

Chapter 6

GOVERNING EQUATIONS AND COMPUTATIONAL STRUCTURE OF THE COMMUNITY MULTISCALE AIR QUALITY (CMAQ) CHEMICAL TRANSPORT MODEL

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ABSTRACT

The chemical transport model (CTM) of the Models-3/CMAQ (Community Multiscale Air Quality) modeling system can be configured to follow the dynamics of the preprocessor meteorological model. A science process module in the CMAQ CTM is not specific to a coordinate system. The generality is accomplished through the use of the coordinate transformation Jacobian within the CMAQ CTM. In this chapter, we derive the governing diffusion equation in a generalized coordinate system, which is suitable for multiscale atmospheric applications. We describe the CMAQ system's modularity concepts, fractional time-step formulation, and key science processes implemented in the current version of the CMAQ CTM. We examine dynamic formulations of several popular Eulerian air quality models as emulated by the governing diffusion equations in the generalized coordinate system. Also, a nesting technique for the CMAQ CTM is introduced. Finally, because the amount of a substance in the atmosphere can be expressed in many different ways, we summarize the most popular expressions for concentration and their transformation relations.

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6.0 GOVERNING EQUATIONS AND COMPUTATIONAL STRUCTURE OF THE COMMUNITY MULTISCALE AIR QUALITY (CMAQ) CHEMICAL TRANSPORT MODEL

In Chapter 5, “Fundamentals of Atmospheric Modeling ...” we discussed the fundamental set of equations for atmospheric dynamics and thermodynamics in a generalized coordinate system. In this Chapter, we investigate the diffusion equation for the trace species in the atmosphere in the generalized coordinate system and the computational structure of the Community Multiscale Air Quality chemical transport model (CMAQ CTM or, hereafter, CCTM).

One requirement of the CMAQ modeling system is to maintain a consistent description of the atmosphere for different meteorological and chemical transport models. This is a feature that is essential for spatial scalability. Various coordinate systems are used in atmospheric models. Selection of a suitable coordinate system is an important step of model formulation. There are numerous criteria to be considered in selecting a coordinate system, such as the dynamic characteristics it can handle and how well it can deal with curvature of the earth’s surface and features of the terrain. Formulation of the models may vary substantially for different coordinate systems. If a CTM can be formulated and coded using a generalized coordinate system, it would be easy to switch from one coordinate to another depending on the application. The generalized coordinate concept is useful because a single CTM formulation can adapt to any of the coordinates commonly used in meteorological models. It is also desirable to compare the benefits of various coordinate systems and to be able to link the CTMs to meteorological models and databases in different coordinates.

Conformity of the coordinates to the physics of the problem is very important. Unlike a model with a fixed coordinate system, a generalized coordinate system allows use of generic coordinates for the specific science processes within a model. Although the model’s overall structure is determined by the choice of a coordinate system, the individual science modules can still use their own generic coordinates that best suit the physical processes they model. This means that each science process can utilize the parameterizations based on the best coordinate to represent the problem. For example, the planetary boundary layer (PBL) parameterizations can be expressed in terms of geometric height, or dimensionless height scaled with PBL height, while for cloud physics, they can be represented in terms of pressure. The linkages between the generic coordinate parameterizations in the science processes and the governing conservation equation in the generalized coordinates are established through the application of appropriate coordinate transformation rules.

Here, we intend to provide a comprehensive and rational development of the governing conservation equation in generalized coordinates, which can be readily implemented in an Eulerian model. The operating assumptions used for the derivations are listed below (see Srivastava et al., 1995).

- **Assumption 1:** Pollutant concentrations are sufficiently small, such that their presence would not affect the meteorology to any detectable extent. Hence, the species

conservation equations can be solved independently of the Navier-Stokes and energy equations. The conditions which could invalidate this assumption are for cases where sufficient heat is generated by chemical reactions to influence the temperature of the medium or where an atmospheric layer become so concentrated with pollutants that absorption, reflection, and scattering of radiation alter the air flow (Seinfeld, 1986).

- **Assumption 2:** The velocities and concentrations of the various species in atmospheric flow are turbulent quantities and undergo turbulent diffusion. Because turbulent diffusion is much greater than molecular diffusion for most trace species, the latter can be ignored.
- **Assumption 3:** The metric tensor that defines the coordinate transformation rules is not a turbulent variable. This means that we can define the coordinates based on the Reynolds averaged quantities. The vertical grids will be defined incrementally between time steps when a time-dependent vertical coordinate is used.
- **Assumption 4:** The ergodic hypothesis holds for the ensemble averaging process. This means that the ensemble average of a property can be substituted with the time average of that property.
- **Assumption 5:** The turbulence is assumed stationary for the averaging time period of interest (say 30 minutes to one hour for atmospheric applications).
- **Assumption 6:** The source function (i.e., emissions of pollutants) is deterministic for all practical purposes and there is no turbulent component.
- **Assumption 7:** The effect of concentration fluctuation on the rate of chemical reaction is negligible, i.e., contributions of covariance effects among tracer species are neglected.
- **Assumption 8:** Because the large-scale motions of the atmosphere are quasi-horizontal with respect to the earth's surface, science processes can be separately represented in horizontal and vertical directions (i.e., quasi-orthogonal in transformed coordinates).

6.1 Derivation of the Atmospheric Diffusion Equation

In Chapter 5, we derived the species continuity equation in generalized coordinates. It is given as:

$$\frac{\partial(\varphi_i J_s)}{\partial t} + m^2 \nabla_s \cdot \left(\frac{\varphi_i J_s \hat{\mathbf{V}}_s}{m^2} \right) + \frac{\partial(\varphi_i J_s \dot{s})}{\partial s} = J_s Q_{\varphi_i} \quad (6-1)$$

where φ_i is the trace species concentration in density units (e.g., kg m^{-3}), J_s is the vertical Jacobian of the terrain-influenced coordinate s , m is the map scale factor, $\hat{\mathbf{V}}_s$ and \dot{s} are horizontal and vertical wind components in the generalized coordinates, and Q_{φ_i} is the source or sink term.

To make the instantaneous species continuity equation useful for air quality simulation, we need to derive the governing diffusion equation. This is done by decomposing the variables in Equation 6-1, except for the Jacobian and map scale factor, in terms of mean and turbulent components. The Reynolds decompositions of species concentration and mixing ratio are expressed as:

$$\varphi_i = \bar{\varphi}_i + \varphi_i'' \quad (6-2a)$$

$$q_i = \bar{q}_i + q_i'' \quad (6-2b)$$

$$\bar{\varphi}_i + \varphi_i'' = \bar{q}_i \bar{\rho} + q_i'' \bar{\rho} + \bar{q}_i \rho'' + q_i'' \rho'' \quad (6-2c)$$

where $q_i = \frac{\varphi_i}{\rho}$ is the species mass mixing ratio and a stochastic quantity is decomposed into mean, $(\bar{\quad})$, and turbulent, $(\quad)''$, components. Stationary turbulence assumption 5 implies that a turbulent component has a zero mean for the averaging period. Following Venkatram (1993), we can estimate the mean and turbulent components of species and air concentrations as

$$\bar{\varphi}_i \approx \bar{q}_i \bar{\rho} \quad (6-3a)$$

$$\varphi_i'' = q_i'' \bar{\rho} + \bar{q}_i \rho'' + q_i'' \rho'' \quad (6-3b)$$

$$\frac{\overline{q_i'' \rho''}}{\bar{q}_i \bar{\rho}} \approx \frac{\overline{\rho''^2}}{(\bar{\rho})^2} \ll 1 \quad (6-3c)$$

Without loss of generality, we redefine the terrain-influenced vertical coordinate s with a coordinate \hat{x}^3 , whose value is increasing monotonically with height, as:

$$\hat{x}^3 = \xi = \begin{cases} s & (\text{if } s \text{ increases with height}) \\ 1-s & (\text{if } s \text{ decreases with height}) \end{cases} \quad (6-4)$$

The choice of a generalized vertical coordinate which increases monotonically with height simplifies the derivation of the governing equation and thus reduces the likelihood of making sign errors in the formulas and in computer codes. The transformation does not change the horizontal wind components or the Jacobian, which is always defined to be a positive quantity. Hereafter, the subscript s is replaced with ξ to reflect modification of the vertical coordinate. Subsequently, the vertical velocity is represented with $\hat{v}^3 = d\xi/dt = \dot{\xi}$, which is positive for upward motion.

Application of decomposition of velocity components in Equation 6-1 and ensemble averaging produces Reynolds flux terms in the mass conservation equation as:

$$\begin{aligned} \frac{\partial(\overline{\varphi}_i J_\xi)}{\partial t} + m^2 \nabla_\xi \cdot \left(\frac{(\overline{\varphi}_i + \varphi_i'')(\overline{\hat{V}}_\xi + \hat{V}_\xi'') J_\xi}{m^2} \right) \\ + \frac{\partial}{\partial \hat{x}^3} \left[(\overline{\varphi}_i + \varphi_i'')(\overline{\hat{v}}^3 + \hat{v}^3'') J_\xi \right] = J_\xi Q_{\varphi_i} \end{aligned} \quad (6-5)$$

where we used $J_\xi = \overline{J}_\xi$ and $Q_{\varphi_i} = \overline{Q}_{\varphi_i}$ based on Assumption 3 and Assumption 6, respectively. The Reynolds flux terms in Equation 6-5 can be approximated in terms of the mixing ratio as:

$$\overline{\varphi_i'' \hat{V}_\xi''} \approx \overline{\rho} \overline{q_i'' \hat{V}_\xi''} + \overline{q_i''} \overline{\hat{V}_\xi''} \approx \overline{\rho} \overline{q_i'' \hat{V}_\xi''} \quad (6-6a)$$

$$\overline{\varphi_i'' \hat{v}^3''} \approx \overline{\rho} \overline{q_i'' \hat{v}^3''} + \overline{q_i''} \overline{\hat{v}^3''} \approx \overline{\rho} \overline{q_i'' \hat{v}^3''} \quad (6-6b)$$

$$\overline{q_i'' \hat{V}_\xi''} \ll 1 \quad (6-6c)$$

$$\overline{q_i'' \hat{v}^3''} \ll 1 \quad (6-6d)$$

in which we have neglected the second order perturbation terms based on the scale analysis of the equations. Equation 6-5 can be rewritten using Equations 6-3a-c and 6-6a-c to give:

$$\begin{aligned} \frac{\partial(\overline{\varphi}_i J_\xi)}{\partial t} + m^2 \nabla_\xi \cdot \left(\frac{\overline{\varphi}_i \overline{\hat{V}}_\xi J_\xi}{m^2} \right) + \frac{\partial(\overline{\varphi}_i \overline{\hat{v}}^3 J_\xi)}{\partial \hat{x}^3} \\ + m^2 \nabla_\xi \cdot \left(\frac{\overline{\rho} \overline{q_i'' \hat{V}_\xi''} J_\xi}{m^2} \right) + \frac{\partial(\overline{\rho} \overline{q_i'' \hat{v}^3''} J_\xi)}{\partial \hat{x}^3} = J_\xi Q_{\varphi_i} \end{aligned} \quad (6-7)$$

The turbulence flux terms can be parameterized using a simple closure scheme such as the eddy diffusion concept (K-theory):

$$\overline{q_i'' \hat{u}_\xi''} = -\hat{K}^{1l} \frac{\partial \overline{q_i}}{\partial \hat{x}^l}; \quad \overline{q_i'' \hat{v}_\xi''} = -\hat{K}^{2l} \frac{\partial \overline{q_i}}{\partial \hat{x}^l}; \quad \overline{q_i'' \hat{v}^3''} = -\hat{K}^{3l} \frac{\partial \overline{q_i}}{\partial \hat{x}^l} \quad (6-8)$$

where \hat{K}^{jl} denotes the eddy diffusivity tensor in the transformed coordinate. The eddy diffusivity tensor for the generalized meteorological coordinates is related to the diffusivity tensor in Cartesian coordinates as:

$$\hat{K}^{kl} = \frac{\partial \hat{x}^k}{\partial x^i} \frac{\partial \hat{x}^l}{\partial x^j} K^{ij} \quad (6-9)$$

