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Chapter 5

FUNDAMENTALS OF ONE-ATMOSPHERE DYNAMICS FOR MULTISCALE AIR QUALITY MODELING

Daewon W. Byun*
Atmospheric Modeling Division
National Exposure Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

ABSTRACT

This chapter provides essential information needed for the proper use of meteorological data in air quality modeling systems. Sources of meteorological data are diverse and many difficulties can arise while linking these with air quality models. To provide an integral view of atmospheric modeling, a robust and fully compressible governing set of equations for the atmosphere is introduced. Limitations of several simplifying assumptions on atmospheric dynamics are presented. Also, concepts of on-line and off-line coupling of meteorological and air quality models are discussed.

When the input meteorological data are recast with the proposed set of governing equations, chemical transport models can follow the dynamic and thermodynamic descriptions of the meteorological data closely. In addition, this chapter introduces a procedure to conserve mixing ratio of trace species even in the case meteorological data are not mass consistent. In summary, it attempts to bridge the information gap between dynamic meteorologists and air quality modelers by highlighting the implication of using different meteorological coordinates and dynamic assumptions for air quality simulations.

* On assignment from the National Oceanic and Atmospheric Administration, U.S. Department of Commerce. Corresponding author address: Daewon W. Byun, MD-80, Research Triangle Park, NC 27711. E-mail: bdx@hpcc.epa.gov

5.0 FUNDAMENTALS FOR ONE-ATMOSPHERE MODELING FOR MULTISCALE AIR QUALITY MODELING

To simulate weather and air quality phenomena realistically, adaptation of a one-atmosphere perspective based mainly on "first principles" description of the atmospheric system (Dennis, 1998) is necessary. The perspective emphasizes that the influence of interactions at different dynamic scales and among multi-pollutants cannot be ignored. For example, descriptions of processes critical to producing oxidants, acid and nutrient depositions, and fine particles are too closely related to treat separately. Proper modeling of these air pollutants requires that the broad range of temporal and spatial scales of multi-pollutant interactions be considered simultaneously. Several chapters (Chapters 4, 8, 9, 11 and 16) of this document present the one-atmosphere modeling perspective related with the multi-pollutant chemical interactions. Another key aspect of the one-atmosphere perspective is the dynamic description of the atmosphere. This is the focus of the present chapter.

Air quality modeling should be viewed as an integral part of atmospheric modeling and the governing equations and computational algorithms should be consistent and compatible. Previously, many atmospheric models have been built with limited atmospheric dynamics assumptions. To simplify the model development process, the governing equations were first simplified to match with the target problems, then computer codes were implemented. This approach enabled rapid development of models. However, we believe that dynamic assumptions and choice of coordinates should not precede the computational structure of the modeling system. To provide the scalability in describing dynamics, a fully compressible governing set of equations in a generalized coordinate system is preferable. Once the system is based on the fully compressible governing equations, simpler models can be built readily. The characteristics of the vertical coordinates and other simplifying assumptions need to be considered as well. For successful one-atmosphere simulations, it is imperative to have consistent algorithmic linkage between meteorological and chemical transport models (CTMs).

The present chapter addresses the issue of consistent description of physical processes across scales in meteorological and air quality modeling systems. It intends to provide appropriate background information to properly link air quality and meteorological models at a fundamental level. It deals with dynamic scalability issues, such as hydrostatic and nonhydrostatic modeling covering wide range of both temporal and spatial scales. Some of the contents are extracts from Byun (1999a and b) and others are complementary information to them. It includes mass correction methods, mass conservative temporal interpolation method, and the coupling paradigm for meteorology and chemical transport models.

