of 3, plus 1.

3.3.6 Four-Dimensional Data Assimilation

The four-dimensional data assimilation (FDDA) scheme included in MM5 is based on Newtonian relaxation or "nudging". Nudging is a continuous form of FDDA where artificial (non-physical) forcing functions are added to the model's prognostic equations to nudge the solutions toward either a verifying analysis or toward observations. The artificial forcing terms are scaled by a nudging coefficient that is selected so that the nudging term will not dominate the prognostic equations. The nudging terms tend to be one order of magnitude smaller than the dominant terms in the prognostic equations and represent the inverse of the *e*-folding time of the phenomena captured by the observations.

There are two types of nudging in MM5: analysis nudging and observation nudging ("obs nudging"). Analysis nudging gently forces the model solution toward gridded fields. Analysis nudging can make use of three-dimensional analyses and some surface analyses. Analysis nudging is generally used for scales where synoptic and mesoalpha forcing are dominant. Obs nudging gently forces the model solution toward individual observations, with the influence of the observations spread in space and time. Obs nudging is better suited for assimilating high frequency, asynoptic data that may not otherwise be included in an analysis.

Nudging in MM5 is extensively discussed in Stauffer and Seaman (1990, 1994) and Stauffer et al. (1991). The data assimilation is generally used throughout the MM5 simulation period for air quality simulations. Three-dimensional analyses of wind, temperature, and moisture are assimilated, and only surface analyses of wind are assimilated, following Stauffer et al. (1991).

3.4 Meteorology Model Post-Processing

Since the output variables that are generated by an MM5 simulation are not always useful in their raw form, those variables must be converted into fields that are required by the chemistry and emission models. The conversion of MM5 output to useful fields for the other Models-3 programs is accomplished in the Meteorology Chemistry Interface Processor (MCIP), which is discussed in Chapter 12. MCIP computes variables that are useful to the subsequent models in Models-3, and it creates an output file written with the I/O API libraries in netCDF format that is standard in the Models-3/CMAQ modeling system.

3.5 Changes to the MM5 System's Software for Models-3

The version of MM5 included with the initial release of Models-3 is MM5 Version 2, Release 6. The system is complete with “bug fixes” included through October 1997. Only selected “bug fixes” and upgrades have been included beyond October 1997. (Including all of the changes to MM5 would have jeopardized testing and evaluation of CMAQ, which uses the MM5 output.) The version of MM5 in the Models-3 release includes most of the science options in NCAR’s current version. The omission of upgrades should not result in substandard or corrupted meteorological simulations.

The following is a summary of EPA-initiated changes that were made to the NCAR release of MM5 and its supporting software to support air quality modeling with CMAQ:

All Programs:

- Standardized the radius of the earth as 6370.997 km to be consistent with chemistry and emission models.

TERRAIN:

- Set terrain height over ocean to zero when using the 1-minute terrain database.
- Improved representation of urban areas along coasts.

INTERP:

- Increased loop indices and parameter sizes to accommodate 120-hour simulation.

MM5:

- Modified script and source code to enable analysis nudging on a one-way nested simulation.

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