If we postulate that the diffusivity tensor in Cartesian coordinates is diagonal (i.e., all the off-diagonal components vanish), then the eddy diffusivity tensor in the generalized meteorological coordinates becomes:

$$\hat{\mathbf{K}} = \begin{pmatrix} m^2 K_{xx} & 0 & m \frac{\partial \hat{x}^3}{\partial x} K_{xx} \\ 0 & m^2 K_{yy} & m \frac{\partial \hat{x}^3}{\partial y} K_{yy} \\ m \frac{\partial \hat{x}^3}{\partial x} K_{xx} & m \frac{\partial \hat{x}^3}{\partial y} K_{yy} & \left(\frac{\partial \hat{x}^3}{\partial x}\right)^2 K_{xx} + \left(\frac{\partial \hat{x}^3}{\partial y}\right)^2 K_{yy} + \left(\frac{\partial \hat{x}^3}{\partial z}\right)^2 K_{zz} \end{pmatrix} \quad (6-10)$$

where $K_{xx} = K^{11}$, $K_{yy} = K^{22}$, and $K_{zz} = K^{33}$ are the diagonal components of eddy diffusivity tensor in the Cartesian coordinate. To match with the computational grid, the gradient terms in Equation 6-10 must be rewritten in terms of the generalized coordinates \hat{x}^3 (defined based on height above ground $h_{AGL} = h - z_{sfc}$, where z_{sfc} represents the height of topography) using the appropriate chain rules, for example, $\frac{1}{m} \left(\frac{\partial A}{\partial x} \right)_z = \left(\frac{\partial A}{\partial \hat{x}^1} \right)_{\hat{x}^3} - \frac{\partial A}{\partial z} \left(\frac{\partial A}{\partial \hat{x}^3} \right) \left(\frac{\partial h}{\partial \hat{x}^1} \right)_{\hat{x}^3}$. When $A = \hat{x}^3$, we get

$$\hat{\mathbf{K}} = \begin{pmatrix} m^2 K_{xx} & 0 & -m^2 \frac{\partial \hat{x}^3}{\partial z} \frac{\partial h}{\partial \hat{x}^1} K_{xx} \\ 0 & m^2 K_{yy} & -m^2 \frac{\partial \hat{x}^3}{\partial z} \frac{\partial h}{\partial \hat{x}^2} K_{yy} \\ -m^2 \frac{\partial \hat{x}^3}{\partial z} \frac{\partial h}{\partial \hat{x}^1} K_{xx} & -m^2 \frac{\partial \hat{x}^3}{\partial z} \frac{\partial h}{\partial \hat{x}^2} K_{yy} & \left(\frac{\partial \hat{x}^3}{\partial z}\right)^2 \left[\left(m \frac{\partial h}{\partial \hat{x}^1}\right)^2 K_{xx} + \left(m \frac{\partial h}{\partial \hat{x}^2}\right)^2 K_{yy} + K_{zz} \right] \end{pmatrix} \quad (6-11).$$

Then the non-zero diffusion terms in Equation 6-7 can be parameterized with the eddy diffusion theory as follows:

$$m^2 \nabla_{\xi} \cdot \left(\overline{\rho q_i \hat{\mathbf{V}}_{\xi} J_{\xi}} \right) = m^2 \frac{\partial}{\partial \hat{x}^1} \left[-\frac{\bar{\rho} J_{\xi}}{m^2} (\hat{K}^{11} \frac{\partial \bar{q}_i}{\partial \hat{x}^1} + \hat{K}^{13} \frac{\partial \bar{q}_i}{\partial \hat{x}^3}) \right] \\ + m^2 \frac{\partial}{\partial \hat{x}^2} \left[-\frac{\bar{\rho} J_{\xi}}{m^2} (\hat{K}^{22} \frac{\partial \bar{q}_i}{\partial \hat{x}^2} + \hat{K}^{23} \frac{\partial \bar{q}_i}{\partial \hat{x}^3}) \right] \quad (6-12)$$

and

$$\frac{\partial (\overline{\rho q_i \hat{v}^3} J_{\xi})}{\partial \hat{x}^3} = \frac{\partial}{\partial \hat{x}^3} \left[-\bar{\rho} J_{\xi} (\hat{K}^{31} \frac{\partial \bar{q}_i}{\partial \hat{x}^1} + \hat{K}^{32} \frac{\partial \bar{q}_i}{\partial \hat{x}^2} + \hat{K}^{33} \frac{\partial \bar{q}_i}{\partial \hat{x}^3}) \right] \quad (6-13)$$

Rewriting Equation 6-7 with Equations 6-12 and 6-13, and separating the diagonal and off-diagonal diffusion terms with an explicit description of the source terms, one can obtain the governing atmospheric diffusion equation in the generalized coordinates where the turbulent flux terms are expressed with the eddy diffusion theory:

$$\begin{aligned}
 & \frac{\partial(\bar{\varphi}_i J_\xi)}{\partial t} + m^2 \nabla_\xi \bullet \left(\frac{\bar{\varphi}_i \hat{\mathbf{V}}_\xi J_\xi}{m^2} \right) + \frac{\partial(\bar{\varphi}_i \hat{v}^3 J_\xi)}{\partial \hat{x}^3} \\
 & \quad \text{(a)} \qquad \qquad \qquad \text{(b)} \qquad \qquad \qquad \text{(c)} \\
 & -m^2 \frac{\partial}{\partial \hat{x}^1} \left[\frac{\bar{\rho} J_\xi}{m^2} (\hat{K}^{11} \frac{\partial \bar{q}_i}{\partial \hat{x}^1}) \right] - m^2 \frac{\partial}{\partial \hat{x}^2} \left[\frac{\bar{\rho} J_\xi}{m^2} (\hat{K}^{22} \frac{\partial \bar{q}_i}{\partial \hat{x}^2}) \right] - \frac{\partial}{\partial \hat{x}^3} \left[\bar{\rho} J_\xi (\hat{K}^{33} \frac{\partial \bar{q}_i}{\partial \hat{x}^3}) \right] \\
 & \quad \qquad \qquad \qquad \qquad \text{(d)} \qquad \qquad \qquad \qquad \qquad \qquad \qquad \text{(e)} \\
 & -m^2 \frac{\partial}{\partial \hat{x}^1} \left[\frac{\bar{\rho} J_\xi}{m^2} (\hat{K}^{13} \frac{\partial \bar{q}_i}{\partial \hat{x}^3}) \right] - m^2 \frac{\partial}{\partial \hat{x}^2} \left[\frac{\bar{\rho} J_\xi}{m^2} (\hat{K}^{23} \frac{\partial \bar{q}_i}{\partial \hat{x}^3}) \right] \\
 & \quad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \text{(f)} \\
 & - \frac{\partial}{\partial \hat{x}^3} \left[\bar{\rho} J_\xi (\hat{K}^{31} \frac{\partial \bar{q}_i}{\partial \hat{x}^1} + \hat{K}^{32} \frac{\partial \bar{q}_i}{\partial \hat{x}^2}) \right] \\
 & \quad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \text{(g)} \\
 & = J_\xi R_{\varphi_i} (\bar{\varphi}_1, \dots, \bar{\varphi}_N) + J_\xi Q_{\varphi_i} + \frac{\partial(\bar{\varphi}_i J_\xi)}{\partial t} \Big|_{cld} + \frac{\partial(\bar{\varphi}_i J_\xi)}{\partial t} \Big|_{aero} + \frac{\partial(\bar{\varphi}_i J_\xi)}{\partial t} \Big|_{ping} \\
 & \quad \text{(h)} \qquad \qquad \text{(i)} \qquad \qquad \text{(j)} \qquad \qquad \text{(k)} \qquad \qquad \text{(l)} \qquad \qquad \qquad \text{(6-14)}
 \end{aligned}$$

The terms in Equation 6-14 are summarized as follows:

- (a) time rate of change of pollutant concentration;
- (b) horizontal advection;
- (c) vertical advection;
- (d) horizontal eddy diffusion (diagonal term);
- (e) vertical eddy diffusion (diagonal term);
- (f) off-diagonal horizontal diffusion;
- (g) off-diagonal vertical diffusion;
- (h) production or loss from chemical reactions;
- (i) emissions;
- (j) cloud mixing and aqueous-phase chemical production or loss;
- (k) aerosol process; and

(1) plume-in-grid process.

Note that the dry deposition process can be included in the vertical diffusion process as a flux boundary condition at the bottom of the model layer.

Alternatively, we can express the turbulent flux terms in Equation 6-7 using the Reynolds flux terms defined as:

$$\overline{q_i'' \hat{u}_\xi''} = \hat{F}_{q_i}^1, \quad \overline{q_i'' \hat{v}_\xi''} = \hat{F}_{q_i}^2, \quad \overline{q_i'' \hat{v}_\xi^3} = \hat{F}_{q_i}^3 \quad (6-15)$$

and the turbulent flux terms are related with the Cartesian counterpart using $\hat{F}_{q_i}^k = \frac{\partial \hat{x}^k}{\partial x^j} F_{q_i}^j$:

$$\hat{F}_{q_i}^1 = mF_{q_i}^x, \quad \hat{F}_{q_i}^2 = mF_{q_i}^y, \quad \hat{F}_{q_i}^3 = \left(\frac{\partial \hat{x}^3}{\partial x}\right)F_{q_i}^x + \left(\frac{\partial \hat{x}^3}{\partial y}\right)F_{q_i}^y + \left(\frac{\partial \hat{x}^3}{\partial z}\right)F_{q_i}^z \quad (6-16)$$

In comparison with Equation 6-14, the Reynolds flux terms shown in Equation 6-15 include the off-diagonal components. One can now rewrite the governing conservation equation for trace species equivalently to Equation 6-14 in terms of the Reynolds flux terms:

$$\begin{aligned} & \frac{\partial(\overline{\varphi_i} J_\xi)}{\partial t} + m^2 \nabla_\xi \cdot \left(\frac{\overline{\varphi_i} \widehat{\mathbf{V}}_\xi J_\xi}{m^2} \right) + \frac{\partial(\overline{\varphi_i} \widehat{v}_\xi^3 J_\xi)}{\partial \hat{x}^3} \\ & + m^2 \frac{\partial}{\partial \hat{x}^1} \left[\frac{\overline{\rho} J_\xi}{m^2} \hat{F}_{q_i}^1 \right] + m^2 \frac{\partial}{\partial \hat{x}^2} \left[\frac{\overline{\rho} J_\xi}{m^2} \hat{F}_{q_i}^2 \right] + \frac{\partial}{\partial \hat{x}^3} \left[\overline{\rho} J_\xi \hat{F}_{q_i}^3 \right] \\ & = J_\xi R_{\varphi_i}(\overline{\varphi}_1, \dots, \overline{\varphi}_N) + J_\xi Q_{\varphi_i} + \left. \frac{\partial(\overline{\varphi_i} J_\xi)}{\partial t} \right|_{cld} + \left. \frac{\partial(\overline{\varphi_i} J_\xi)}{\partial t} \right|_{aero} + \left. \frac{\partial(\overline{\varphi_i} J_\xi)}{\partial t} \right|_{ping} \end{aligned} \quad (6-17)$$

The governing equation can be simplified for a domain with gentle topography for which one may ignore all the terms involved with the horizontal gradients of the surface normal to the vertical coordinate. This forces the vertical diffusion terms in the curvilinear coordinate system to be identical to those of the orthogonal Cartesian coordinate system. Then the trace species conservation equation can be written in a simpler form:

$$\begin{aligned} & \frac{\partial \varphi_i^*}{\partial t} + \widehat{\mathbf{V}}_\xi \cdot \left[\varphi_i^* \widehat{\mathbf{V}}_\xi \right] + \frac{\partial(\varphi_i^* \widehat{v}_\xi^3)}{\partial \hat{x}^3} + \widehat{\mathbf{V}}_\xi \cdot \left[\overline{\rho} \sqrt{\widehat{\gamma}} \widehat{\mathbf{F}}_{q_i} \right] + \frac{\partial(\overline{\rho} \sqrt{\widehat{\gamma}} \widehat{F}_{q_i}^3)}{\partial \hat{x}^3} \\ & = \sqrt{\widehat{\gamma}} R_{\varphi_i}(\overline{\varphi}_1, \dots, \overline{\varphi}_N) + \sqrt{\widehat{\gamma}} S_{\varphi_i} + \left. \frac{\partial(\varphi_i^*)}{\partial t} \right|_{cld} + \left. \frac{\partial(\varphi_i^*)}{\partial t} \right|_{ping} + \left. \frac{\partial(\varphi_i^*)}{\partial t} \right|_{aero} \end{aligned} \quad (6-18)$$

where $\phi_i^* = \sqrt{\hat{\gamma}} \bar{\phi}_i = (J_\xi / m^2) \bar{\phi}_i$. In writing Equation 6-18, we have explicitly identified terms to directly relate to science process modules implemented in the CMAQ. Equation 6-18 is similar to the conservation equation in the generalized coordinates as suggested by Toon et al. (1988).