5.1 Governing Equations and Approximations for the Atmosphere

In most weather prediction models, temperature and pressure, as well as moisture variables, are used to represent thermodynamics of the system. Often these thermodynamic parameters are represented with the advective form equations in meteorological models. Most of time, the density is diagnosed as a byproduct of the simulation, usually through the ideal gas law. For multiscale air quality applications where the strict mass conservation is required, prognostic equations for the thermodynamic variables are preferably expressed in a conservative form similar to the continuity equation. Recently, Ooyama (1990) has proposed the use of prognostic equations for entropy and air density in atmospheric simulations by highlighting the thermodynamic nature of pressure. Entropy is a well-defined state function of the thermodynamic variables such as pressure, temperature, and density. Therefore, entropy is a field variable that depends only on the state of the fluid. The principle he uses is the separation of dynamic and thermodynamic parameters into their primary roles. An inevitable interaction between dynamics and thermodynamics occurs in the form of the pressure gradient force.

In this section, a set of governing equations for fully compressible atmosphere is presented. Here, density and entropy are used as the primary thermodynamic variables. For simplicity, a dry adiabatic atmosphere is considered. Most of the discussions in this section should be extensible for moist atmosphere if Ooyama's approach is followed.

5.1.1 Governing Equations in a Generalized Curvilinear Coordinate System

Using tensor notation, the governing set of equations for the dry atmosphere in a generalized curvilinear coordinate system can be written as:

$$\frac{\partial \hat{v}^j}{\partial t} + \hat{v}^k \hat{v}^j_{;k} + \hat{g}^{jk}\left(\frac{1}{\rho}\frac{\partial p}{\partial \hat{x}^k} + \frac{\partial \Phi}{\partial \hat{x}^k}\right) + 2\hat{\varepsilon}^{jkl}\Omega_k \hat{v}_l = \hat{F}^j_r \tag{5-1}$$

$$\frac{\partial(\rho\sqrt{\hat{\gamma}})}{\partial t} + \frac{\partial(\rho\sqrt{\hat{\gamma}}\hat{v}^j)}{\partial \hat{x}^j} = \hat{Q}_\rho = \sqrt{\hat{\gamma}}Q_\rho \tag{5-2}$$

$$\frac{\partial(\zeta\sqrt{\hat{\gamma}})}{\partial t} + \frac{\partial(\zeta\sqrt{\hat{\gamma}}\hat{v}^j)}{\partial \hat{x}^j} = \hat{Q}_\zeta = \sqrt{\hat{\gamma}}Q_\zeta \tag{5-3}$$

$$\frac{\partial(\varphi_i\sqrt{\hat{\gamma}})}{\partial t} + \frac{\partial(\varphi_i\sqrt{\hat{\gamma}}\hat{v}^j)}{\partial \hat{x}^j} = \hat{Q}_{\varphi_i} = \sqrt{\hat{\gamma}}Q_{\varphi_i} \tag{5-4}$$

where $\hat{v}^j$ and $\hat{v}_k$ are contravariant and covariant wind components, respectively, $\hat{v}^j_{;k}$ represents the covariant derivative of contravariant vector, $\hat{\varepsilon}^{jkl}$ is the Levi-Cevita symbol, Ω_k is the angular velocity of earth's rotation, $\hat{F}^j_r$ represents frictional forcing terms, $\sqrt{\hat{\gamma}}$ is the Jacobian of coordinate transformation, Φ is geopotential height, ρ is air density, and $\hat{g}^{jk}$ represents components of gravity vector in tensor form. Refer to Appendix 5A for the tensor primer and the derivation of the continuity equation in a generalized curvilinear coordinate system. φ_i represents trace species concentration, and ζ is (dry air) entropy per unit volume (entropy density), given as

$$\zeta = \rho C_{vd} \ln(\frac{T}{T_{oo}}) - \rho R_d \ln(\frac{\rho}{\rho_{oo}}) \tag{5-5}$$

where T is temperature, T_{oo} and ρ_{oo} are temperature and density of the reference atmosphere, respectively, at pressure p_{oo} = 1000 mb = 10^5 Pascal, C_{vd} is the specific heat capacity at constant volume, and R_d is the gas constant for dry air. The Q-terms represent sources and sinks of each conservative property. Although the source term for air density (Q_ρ) should be zero in an ideal case, it is retained here to capture the possible density error originating from numerical procedures in meteorological models. It is important to understand how this error term influences computations of other parameters such as vertical velocity component. Effects of the error term on trace gas simulation are discussed later.