6.2 Representation of Science Processes in CMAQ Modeling System

This section describes how the CMAQ modeling system is structured to accommodate many different science process modules that provide a one-atmosphere, multiscale and multi-pollutant modeling capability to the CMAQ system. First, we describe the modularity concepts and key science processes implemented in the current version of CMAQ. Then the governing fractional time-step formulation for each science process is presented.

6.2.1 Supporting Models and Interface Processors

Key supporting models for the current version of the CMAQ modeling system are the Mesoscale Model Version 5 (MM5) (Seaman et al., 1995) and Models-3 Emissions Processing and Projection System (MEPPS). The CMAQ modeling system is comprised of the main CMAQ chemical transport model (CCTM) and several interface processors that link other model input data to the CCTM. The Meteorology-Chemistry Interface Processor (MCIP) processes MM5 output to provide a complete set of meteorological data required for CCTM. MCIP is designed in such a way that other meteorological models can be linked with minimal effort. Initial and boundary conditions are generated with the ICON and BCON processors, respectively, and the Emissions-Chemistry Interface Processor (ECIP) combines area and point source emissions to generate three-dimensional gridded emissions data for CCTM. In addition, a plume dynamics model (PDM) is used to provide dimensions and positions of plumes from major elevated point-sources. The PDM data are used for driving the plume-in-grid processing in CCTM. A photolytic rate constant processor (JPROC) which is based on the RADM (Chang et al., 1987) approach, computes species specific photolysis rates for a set of predefined zenith angles, latitude, and altitudes. An alternative detailed-science version adopts state-of-the-science radiative transfer models that can take into account the total ozone column (TOMS data) and turbidity. Refer to Table 6-1 for the list of the interface processors in CMAQ and Figure 6-1 for the data linkage among these interface processors.

By assembling appropriate science modules available in the CMAQ system, users can build a specific CCTM's that may include all or some of the critical science processes, such as atmospheric transport, deposition, cloud mixing, emissions, gas- and aqueous-phase chemical transformations, and aerosol dynamics and chemistry. One of the features of CMAQ that distinguishes it from other air quality models is the hierarchical functional modularity of the science processor codes. We define the levels of modularity in the science model based on the granularity of the modeling components. The coarsest level of modularity is the distinction between the system framework and science models. The second level is the division of science sub-models (MM5, MEPPS, and CMAQ). The third level of modularity involves a driver module, processor modules, data provider modules, and a utility module (a collection of assisting

subroutines) in a CTM. While the emissions processing and the meteorology model are modular at the second level, the CCTM achieves the third-level of modularity by employing the operator splitting, or fractional time step, concept in the science processes. The next level of modularity is based on the computational functionality in a processor module, e.g., science parameterization, numerical solver, processor analysis, and input/output routines. The lowest meaningful modularization level is the isolation of sections of code that can benefit from machine dependent optimization.

6.2.2 Modularity Concept of CMAQ

To allow for both the continuous improvement of science and for the addition of new capabilities in a unified fashion, it is critical to have efficient modular schemes in the CMAQ design. Currently, the modularity within CMAQ is based mostly on the fractional time-step implementation of the science processes. This level of modularity involves the distinction of a driver, processor modules, data provider modules, and utility subroutines in CMAQ. We have chosen this method because it provides a natural disciplinary distinction for different science processes through which developments in specific research areas can readily be incorporated (Refer to Figure 6-2).

In some of the process modules, such as the aqueous-phase chemistry module, the science algorithms and numerical solvers are tightly linked. For other types of modules, the science parameterization components and numerical solvers have a looser association. In such cases the modularity can be defined either at the parameterization level, the numerical algorithm level, or both. For example, the module definition for the advection process is based on the numerical advection algorithm used. For the gas-phase chemistry process, the modularity is based on the ordinary differential equation numerical solvers. The chemistry mechanism description is generalized and the Models-3/CMAQ framework provides a straightforward method to link model species surrogate names with the species names in the data set. See Chapter 15 for details. The use of different chemical mechanisms is accommodated through the mechanism reader and generalized codes for setting up the production and loss terms of the chemistry reactions. Therefore, the CCTM does not require different gas-phase chemistry modules for different mechanisms.

The vertical diffusion process can be formulated using either local- or non-local-mixing parameterization schemes. The current classification of vertical diffusion modules is based on the process parameterization methods. The modularity of this process can be enhanced if we distinguish the method used for computing the vertical diffusivities for local-mixing. In this case, the modularity is defined at the level of data provider modules. The modularity level can be deepened further if we identify different numerical solution methods for the diffusion.

With the current version of CMAQ, the level of science modularity is subordinated by the way the science process codes are archived in the system. Here, we define a class as a collection of different modules for a given science process. The science classes are identified with the grouping

of the terms in the governing conservation equation, Equation 6-18. Currently, nine science process classes are defined in CCTM:

- **DRIVER** controls model data flows and synchronizes fractional time steps;
- **HADV** computes the effects of horizontal advection;
- **VADV** computes the effects of vertical advection;
- **ADJCON** adjusts mixing ratio conservation property of advection processes;
- **HDIFF** computes the effects of horizontal diffusion;
- **VDIFF** computes the effects of vertical diffusion and deposition;
- **CHEM** computes the effects of gas-phase chemical reactions;
- **CLOUD** computes the effects of aqueous-phase reactions and cloud mixing;
- **AERO** computes aerosol dynamics and size distributions; and
- **PING** computes the effects of plume chemistry.

CCTM does not have emissions as a separate science process because it can be either a part of the vertical diffusion or the gas-phase chemical reaction process. It is worthwhile to mention here that the current modular paradigm does not prevent establishment of combination of processes in a larger single module. For example, one can develop a module describing the vertical transport, chemistry, and emissions simultaneously when time scales of those processes become comparable. Users could experiment with the combination of modules to best fit to their problems at hand.

In addition to nine science process modules, CCTM includes two science process classes. The PHOT computes photolysis rates, and AERO_DEPV computes particle size-dependent dry deposition velocities. These are typical “data-provider” science process classes, which do not involve updating concentrations directly. There are some other classes that do not fall in any of the above definitions. We have grouped these auxiliary routines as the UTIL class, which is a collection of utility subroutines. As one can see, the current modularity of the CCTM is implemented more on a practical basis rather than by strictly following a design paradigm. One can also see that the present modularity definition of CMAQ is somewhat subjective. In the future we intend to allow definition of the modularity at the user-defined granularity level.

Figure 6-1 describes the key science process modules in CCTM and their data linkage with CMAQ’s preprocessors, whose descriptions are available in other chapters. The only data dependencies among the CCTM science modules are the trace species concentration field as seen in the diagram and the model integration time step. Figure 6-2 shows the distinct data

dependencies within the CCTM. To facilitate modularity and to minimize data dependency in CCTM, we store concentrations in global memory while the environmental input data are obtained from random-access files and interpolated to the appropriate computational (synchronization) time step. This realizes the recommended “thin-interface” structure of the model:

- Common timing data are managed through the science process main subroutine’s call arguments;
- Concentrations are the object of all process operations;
- Environmental data are provided through a standard I/O interface;
- Model structure data are provided through shared include files; and
- Standard physical constants are obtained from shared include files.

See Chapter 18 for further details on how the science codes are integrated in the Models-3 CMAQ system.

CMAQ Science Processors

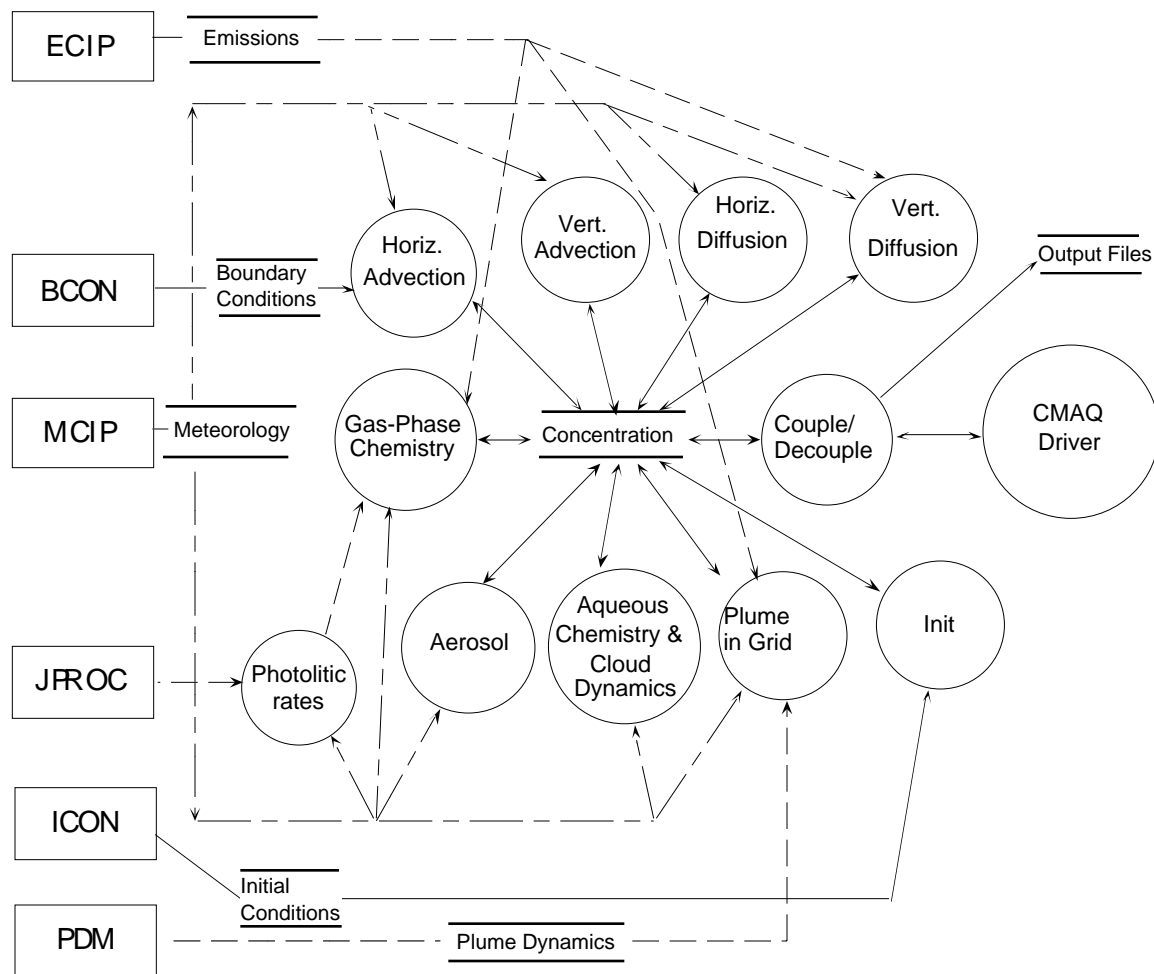


Figure 6-1. Science Process Modules in CMAQ. Interface processes are shown with rectangular boxes. Typical science process modules are updating the concentration field directly and the data-provider modules include routines to feed appropriate environmental input data to the science process modules. Driver module orchestrates the synchronization of numerical integration across the science processes. Concentrations are linked with solid lines and other environmental data with broken lines. (From Byun et al., 1998.)

Table 6-1. Interface Processors for the CMAQ Modeling System

Interface Processor	Description	Reference
ICON	Provides initial three-dimensional fields of trace species concentrations for modeling domain	Chapter 13
BCON	Provides concentrations of trace species for the boundary cells	Chapter 13
ECIP	Incorporates emissions from separate area and major point sources to generate hourly 3-D emissions input file	Chapter 3
MCIP	Processes the output of a meteorological model to provide the necessary meteorological data for CMAQ models	Chapter 12
JPROC	Computes photolysis rates for various altitudes, latitudes, and sun zenith angle	Chapter 14
PDM	Generates plume information needed to apply plume-in-grid (PinG) processing in CCTM	Chapter 9

6.2.3 Description of Science Processes

In this section we describe individual science processes, shown in Figure 6-1, associated with the groups of individual terms in the governing diffusion equation. Note that different concentration units are used for different science processes in CMAQ CTMs. Appendix 6A provides the relationships among the concentration units and their conversion factors from one unit to another.

CMAQ CTM 's Data Flow

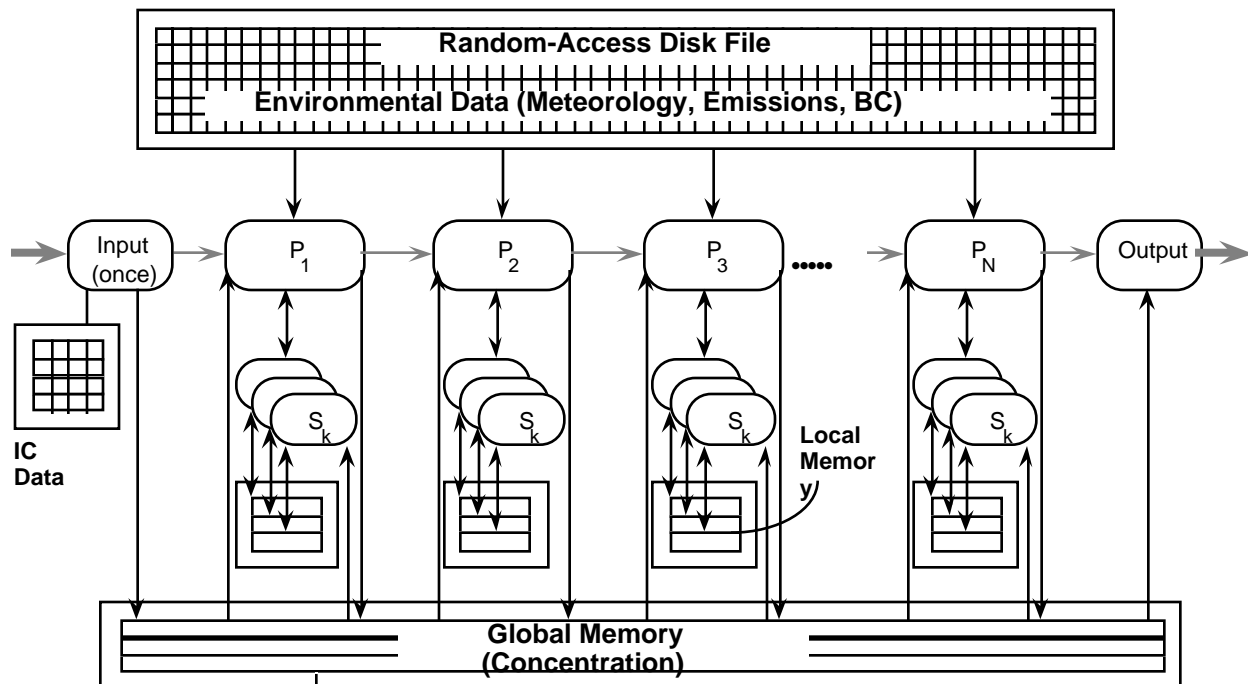


Figure 6-2. Data Dependencies Among Modules in CCTM. P and S_k represent a science process module and the related subroutines for the module, respectively. (From Byun et al., 1995.)

6.2.3.1 Driver Class for CCTM

The key function of the driver class module is hosting the science processors. It is responsible for coordinating model integration time (synchronizing fractional-time steps of science process call) and some input/output sequences. The driver structure of the current CCTM is given in Figure 6-3. A synchronization time step is used to ensure the global stability of the CCTM's numerical integration at the advection time step, which is based on a Courant number limit. Nesting requires finer synchronization time steps for the fine grid domain. The CCTM's process synchronization time steps are represented as integer seconds because the Models-3 I/O API can only handle integer seconds for I/O data. All the needed data are appropriately interpolated based on the synchronization time step. For maintaining numerical stability and for other reasons, an individual process module may have its own internal time steps. In general, each science process module uses the synchronization time step (Δt_{sync}) as the input time step of required environmental data. The global output time steps can be set differently from the

synchronization time step. Usually, the output time step (Δt_{out}) is set as one hour, but sub-hourly output down to the synchronization time step is possible.

Table 6-2. List of Science Process Subroutines Called by the CMAQ Driver

Subroutine	Science Class	Description
CGRID_MAP	UTIL	Sets up pointers for different concentration species: gas chemistry, aerosol, non-reactive, and tracer species
INITSCEN	INIT*	Initializes simulation time period, time stepping constants, and concentration arrays for the driver
ADVSTEP	DRIVER	Computes the model synchronization time step and number of repetitions for the output time step
COUPLE/ DECOUPLE	COUPLE*	Converts units and couples or de-couples concentration values with the density and Jacobian for transport
SCIPROC	DRIVER	Controls all of the physical and chemical processes for a grid (currently, two versions are available: symmetric and asymmetric around the chemistry processes)
XADV, YADV ZADV	HADV VADV	Computes advection in horizontal plane (x- and y-directions) Computes advection in the vertical direction in the generalized coordinate system
ADJADV	ADJCON	Adjusts concentration fields to ensure mixing ratio conservation given mass consistency error in meteorology data
HDIFF	HDIFF	Computes horizontal diffusion
VDIFF	VDIFF	Computes vertical diffusion and deposition
CHEM	CHEM	Solves gas-phase chemistry
PING	PING	Computes effects of plume-in-grid process
AERO	AERO	Computes aerosol dynamics, particle formation, and deposition
CLDPRC	CLOUD	Computes cloud mixing and aqueous chemistry

* represents a process class that is part of DRIVER function.

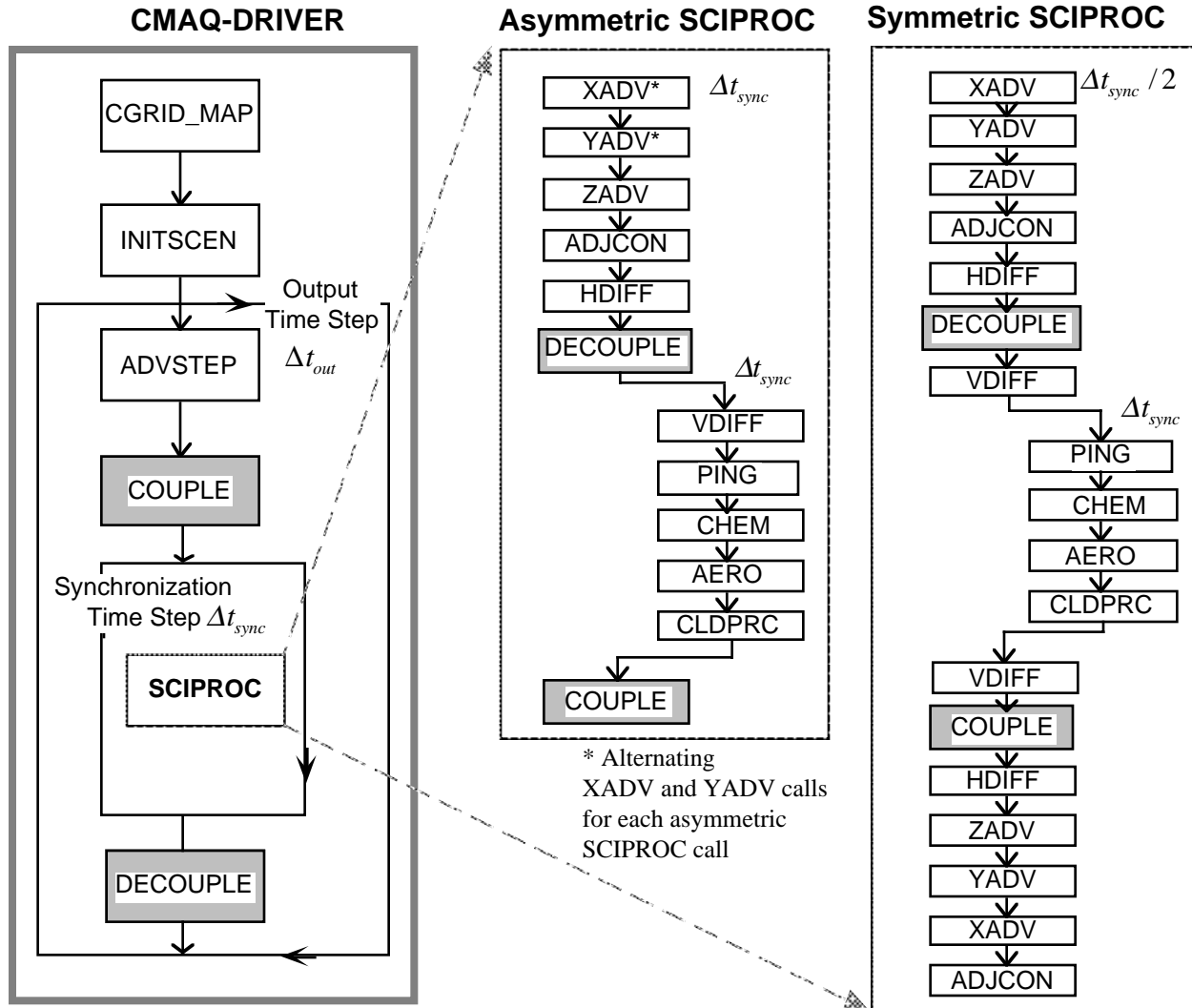


Figure 6-3. Driver Module and Its Science Process Call Sequence.

Both asymmetric and symmetric call sequences in SCIPROC are presented. Δt_{sync} and Δt_{out} are model synchronization and output time steps, respectively. Refer to Table 6-2 for the description of the subroutines.

The DRIVER program calls initialization routines to set up CCTM runs. It initializes the concentration field and checks if the input files, run time, and grid/coordinate information are consistent for a given scenario. Subroutines used for the initialization process are grouped into the INIT class. Usually, initial concentrations for gaseous species are in molar mixing ratio units (ppm) and aerosol species in density units ($\mu\text{g m}^{-3}$), the same as the output units of CMAQ. Also, DRIVER calls couple/decouple subroutines to convert concentration units for appropriate data processing. The pair of couple/decouple calls, which are available in the class COUPLE, limit the interchange of process modules between two different concentration units, such as density versus mixing ratio. The classes INIT and COUPLE are introduced just for the

convenience of code management from the point of view of science process modularity, and they should be considered as part of the DRIVER class modules.

6.2.3.2 Advection Processes for CCTM: HADV, VADV and ADJCON

For convenience, the advection process is divided into horizontal and vertical components. This distinction is possible because the mean atmospheric motion is mostly in horizontal planes. Usually the vertical motion is related with the interaction of dynamics and thermodynamics. The advection process relies on the mass conservation characteristics of the continuity equation:

$$\frac{\partial(\sqrt{\hat{\gamma}}\bar{\varphi}_i)}{\partial t} = -\nabla_{\xi} \cdot \left(\sqrt{\hat{\gamma}}\bar{\varphi}_i \bar{\mathbf{V}}_{\xi} \right) - \frac{\partial(\sqrt{\hat{\gamma}}\bar{\varphi}_i \hat{v}^3)}{\partial \hat{x}^3} \quad (6-19)$$

Using the dynamically and thermodynamically consistent meteorology data from MCIP, we can maintain data consistency for air quality simulations at the synchronization time step. In case the meteorological data provided and the numerical advection algorithms are not exactly mass consistent, we need to solve a modified advection equation:

$$\frac{\partial(\sqrt{\hat{\gamma}}\bar{\varphi}_i)}{\partial t} = -\nabla_{\xi} \cdot \left(\sqrt{\hat{\gamma}}\bar{\varphi}_i \bar{\mathbf{V}}_{\xi} \right) - \frac{\partial(\sqrt{\hat{\gamma}}\bar{\varphi}_i \hat{v}^3)}{\partial \hat{x}^3} + \bar{\varphi}_i \sqrt{\hat{\gamma}} \frac{Q_p}{\rho} \quad (6-20)$$

where Q_p is mass consistency error term (Byun, 1999). Equation 6-20 ensures conservation of mixing ratio, which is a necessary (though not sufficient) condition for preserving total tracer mass given significant fluctuations of density field in space and time. The equation shows that the correction term has the same form as a first-order chemical reaction whose reaction rate is determined by the mass consistency error (normalized with air density) in the meteorology data.

Modules in HADV class solve for the horizontal advection:

$$\frac{\partial(\sqrt{\hat{\gamma}}\bar{\varphi}_i)}{\partial t} = -\nabla_{\xi} \cdot \left(\sqrt{\hat{\gamma}}\bar{\varphi}_i \bar{\mathbf{V}}_{\xi} \right) \quad (6-21)$$

and modules in VADV class solve for the vertical advection with boundary conditions $\hat{v}^3 = 0$ at the bottom and top of the model.

$$\frac{\partial(\sqrt{\hat{\gamma}}\bar{\varphi}_i)}{\partial t} = - \frac{\partial(\sqrt{\hat{\gamma}}\bar{\varphi}_i \hat{v}^3)}{\partial \hat{x}^3} \quad (6-22)$$

In simulating air quality, one of fundamental characteristic of the model application should be conservation of mass. Therefore, the modules in the ADJCON class solve for the mass correction term:

$$\frac{\partial(\sqrt{\hat{\gamma}}\bar{\varphi}_i)}{\partial t} = \bar{\varphi}_i \sqrt{\hat{\gamma}} \frac{Q_p}{\rho} \quad (6-23)$$

We wish to emphasize that the artificial distinction of advection modules between horizontal and vertical processes is not adequate and that all three modules (HADV, VADV, and ADJCON) should be considered as an integral unit for solving the physical advection process of trace species. The advection and mass adjustment algorithms are described in detail in Chapter 7.

6.2.3.3 Diffusion Process Classes for CCTM: HDIFF and VDIFF

For convenience the atmospheric diffusion process is divided into horizontal and vertical components. This distinction is needed because the vertical diffusion mostly represents the thermodynamic influence on the atmospheric turbulence by the air-surface energy exchange processes while the horizontal diffusion represents subgrid scale mixing due to the unresolved wind fluctuations. To handle the atmospheric diffusion processes in the generalized coordinates, we need to carefully examine the governing equation to properly set up the diffusion solver.

We start from the atmospheric diffusion equation in the same concentration units as used in advection:

$$\left. \frac{\partial \varphi_i^*}{\partial t} \right|_{diff} = \left. \frac{\partial (\sqrt{\hat{\gamma}} \bar{\rho} \bar{q}_i)}{\partial t} \right|_{diff} = -\hat{\mathbf{V}}_s \cdot [\sqrt{\hat{\gamma}} \bar{\rho} \hat{\mathbf{F}}_{q_i}] - \frac{\partial (\sqrt{\hat{\gamma}} \bar{\rho} \hat{F}_{q_i}^3)}{\partial \hat{x}^3} + \sqrt{\hat{\gamma}} \bar{\rho} \left(\frac{Q_{\varphi_i}}{\bar{\rho}} \right) \quad (6-24)$$

where $\varphi_i^* = \sqrt{\hat{\gamma}} \bar{\varphi}_i$, and the term $(Q_{\varphi_i} / \bar{\rho})$ is the time rate change of mass mixing ratio due to emissions of species i . Initially, it is assumed that we can decompose the diffusion into the horizontal and vertical components with respect to the curvilinear coordinates:

$$\left. \frac{\partial \varphi_i^*}{\partial t} \right|_{hdiff} = \left. \frac{\partial (\sqrt{\hat{\gamma}} \bar{\rho} \bar{q}_i)}{\partial t} \right|_{hdiff} = -\hat{\mathbf{V}}_\xi \cdot [\sqrt{\hat{\gamma}} \bar{\rho} \hat{\mathbf{F}}_{q_i}] \quad (6-25)$$

$$\left. \frac{\partial \varphi_i^*}{\partial t} \right|_{vdiff} = \left. \frac{\partial (\sqrt{\hat{\gamma}} \bar{\rho} \bar{q}_i)}{\partial t} \right|_{vdiff} = -\frac{\partial (\sqrt{\hat{\gamma}} \bar{\rho} \hat{F}_{q_i}^3)}{\partial \hat{x}^3} + \sqrt{\hat{\gamma}} \bar{\rho} \left(\frac{Q_{\varphi_i}}{\bar{\rho}} \right) \quad (6-26)$$

Emissions can be included either in vertical diffusion or gas-phase chemistry module. If we can parameterize the turbulent fluxes directly in the curvilinear coordinates, we can implement HDIFF and VDIFF modules following Equations 6-25 and 6-26. When the turbulent fluxes are parameterized with eddy diffusion theory, the contributions of the off-diagonal (cross-directional) diffusion terms show up explicitly as shown in Equation 6-14:

$$\left. \frac{\partial \varphi_i^*}{\partial t} \right|_{cdiff} = \frac{\partial}{\partial \hat{x}^1} \left[\sqrt{\hat{\gamma}} \bar{\rho} (\hat{K}^{13} \frac{\partial \bar{q}_i}{\partial \hat{x}^3}) \right] + \frac{\partial}{\partial \hat{x}^2} \left[\sqrt{\hat{\gamma}} \bar{\rho} (\hat{K}^{23} \frac{\partial \bar{q}_i}{\partial \hat{x}^3}) \right]$$

$$+ \frac{\partial}{\partial \hat{x}^3} \left[\sqrt{\hat{\gamma} \bar{\rho}} \left(\hat{K}^{31} \frac{\partial \bar{q}_i}{\partial \hat{x}^1} + \hat{K}^{32} \frac{\partial \bar{q}_i}{\partial \hat{x}^2} \right) \right] \quad (6-27)$$

For a domain with a significant topographic feature, the module CDIFF must be implemented. However, the current CMAQ version does not include CDIFF module as the off-diagonal terms are often neglected in operational air quality models. In such a case, the HDIFF and VDIFF modules solve for diagonal terms (with respect to the curvilinear coordinates) as follows:

$$\left. \frac{\partial \varphi_i^*}{\partial t} \right|_{\text{hdiff}} = \frac{\partial}{\partial \hat{x}^1} \left[\sqrt{\hat{\gamma} \bar{\rho}} \left(\hat{K}^{11} \frac{\partial \bar{q}_i}{\partial \hat{x}^1} \right) \right] + \frac{\partial}{\partial \hat{x}^2} \left[\sqrt{\hat{\gamma} \bar{\rho}} \left(\hat{K}^{22} \frac{\partial \bar{q}_i}{\partial \hat{x}^2} \right) \right] \quad (6-25')$$

$$\left. \frac{\partial \varphi_i^*}{\partial t} \right|_{\text{vdiff}} = \frac{\partial}{\partial \hat{x}^3} \left[\sqrt{\hat{\gamma} \bar{\rho}} \left(\hat{K}^{33} \frac{\partial \bar{q}_i}{\partial \hat{x}^3} \right) \right] \quad (6-26')$$

Compared with above formulations, let's consider the case that we approximate the quantity $\sqrt{\hat{\gamma} \bar{\rho}}$, which defines the computational grid, to be constant for the duration of synchronization time step for integrating the diffusion process with the fractional time-step method. Then, the problem becomes equivalent to solving for the diffusion equations in terms of the mass mixing ratio instead of density:

$$\left. \frac{\partial \bar{q}_i}{\partial t} \right|_{\text{diff}} = -\hat{V}_\xi \cdot [\hat{\mathbf{F}}_{q_i}] - \frac{\partial(\hat{F}_{q_i}^3)}{\partial \hat{x}^3} + \left(\frac{Q_{\varphi_i}}{\bar{\rho}} \right) - \hat{\mathbf{F}}_{q_i} \cdot \hat{V}_\xi \left[\ln(\sqrt{\hat{\gamma} \bar{\rho}}) \right] - \hat{F}_{q_i}^3 \frac{\partial \left[\ln(\sqrt{\hat{\gamma} \bar{\rho}}) \right]}{\partial \hat{x}^3} \quad (6-28)$$

If we rely on Equation 6-28 for representing the atmospheric diffusion process, the concentration must first be decoupled to obtain mass mixing ratio, q_i . Once the new mixing ratio is computed, it needs to be coupled with $\sqrt{\hat{\gamma} \bar{\rho}}$ to give the updated concentration in terms of φ_i^* . This means that the operator for the horizontal diffusion process should compute:

$$\left. \frac{\partial \bar{q}_i}{\partial t} \right|_{\text{hdiff}} = -\hat{V}_\xi \cdot [\hat{\mathbf{F}}_{q_i}] - \hat{\mathbf{F}}_{q_i} \cdot \hat{V}_\xi \left[\ln(\sqrt{\hat{\gamma} \bar{\rho}}) \right] \quad (6-29)$$

and the vertical diffusion process should solve for:

$$\left. \frac{\partial \bar{q}_i}{\partial t} \right|_{\text{vdiff}} = -\frac{\partial(\hat{F}_{q_i}^3)}{\partial \hat{x}^3} + \left(\frac{Q_{\varphi_i}}{\bar{\rho}} \right) - \hat{F}_{q_i}^3 \frac{\partial \left[\ln(\sqrt{\hat{\gamma} \bar{\rho}}) \right]}{\partial \hat{x}^3} \quad (6-30)$$

This approach is more convenient in numerically solving the flux-form turbulence mixing representation because most of the flux-based closure algorithms use parameterizations of turbulent fluxes in terms of conserving quantities, such as the mass mixing ratio, q_i . A considerable amount of meteorological and air quality literature on turbulence diffusion fails to clarify this important point. Especially for the case of multiscale applications, the representation of diffusion in terms of a conserving quantity is critical as shown by Venkatram (1993).

The effects of turbulence flux caused by the divergence of the grid boxes in the coordinate system need to be included in order to describe the turbulence exchange processes precisely. One can readily show that the coordinate-divergence term in Equation 6-30 vanishes for a mass conserving vertical coordinate. Similarly, when topographical features vary significantly and horizontal variations of the quantity $\sqrt{\hat{\gamma}\bar{\rho}}$ are large, one cannot neglect the last term in Equation 6-29. Chapter 7 of this document describes physical parameterization schemes and numerical algorithms for the horizontal and vertical diffusion processes in the CCTM.

One may wonder how deposition should be represented in the generalized coordinate system. In Eulerian air quality models, the deposition process affects the concentration in the lowest layer as a boundary flux condition. Considering the deposition process as the diffusion flux at the bottom of the model, we can relate the boundary condition in the generalized coordinate system to that of the Cartesian coordinate system as:

$$\hat{F}_{q_i}^3 \Big|_{dep} = \left(\frac{\partial \hat{x}^3}{\partial x} \right) F_{q_i}^x \Big|_{dep} + \left(\frac{\partial \hat{x}^3}{\partial y} \right) F_{q_i}^y \Big|_{dep} + \left(\frac{\partial \hat{x}^3}{\partial z} \right) F_{q_i}^z \Big|_{dep} = \left(\frac{\partial \hat{x}^3}{\partial z} \right) F_{q_i}^z \Big|_{dep} \quad (6-31)$$

because $F_{q_i}^x \Big|_{dep}$ and $F_{q_i}^y \Big|_{dep}$ do not exist. Then, the effects of dry deposition on the species concentration is accounted for by the following relationship:

$$\begin{aligned} \frac{\partial \phi_i^*}{\partial t} \Big|_{dep} &= \frac{\partial (\sqrt{\hat{\gamma}\bar{\rho}} \bar{q}_i)}{\partial t} \Big|_{dep} = - \frac{\partial (\sqrt{\hat{\gamma}\bar{\rho}} \hat{F}_{q_i}^3)}{\partial \hat{x}^3} \Big|_{dep} = - \frac{\partial}{\partial \hat{x}^3} \left(\sqrt{\hat{\gamma}\bar{\rho}} \left(\frac{\partial \hat{x}^3}{\partial z} \right) F_{q_i}^z \right) \Big|_{dep} \\ &\approx - \frac{\left(\frac{\partial \hat{x}^3}{\partial z} \right)_{dep} (\sqrt{\hat{\gamma}\bar{\rho}}) (F_{q_i}^z)_{dep}}{(\Delta \hat{x}^3)_{dep}} = - \frac{v_d}{h_{dep}} (\sqrt{\hat{\gamma}\bar{\rho}}) \bar{q}_i \Big|_{layer1} = - \frac{v_d}{h_{dep}} \phi_i^* \Big|_{layer1} \end{aligned} \quad (6-32)$$

where $h_{dep} = \left(\frac{\partial z}{\partial \hat{x}^3} \right)_{dep} (\Delta \hat{x}^3)_{dep}$ is the thickness of the lowest model layer in the geometric height coordinate. In the derivation of Equation 6-32, we assume that the deposition flux is constant in the lower part of the surface layer (i.e., a constant flux layer). Thus, the deposition velocities are computed at the middle (in terms of the generalized coordinate, ξ) of the lowest model layer at which the concentrations are represented. For the case in which the mass mixing ratio is used as the concentration variable for solving the diffusion equation, the deposition should be implemented as a boundary condition for the vertical diffusion (VDIFF) in the following manner:

$$\frac{\partial \bar{q}_i}{\partial t} \Big|_{dep} = - \frac{\partial (\hat{F}_{q_i}^3)}{\partial \hat{x}^3} \Big|_{dep} = - \frac{\partial}{\partial \hat{x}^3} \left(\left(\frac{\partial \hat{x}^3}{\partial z} \right) F_{q_i}^z \right) \Big|_{dep} \quad (6-33)$$

Therefore, the bottom boundary condition for the VDIFF module is given as:

$$\left. \frac{\partial \bar{q}_i}{\partial t} \right|_{dep} = -\frac{\partial}{\partial \hat{x}^3} \left(\left(\frac{\partial \hat{x}^3}{\partial z} \right) F_{q_i}^z \right)_{dep} \approx -\frac{\left(\frac{\partial \hat{x}^3}{\partial z} \right)_{bottom} (F_{q_i}^z)_{dep}}{(\Delta \hat{x}^3)_{dep}} = \frac{(F_{q_i}^z)_{dep}}{h_{dep}} = -\frac{v_d}{h_{dep}} \bar{q}_i \Big|_{layer1} \quad (6-33')$$

Equations 6-32 and 6-33 show that we do not need to estimate contravariant deposition velocities if the deposition process is implemented as a bottom boundary condition in the generalized coordinate formulation.

In the current CCTM implementation, the concentration units for horizontal and vertical diffusion processes are density (coupled with Jacobian) and molar mixing ratio, $m_i = q_i \frac{M_{air}}{M_i}$, respectively. We have chosen m_i as the generic concentration unit for the vertical diffusion to coordinate with the emissions units in the data. Subsection 6.2.3.6 provides a detailed explanation for this. Therefore, HDIFF is placed outside and VDIFF is placed in between the pair of couple/decouple calls. Because the ratio of molecular weights are constant, equations for the vertical diffusion in terms of molar mixing ratio are equivalent to those in terms of mass mixing ratio, q_i . Refer to Chapter 7 for details of the computational algorithms for HDIFF and VDIFF.

6.2.3.4 Gas-phase Chemistry Process for CCTM

Instead of directly computing the time rate of change of φ_i^* , as is given by:

$$\left. \frac{\partial (\varphi_i^*)}{\partial t} \right|_{chem} = \sqrt{\hat{\gamma}} R_{\varphi_i} (\bar{\varphi}_1, \dots, \bar{\varphi}_N) + \sqrt{\hat{\gamma}} Q_{\varphi_i} \quad (6-34),$$

we need to decouple the Jacobian and air density in $\sqrt{\hat{\gamma}} \bar{\varphi}_i$ before computing gas-phase chemistry. This is useful because we can approximate that the computational grid remains constant for the duration of a synchronization time step, which is set by the Courant conditions for the fractional time step numerical integration schemes. Because the concentration unit required in the gas-phase chemistry is the volumetric mixing ratio, we rewrite the concentration φ_i^* as follows:

$$\begin{aligned} \varphi_i^* &= \sqrt{\hat{\gamma}} \bar{\varphi}_i = \sqrt{\hat{\gamma}} \bar{\rho} \bar{q}_i \frac{M_{air}}{M_i} \frac{M_i}{M_{air}} = \bar{q}_i \frac{M_{air}}{M_i} \left[\sqrt{\hat{\gamma}} \bar{\rho} \frac{M_i}{M_{air}} \right] \\ &= \bar{m}_i \left[\sqrt{\hat{\gamma}} \bar{\rho} \frac{M_i}{M_{air}} \right] \end{aligned} \quad (6-35)$$

where $\bar{m}_i = \bar{q}_i \frac{M_{air}}{M_i}$ is used as the definition of the volumetric or molar mixing ratio. The time rate of change of the volumetric mixing ratio due to the gas-phase chemistry is evaluated with the following equation:

$$\left. \frac{\partial \bar{m}_i}{\partial t} \right|_{chem} = \hat{R}_{m_i}(\bar{m}_1, \dots, \bar{m}_N) + \hat{Q}_{m_i}(\bar{m}_i) \quad (6-36)$$

where \hat{R}_{m_i} and \hat{Q}_{m_i} represent chemistry reactions and source terms in molar mixing ratio units, respectively.

CMAQ employs generalized chemistry solvers, such as QSSA (Young et al., 1993) and SMVGEAR (Jacobson and Turco, 1994), which are designed to solve the nonlinear set of stiff ordinary equations presented in Equation 6-36. They can be applied independent of the coordinate and grid descriptions. To accommodate the need for modified or new chemical mechanisms, the CMAQ system is equipped with a generalized chemical mechanism processor. Refer to Chapter 8 for detailed description of numerical solvers used for gas-phase chemistry.

The Models-3 framework provides a mapping table to link chemistry mechanism species with surrogate species names in the initial and boundary condition files and emissions files. See Chapter 15 for details. When a new mechanism is used, appropriate emissions data must be supplied. It is possible to include emissions either in the gas-phase chemistry or in the vertical diffusion process. It is preferable that the emissions are interpolated with the same temporal interpolation schemes used in the transport processes.

6.2.3.5 Aerosol Process Class for CCTM

The fractional time step implementation solves for the effects of aerosol chemistry and dynamics on trace gas and aerosol species concentrations with:

$$\left. \frac{\partial \varphi_i^*}{\partial t} \right|_{aero} = \sqrt{\hat{\gamma}} R_{aero_i}(\bar{\varphi}_1, \dots, \bar{\varphi}_N) + \sqrt{\hat{\gamma}} Q_{aero_i} - \hat{v}_g \frac{\partial \varphi_i^*}{\partial \xi} \quad (6-37)$$

where R_{aero_i} represents processes such as new particle formation and growth and depletion of existing particles. Q_{aero_i} stands for all the external sink and source terms, and \hat{v}_g is the contravariant sedimentation velocity. The generic concentration units for the aerosol process are [$\mu\text{g m}^{-3}$] (density) for aerosol mass and [number m^{-3}] for aerosol particle number density. Because the aerosol process is called within the pair of couple/decouple calls, the input concentration is already decoupled and the following set of governing equations are solved in the aerosol process module:

$$\left. \frac{\partial \varphi_i}{\partial t} \right|_{aero} = R_{aero_i}(\bar{\varphi}_1, \dots, \bar{\varphi}_N) + Q_{aero_i} - \hat{v}_g \frac{\partial \varphi_i}{\partial \xi} \quad (6-38)$$

The present implementation of the aerosol module in CCTM is derived from the Regional Particulate Model (Binkowski and Shankar, 1995). Here, primary particles are divided into two groups: fine particles and coarse particles. The fine particles result from combustion and secondary production processes and the coarse group is composed of materials such as wind-

blown dust and marine particles. The key scientific algorithms simulating aerosol processes for the CCTM are: (1) aerosol removal by size-dependent dry deposition; (2) aerosol-cloud droplet interaction and removal by precipitation; (3) new particle formation by binary homogeneous nucleation in a sulfuric acid/water vapor system; (4) the production of an organic aerosol component from gas-phase precursors; and (5) particle coagulation and condensation growth. Refer to Chapter 10 for details on aerosol process implemented in CCTM.

6.2.3.6 Emissions Process for CCTM

As mentioned earlier, the emissions process does not have its own science process class. Instead, it is included either in vertical diffusion or in the gas-phase chemistry process. In the governing conservation equations for the trace gases, the emissions process is represented simply as source terms.

If emissions data are given in the unit of time rate of change of mass, for example for particulate species, such as PM2.5 and PM10 in [$g\ s^{-1}$], they are expressed as:

$$Q_{\varphi_i} = \frac{E_i}{\delta V} = \frac{1}{\delta V} \left. \frac{\partial(\varphi_i \delta V)}{\partial t} \right|_{emis} = \frac{1}{\delta V} \left. \frac{\partial(\rho q_i \delta V)}{\partial t} \right|_{emis} \quad (6-39)$$

where δV is volume of the cell and $E_i = \left. \frac{\partial(\varphi_i \delta V)}{\partial t} \right|_{emis}$ represents the emissions rate into the cell. If the mass of air in the cell does not change for each time step (usually one hour), the concentration expression, either as the time rate of change of density or as the mass mixing ratio can be used. Otherwise, when the volume and density of a cell change substantially with time, the effect of change in air mass must be accounted for in determining the emissions rates.

For gaseous species, the time rate of change of E_i for each hour and each grid cell are provided in the three-dimensional emissions data files in molar units, (i.e., $mole\ s^{-1}$):

$$E_i = \left(\frac{M_{air}}{M_i} \frac{Q_{\varphi_i}}{\rho} \right) \delta V \quad (6-40)$$

Emissions for gaseous species in molar units are preferred to those in mass units because molar units are the natural units for chemistry and mass units must be transformed into [$mole\ s^{-1}$] eventually for the gas-phase chemistry process. For gaseous species the molar mixing ratio and mass mixing ratio differ only by a simple multiplication factor, the ratio of molecular weights. However, for lumped species, the molecular weights are variable depending on the fractional compositions of the categorized hydrocarbon species in the emissions data. Therefore, transformation of emissions in mass units into the molar units for the lumped species can introduce misrepresentation of emissions amount. The data for the fractional compositions of the categorized hydrocarbon species are available in the emissions processor, Models-3 Emissions Projection and Processing System (MEPPS) (See Chapter 4). Thus, when emissions

data are processed in [*mole s⁻¹*] units, we do not have this conversion problem. Then the emissions process is represented as:

$$\left. \frac{\partial \bar{m}_i}{\partial t} \right|_{emiss} \approx \frac{M_{air}}{M_i} \frac{Q_{\varphi_i}}{\bar{\rho}} \quad (6-41)$$

An additional benefit is that the same transformation rule can be applied when emissions are included either in the vertical diffusion or in the chemistry.

6.2.3.7 Cloud Mixing and Aqueous-phase Chemistry (CLOUD) for CCTM

The rate of change in pollutant concentrations due to cloud processes is given by:

$$\left. \frac{\partial \bar{m}_i}{\partial t} \right|_{cld} = \left. \frac{\partial \bar{m}_i}{\partial t} \right|_{subcld} + \left. \frac{\partial \bar{m}_i}{\partial t} \right|_{rescld} \quad (6-42)$$

where subscripts *cld*, *subcld*, and *rescld* represent cloud, subgrid scale cloud, and resolved cloud, respectively. Although calls to the CLOUD module are made at every synchronization time step, the subgrid cloud effects are accounted for once an hour while the resolved cloud effects are impacted at each call. This is equivalent to assuming that the cloud life time of all sub-grid clouds is one hour. The effects of subgrid cloud processes, such as mixing (*mix*), scavenging (*scav*), aqueous-phase chemistry (*aqchem*), and wet deposition (*wdep*) on grid-average concentrations are parameterized with a “representative cloud” within the grid cell:

$$\left. \frac{\partial \bar{m}_i}{\partial t} \right|_{subcld} \sim f(mix, scav, aqchem, wdep) \quad (6-43)$$

where *f* represents a function of its arguments. We chose this expression because of the implicit nature of the algorithm representing the processes. For the resolved cloud, no additional cloud dynamics are considered in CMAQ and only effects of the scavenging and aqueous-phase chemistry are considered:

$$\left. \frac{\partial \bar{m}_i}{\partial t} \right|_{rescld} = \left. \frac{\partial \bar{m}_i}{\partial t} \right|_{scav} + \left. \frac{\partial \bar{m}_i}{\partial t} \right|_{aqchem} \quad (6-44)$$

See Chapter 11 for details of the cloud process descriptions.

6.2.3.8 Plume-in-Grid Process (PING) for CCTM

Anthropogenic precursors of the tropospheric loading of ozone, aerosols, and acidic species are largely emitted from major point sources, mobile sources, and urban-industrial area sources. In particular, inadequate spatial resolution of the major point source emissions can cause inaccurate predictions of air quality in regional and urban Eulerian air quality models. A plume-in-grid

(PinG) approach in CCTM provides a more realistic treatment of the subgrid scale physical and chemical processes for major elevated point source emitters (MEPSEs).

The PING module solves for:

$$\frac{\partial m_p}{\partial t} = \frac{\partial m_p}{\partial t} \Big|_{disp} + \frac{\partial m_p}{\partial t} \Big|_{emis} + \frac{\partial m_p}{\partial t} \Big|_{chem} + \frac{\partial m_p}{\partial t} \Big|_{dep} \quad (6-45)$$

where m_p is concentration of the subgrid plume (in molar mixing ratio) and the time-rate of change terms with subscripts *disp*, *emis*, *chem*, and *dep* represent effects of plume dispersion, point source emissions, plume chemistry, and dry deposition in the plume, respectively. The location and shape of plumes are determined by the PDM and plume chemistry is computed in the CCTM within plume subsections. When the subgrid scale phase of the plume simulation has been completed, the PING module updates grid scale concentrations with:

$$\frac{\partial m_i}{\partial t} \Big|_{ping} = \frac{\delta V_p}{\delta V} \frac{\partial(m_p - m_{ibg})}{\partial t} \quad (6-46)$$

where m_{ibg} is the back ground concentration and δV_p is the volume of plume in a grid cell with volume δV . Currently, only gaseous species are treated with the PING module. Readers are referred to Chapter 9 for the details. The work for the inclusion of particulates in the PING process has been started.

6.3 Equivalent Model Formulations for Different Vertical Coordinates

Because the CCTM is based on a generalized coordinate system, it is possible to emulate the governing equations of other popular Eulerian air quality models. For most urban and regional applications, the choice of horizontal map projection is handled with the map scale factors at the individual grid points. Therefore, there are no real differences in formulations in horizontal directions. One caveat is that the current CMAQ version is not tested with anholonomic coordinates, such as spherical coordinates. A few implementation details must be taken into account to accommodate the spherical coordinates. Most of the distinction of the dynamics is attributed to the choice of the vertical coordinate of the system.

The generalized governing conservation equation for trace species, written in the Reynolds flux form, is given in Equation 6-18. The same equation in eddy-diffusion form, in which the components of the eddy diffusivity tensor are represented in terms of those in Cartesian coordinates, is given below:

$$\frac{\partial}{\partial t} (J_\xi \bar{\varphi}_i) + m^2 \hat{\mathbf{V}}_\xi \cdot \left[\frac{J_\xi \bar{\varphi}_i}{m^2} \hat{\mathbf{V}}_\xi \right] + \frac{\partial (J_\xi \bar{\varphi}_i \bar{v}^3)}{\partial \xi}$$

$$\begin{aligned}
& -m^2 \frac{\partial}{\partial \hat{x}^1} \left[\bar{\rho} J_{\xi} (K_{xx} \frac{\partial \bar{q}_i}{\partial \hat{x}^1}) \right] - m^2 \frac{\partial}{\partial \hat{x}^2} \left[\bar{\rho} J_{\xi} (K_{yy} \frac{\partial \bar{q}_i}{\partial \hat{x}^2}) \right] \\
& - \frac{\partial}{\partial \xi} \left[\frac{\bar{\rho}}{J_{\xi}} \left[\left(\frac{\partial z_{sfc}}{\partial \hat{x}^1} \right)^2 K_{xx} + \left(\frac{\partial z_{sfc}}{\partial \hat{x}^2} \right)^2 K_{yy} + K_{zz} \right] \frac{\partial \bar{q}_i}{\partial \xi} \right] \\
& = J_{\xi} \left[R_{\varphi_i} (\bar{\varphi}_1, \dots, \bar{\varphi}_N) + Q_{\varphi_i} \right] + \frac{\partial (J_{\xi} \bar{\varphi}_i)}{\partial t} \Bigg|_{cld} + \frac{\partial (J_{\xi} \bar{\varphi}_i)}{\partial t} \Bigg|_{ping} + \frac{\partial (J_{\xi} \bar{\varphi}_i)}{\partial t} \Bigg|_{aero} \quad (6-47)
\end{aligned}$$

In most popular air quality models, including the present implementation of the CCTM, the cross-terms from the off-diagonal components of the diffusivity tensor are neglected. Note that some models use wind components defined in Cartesian coordinates. The mass conservation characteristic of Equation 6-47 is heavily dependent on the quality of the wind data provided. In particular, depending on the dynamic assumptions used in atmospheric models, methods for estimating the contravariant vertical velocity component vary considerably. Refer to Chapter 5 for the details.

Formulations of other air quality models with popular meteorological vertical coordinates, such as z , σ_z , σ_{po} , and σ_p ; and the step-mountain eta coordinate, η , can be obtained by substituting the appropriate vertical Jacobian in Equation 6-47. Refer to Table 6-3 for the coordinate definitions, associated Jacobians and contravariant vertical velocity components. Occasionally, one may find discrepancies in the governing equation between the one represented by Equation 6-47 and the one presented in the documentation of a specific model with the same vertical coordinates. Some of these can be attributed to the explicit representation of the dynamic characteristics and other idiosyncratic implementation practices used in those models. In the CCTM, the vertical coordinate is defined to increase with geometric height as given in Equation 6-4. This restriction simplifies interpretation of terms in the governing equations and eventually the computer coding of the algorithms. For example, the sign of the contravariant vertical velocity component is kept the same (i.e., positive value represents upward motion) across the different coordinate systems.

The terrain-influenced height coordinate σ_z has been used often for studying air quality especially with some simplifying conditions such as the Boussinesq approximation and anelastic assumption. For urban air quality simulations, there are a few examples of applying the σ_z coordinate defined with time and space dependent H (thickness of model), which is often related with the boundary layer height. The σ_z coordinate is used in air quality models, such as the Urban Airshed Model (UAM) (Scheffe and Morris, 1993), STEM-II (Carmichael et al., 1991), CIT (Harley et al., 1993), CALGRID (Yamartino et al., 1992), and others. The terrain-influenced reference pressure coordinate is used in SAQM (Chang et al., 1997), which is designed to be consistent with the nonhydrostatic MM5 meteorological model. The terrain-influenced time dependent hydrostatic pressure coordinate is used in RADM (Chang et al., 1987). It is the same coordinate used for MM4 or MM5 hydrostatic applications. Step-mountain eta coordinate is

used for NCEP's Eta meteorological model (Black, 1994, and Mesinger et al., 1988), but no operational air quality model using the eta coordinate is available.

Table 6-3. Vertical Coordinates and Associated Characteristics

CMAQ Coordinate $\hat{x}^3 = \xi$	Definition	Contravariant Vertical Velocity \hat{v}^3	Vertical Jacobian J_ξ	Remarks
Z		$w = \frac{dz}{dt}$	1	Geometric height
σ_z	$\sigma_z = H \frac{z - z_{sfc}}{H - z_{sfc}}$	$\frac{d\sigma_z}{dt}$	$\frac{H - z_{sfc}}{H}$	H is the thickness of model and σ_z is the scaled height
σ_z	$\sigma_z = \frac{z - z_{sfc}}{H - z_{sfc}}$	$\frac{d\sigma_z}{dt}$	$H - z_{sfc}$	Nondimensional height, terrain-influenced
$1 - \sigma_{po}$	$\sigma_{po} = \frac{p_o - p_T}{p_{os} - p_T}$	$-\frac{d\sigma_{po}}{dt}$	$\frac{p_{os} - p_T}{\rho_o g}$	Nondimensional reference pressure
$1 - \sigma_{\tilde{p}}$	$\sigma_{\tilde{p}} = \frac{\tilde{p} - p_T}{\tilde{p}_s - p_T}$	$-\frac{d\sigma_{\tilde{p}}}{dt}$	$\frac{\tilde{p}_s - p_T}{\tilde{\rho} g}$	Nondimensional geostrophic pressure
$1 - \eta$	$\eta = \left(\frac{\pi - \pi_T}{\pi_s - \pi_T} \right) \eta_{sfc}$	$-\frac{d\eta}{dt}$	$\frac{\pi_s - \pi_T}{\tilde{\rho} g \eta_{sfc}}$	Step-mountain ETA $\eta_{sfc} = \left(\frac{p_o(z_{sfc}) - p_T}{p_o(0) - p_T} \right)$

6.4 Nesting Techniques

The nested grid CTM is needed to provide the required high resolution simulations. At present, Models-3 CMAQ allows only static grid nesting. In static grid nesting, finer grids (FGs) are placed (i.e., nested) inside coarser grids (CGs). The resolution and the extent of each grid are determined *a priori* and remain fixed throughout the CTM simulation. Static grid nesting conserves mass and preserves transport characteristics at the interfaces of grids with different resolutions (Odman et al., 1995). It allows for effective interaction between different scales with efficient use of computing resources. On the other hand, the nest domain is redefined during a simulation with the dynamic nesting. Both static and dynamic nesting techniques allow one-way or two-way exchange of information among FGs and the CG and periodically by independently simulating CTMs at each grid (coarse or nested) with its own time step. The dynamic nesting procedure is not implemented in the CMAQ system.

In one-way nesting, the primary concern is the mass conservation at the grid interface where boundary conditions are input to the FG using the CG solution. The advective flux at the inflow

boundaries of the FG is the flux as determined by the CG solution that passes through this interface. We also allow for time variation of the flux during the CG time step. This is performed by computing the departure point of the last particle passing through the interface for each FG time step. In the Lagrangian description, the mass crossing the interface is equal to the spatial integral of the concentration distribution between the departure point and the interface. Most flux-conserving advection schemes use the same Lagrangian concept to calculate the mass transfer between grid cells (e.g., Bott, 1989). During each FG time step, we meter into the FG the exact amount of mass that would have crossed the interface on the CG (Byun et al., 1996).

In two-way nesting, the concentrations are updated in each CG cell by averaging the concentrations of all the FG cells overlapping with the CG cell. Special care is required to assure strict mass conservation at the grid interface. The mass of some species (e.g., radicals) may no longer be conserved because, when advancing the FG solution, we perform nonlinear chemical transformations in addition to transport. However, the mass of the basic chemical elements such as sulfur, nitrogen, and carbon must be conserved. The FG solution is used to compute the flux of each element at the grid interface. When conservation principles are applied to the grid interface, as described above, the CG concentrations near the interface must be corrected (when the Courant stability limit is applied, only the first row of CG cells immediately outside the interface need correction). This is done by renormalizing the concentration of each species based on the assumption that the ratio of the species mass to element mass will remain the same before and after the correction. This method is similar to the renormalization procedure used to make slightly non-conservative chemical solvers strictly conservative. Alapaty et al. (1998) compares different spatial interpolation schemes used for the two-way nesting.

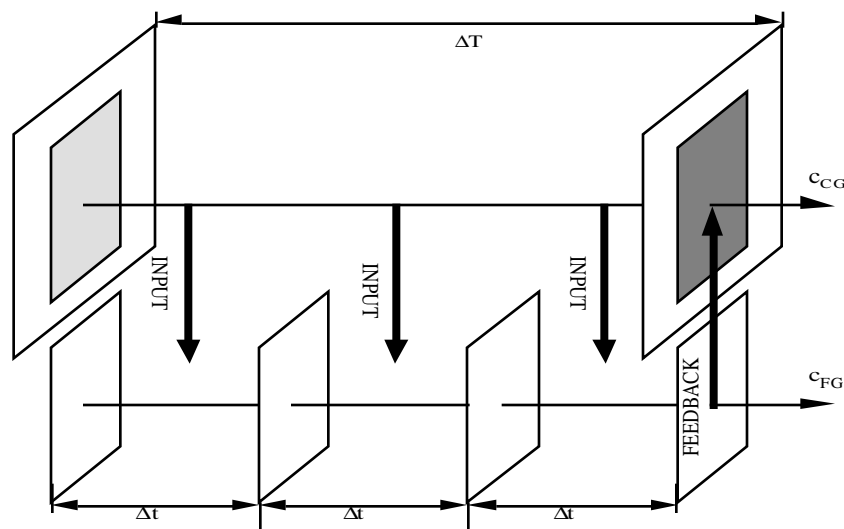


Figure 6-5. Static Grid Nesting Used in CMAQ System

The CCTM provides a static nesting (see Figure 6-5) capability while maintaining a high level of modularity by separately processing object codes for different grid domains and by enforcing the protocol that each module reads its required input data independently from others. The scheme

is also applicable for multiple and multi-level grid nesting. Multi-level nesting is a natural extension of the single static grid nesting. Figure 6-6 presents a schema for multi-level nesting, where three-levels are illustrated. The feedback processes update coarser grid concentrations at each synchronization time steps of the nest grids. The information about the grid is communicated to each process module through a set of FORTRAN include files specific to each grid domain during compilation time. This allows use of the same process modules for different grids. Customizing a nested model is as simple as preparing include files with grid dimensions for each grid and a driver with the appropriate process calling sequence.

As seen in Figure 6-6, the only difference between the one-way and two-way nesting is whether concentrations in coarser grid simulations are updated with the finer grid simulations through the feedback processors or not. Depending on the computer hardware and software configurations, one could build a nested CTM model with one executable collectively simulating all the FGs and CG, or with independent CTM executables for different grids that run simultaneously on multiple CPUs accessing common data through appropriate I/O API. The latter approach relies on the cooperating processors concept in a UNIX environment. As mentioned before, the current CMAQ version lacks a feedback module, which is necessary for the two-way nesting.

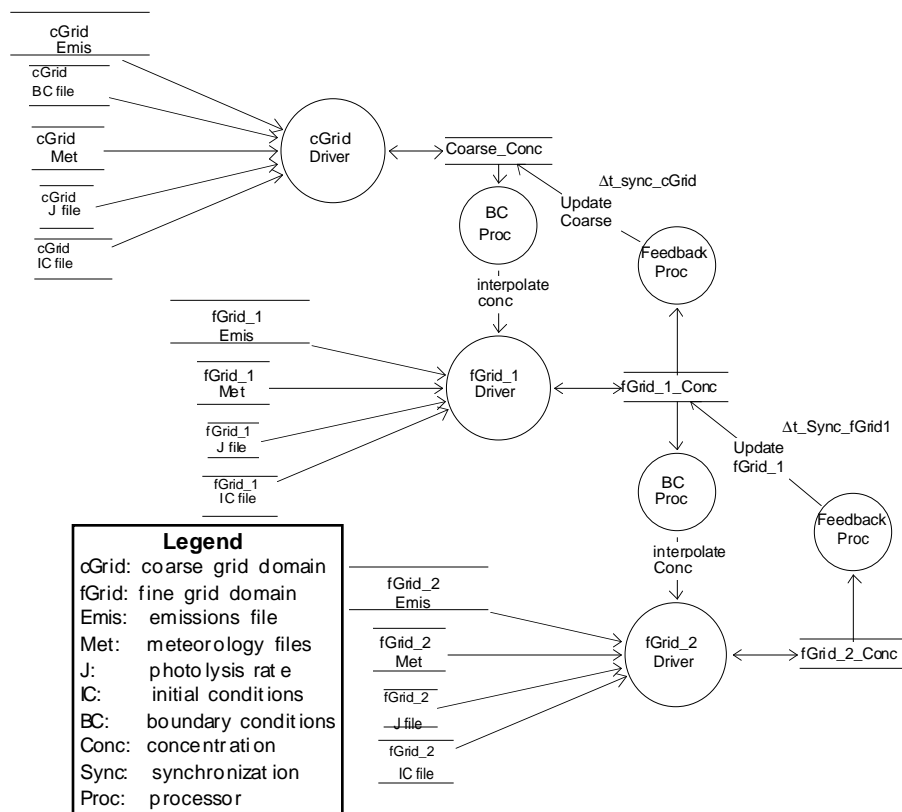


Figure 6-6. Schematics for Multi-level Nesting (three levels illustrated)

6.5 Summary

The CMAQ system achieves multi-pollutant and multiscale capabilities by combining several distinct modeling techniques. The generalized governing conservation equations of the CCTM allow transformation among various vertical coordinates (e.g., terrain-influenced geometric height, or pressure) and transformation among various horizontal coordinates, especially map projections (e.g., rectangular, Mercator, Lambert, and polar stereographic) by simple changes in a few scaling parameters defining the boundary domain, map origin, and orientation. Therefore, CMAQ can be configured to match the dynamic characteristics of the preprocessor meteorological models. The CMAQ system uses a nesting technique and a plume-in-grid approach to handle small scale air quality problems and subgrid scale plume dispersion and chemical reactions, respectively. The multi-pollutant capability is provided by a generalized mechanism reader and generalized chemistry solvers, linked cloud mixing and aqueous reaction processes, and aerosol modules. The CCTM code uses a modular structure that allows for the continuing improvement of the science and addition of new capabilities in a unified fashion. It provides a natural disciplinary distinction among different science processes through which developments in specific research areas can be readily incorporated.

As mentioned above, there remain a few implementation tasks, such as development of feed-back modules for two-way nesting and adaptation of anholonomic coordinates (e.g., latitude-longitude), which will provide additional functionalities in CCTM.

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

Appendix 6A. Concentration Units Used for Air Quality Studies

As we have seen above, many different concentration units are used for air quality studies. In this section we summarize the relations among the concentration units and their conversion factors from one unit to another. For Models-3/CMAQ system we follow the International System of Units (Système International, SI) as a framework for units in the formulations. The fundamental assumption used here is that air and trace gases follow the ideal gas law, i.e.,

$$pV = \nu R_g T, \quad (6A-1)$$

where R_g is the universal gas constant = $8.314510 [J/(mol \cdot K)]$,
 ν is molar number,
 V is volume of the gas [m^3],
 p is pressure [Pa], and
 T is temperature [K].

There are many different ways to express the amount of substance in the atmosphere. We introduce most popular quantities and transformation relations among them are presented below.

Number Density, n

One way to express trace gas quantities is to count number of molecules in the unit volume. For example, number of molecules of air in the unit volume, n_{air} , is expressed as:

$$n_{air} = \frac{\nu_{air} N_A}{V} \quad (6A-2)$$

where ν_{air} is number of moles of air,

N_A is the Avogadro's number = 6.0221367×10^{23} , and

Similarly, number of molecules of trace gas per volume, i.e., number density of species n_i , is defined as:

$$n_i = \frac{\nu_i N_A}{V} = \frac{\nu_i N_A}{\nu_i R_g T / p_i} = \frac{p_i}{k_B T} [molecules \ m^{-3}] \quad (6A-3)$$

where ν_i is number of moles of trace gas i in a given volume, and

$k_B = R_g / N_A$ is Boltzmann's constant

p_i is the partial pressure of species i .

Molar Density, c_i

The number of moles of air (c_{air}) and trace gas (c_i) normalized for a unit volume of air are simply defined as:

$$c_{air} = \frac{V_{air}}{V} \quad (6A-4a)$$

$$c_i = \frac{V_i}{V} \quad (6A-4b)$$

with the unit [*mole m*⁻³]. Because the SI unit for the amount of substance is *mol*, this quantity can be used conveniently for expressing chemical relationships.

Partial Pressure, p_i

Although not used widely in atmospheric chemistry, the partial pressure has been playing an important role specifying thermodynamic properties of the atmosphere, especially for water vapor in the air. The Dalton's law states that the total pressure exerted by a mixture of gases is equal to the sum of the partial pressure exerted by each constituent at the given temperature and volume. Because we assume that each trace gas follows the ideal gas law, the partial pressure can be used to express the trace gas quantity. The partial pressure of atmospheric constituent gas is related to the number of moles per volume as:

$$p_i = \frac{v_i R_g T}{V} = c_i R_g T \quad (6A-5)$$

and the standard SI unit for the partial pressure is Pascal [*Pa*].

Molar Mixing Ratio, m_i

Often, the molar mixing ratio is used as a synonym for the volume mixing ratio, or the mole fraction of a substance in air. Basically it is a unitless quantity. However, it is customary to identify in terms of molar unit as [*mole / mole*]. Because the volume occupied by a mole of ideal gas at given pressure is the same regardless of the constituent, the mole fraction is essentially equal to the volume fraction. However, mole fraction is preferred because it does not require the implicit assumption of the ideality of the gases, and more importantly because it is applicable also to condensed-phase species (Schwartz and Warneck, 1995). For a given volume, the volume mixing ratio of a trace species is expressed in terms of concentration units defined above as:

$$m_i = \frac{V_i}{V_{air} + V_i} = \frac{c_i}{c_{air} + c_i} = \frac{p_i}{p}, \quad (6A-6)$$

where p is the total pressure.

Because $v_i \ll v_{air}$ for trace gases, Equation 6A-6 can be approximated as:

$$m_i \approx \frac{V_i}{V_{air}} = \frac{c_i}{c_{air}} = \frac{p_i}{p_{air}}$$

When dealing with trace gases in the real atmosphere, the contribution of moisture can be used in the definition of mixing ratio. Therefore, p_{air} represents total pressure of the atmosphere which includes vapor pressure of water while the contribution of other trace gases are neglected. Because the variation caused by the moisture can amount to several percent, some researchers prefer to use dry air when expressing trace gas mixing ratios. However, in the Models-3/CMAQ system, we use the trace gas mixing ratio with respect to the moist air because we rely on the continuity equation for the total air density to represent atmospheric mass conservation.

Mass Mixing Ratio, q_i

Mass mixing ratio is used often for describing transport process and is simply related with the volume mixing ratio as:

$$q_i = m_i \frac{M_i}{M_{air}} \quad (6A-7)$$

Density, φ_i

Concentrations of substances in air can be expressed in terms of amount of substance mass per volume of air, i.e. density. Density is a most popular unit for dynamic representation of atmospheric concentration because it is the operating units of the mass continuity equation. Density can be expressed in terms of other concentration units as:

$$\begin{aligned} \varphi_i &= \frac{v_i M_i}{V} = c_i M_i = \frac{c_i}{c_{air}} c_{air} M_i \\ &\approx \left(m_i \frac{M_i}{M_{air}} \right) (c_{air} M_{air}) = q_i \rho_{air} \end{aligned} \quad (6A-8)$$

Table 6A-1 provides cross-reference relationships among the concentration variables described. However, the individual process science area prefers to use certain specific units of decimal multiples of the SI unit suggested. We included the conversion factors among the concentration variables actually implemented in science process modules. Because it is convenient to express the conversion factors in terms of the dry air quantities, the virtual temperature is used in Table 6A-1.

Table 6A.1. Conversion formula among various trace gas concentration units used in the CMAQ system

	number density, N_i [<i>molecules/m³</i>]	molar density, c_i [<i>mol/m³</i>]	partial pressure, p_i [<i>Pascad</i>]	molar mixing ratio, m_i [ppmV]	mass mixing ratio, q_i [ppm]	density, φ_i [<i>μg/m³</i>]
number density, N_i [<i>molecules/m³</i>]	1	$N_i = (N_A) c_i$	$N_i = (k_B T)^{-1} p_i$	$N_i = 10^3 \cdot \left(\frac{\rho_{air}}{M_{air}} \right) m_i$	$N_i = 10^3 \cdot \left(\frac{\rho_{air}}{M_i} \right) q_i$	$N_i = 10^{-6} \cdot \left(\frac{N_A}{M_i} \right) \varphi_i$
molar density, c_i [<i>mol/m³</i>]	$c_i = (N_A)^{-1} N_i$	1	$c_i = (R_g T)^{-1} p_i$	$c_i = 10^{-3} \cdot \left(\frac{\rho_{air}}{M_{air}} \right) m_i$	$c_i = 10^{-3} \cdot \left(\frac{\rho_{air}}{M_i} \right) q_i$	$c_i = 10^{-6} \cdot (M_i)^{-1} \varphi_i$
partial pressure, p_i [Pascad]	$p_i = (k_B T) N_i$	$p_i = (R_g T) c_i$	1	$p_i = 10^{-6} \cdot (p) m_i$	$p_i = 10^{-6} \cdot \left(\frac{M_{air}}{M_i} \right) p q_i$	$p_i = 10^6 \cdot \left(\frac{R_g T}{M_i} \right) \varphi_i$
molar mixing ratio, m_i [ppmV]	$m_i = 10^3 \cdot \left(\frac{M_{air}}{\rho_{air} N_A} \right) N_i$	$m_i = 10^3 \cdot \left(\frac{M_{air}}{\rho_{air}} \right) c_i$	$m_i = 10^6 \cdot (p)^{-1} p_i$	1	$m_i = \left(\frac{M_{air}}{M_i} \right) q_i$	$m_i = 10^{-3} \cdot \left(\frac{M_{air}}{\rho_{air} M_i} \right) \varphi_i$
mass mixing ratio, q_i [ppm]	$q_i = 10^3 \cdot \left(\frac{M_i}{N_A \rho_{air}} \right) N_i$	$q_i = 10^3 \cdot \left(\frac{M_i}{\rho_{air}} \right) c_i$	$q_i = 10^6 \cdot \left(\frac{M_i}{p M_{air}} \right) p_i$	$q_i = \left(\frac{M_i}{M_{air}} \right) m_i$	1	$q_i = 10^3 \cdot (\rho_{air})^{-1} \varphi_i$
density, φ_i [<i>μg/m³</i>]	$\varphi_i = 10^6 \cdot \left(\frac{M_i}{N_A} \right) N_i$	$\varphi_i = 10^6 \cdot (M_i) c_i$	$\varphi_i = 10^6 \cdot \left(\frac{M_i}{R_g T} \right) p_i$	$\varphi_i = 10^3 \cdot \left(\frac{\rho_{air} M_i}{M_{air}} \right) m_i$	$\varphi_i = 10^3 \cdot (\rho_{air}) q_i$	1

Note: Values for the Avogadro's constant (N_A) is 6.0221367x10²³ [number/mol], the universal gas constant (R_g) is 8.314510 [J/mol-K], and the Boltzmann's constant (k_B) is defined with R_g/N_A . Molar mixing ratio is equivalent to volume mixing ratio and their units [ppmV], [ppb], and [ppt] are short hand notations for [], [], and [], respectively. The unit for mass mixing ratio, [ppm], is a short hand for []. Both and may represent values for dry air or moisture air depending on applications. However, in one processing system, their usage should be consistent. and (molecular weight of species i) are in [g mol⁻¹] and is in [kg m⁻³].