To close the system we need to utilize the ideal gas law and the thermodynamic relations for temperature, entropy, pressure gradients, and density. Here, atmospheric pressure is treated as a thermodynamic variable that is fully defined by the density and entropy of the atmosphere. Then, pressure gradient terms can be computed using the thermodynamic relations with the density and entropy (e.g., Batchelor, 1967; Ooyama, 1990; DeMaria, 1995) in terms of the general vertical coordinate $s = \hat{x}^3$, as:

$$p = \rho R_d T \tag{5-6a}$$

$$\nabla_s p = \left(\frac{\partial p}{\partial \rho}\right)\nabla_s \rho + \left(\frac{\partial p}{\partial \zeta}\right)\nabla_s \zeta \tag{5-6b}$$

$$\frac{\partial p}{\partial s} = \left(\frac{\partial p}{\partial \rho}\right)\frac{\partial \rho}{\partial s} + \left(\frac{\partial p}{\partial \zeta}\right)\frac{\partial \zeta}{\partial s} \tag{5-6c}$$

$$\frac{\partial p}{\partial \rho} = \left(C_{pd} - \frac{\zeta}{\rho}\right)\frac{R_d T}{C_{vd}} \tag{5-6d}$$

$$\frac{\partial p}{\partial \zeta} = \frac{R_d T}{C_{vd}}, \tag{5-6e}$$

where C_{pd} is the specific heat capacity at constant pressure for dry air, and $\nabla_s = \hat{\mathbf{i}}\partial / \partial\hat{x}^1\big|_{s=const} + \hat{\mathbf{j}}\partial / \partial\hat{x}^2\big|_{s=const}$. For a conformal map projection, we can relate generalized meteorological curvilinear coordinates $(\hat{x}^1, \hat{x}^2, \hat{x}^3, \hat{t})$ to the reference rotated earth-tangential coordinates (x, y, z, t) as

$$\begin{cases} \hat{x}^1 = mx \\ \hat{x}^2 = my \\ \hat{x}^3 = s \\ \hat{t} = t \end{cases} \qquad \begin{cases} x = m^{-1}\hat{x}^1 \\ y = m^{-1}\hat{x}^2 \\ z = h(\hat{x}^1, \hat{x}^2, \hat{x}^3, \hat{t}) = h_{AGL}(\hat{x}^1, \hat{x}^2, \hat{x}^3, \hat{t}) + z_{sfc}(\hat{x}^1, \hat{x}^2) \\ t = \hat{t} \end{cases} \tag{5-7a, b}$$

where m is the map scale factor, z_{sfc} is the topographic height, and h is the geometric height, and h_{AGL} represents height above the ground (AGL). In the derivation of Equations 5-7a,b, we neglected the first-order variations of the map scale factor in x- and y-directions. The approximation establishes a quasi-orthogonality of the vertical coordinate to the horizontal plane on the confomal map. The covariant metric tensor, for example, and its determinant are given as

$$\hat{\gamma}_{jk} = \begin{bmatrix} m^{-2} + (\frac{\partial h}{\partial \hat{x}^1})^2 & (\frac{\partial h}{\partial \hat{x}^1})(\frac{\partial h}{\partial \hat{x}^2}) & (\frac{\partial h}{\partial \hat{x}^1})(\frac{\partial h}{\partial s}) \\ (\frac{\partial h}{\partial \hat{x}^1})(\frac{\partial h}{\partial \hat{x}^2}) & m^{-2} + (\frac{\partial h}{\partial \hat{x}^2})^2 & (\frac{\partial h}{\partial \hat{x}^2})(\frac{\partial h}{\partial s}) \\ (\frac{\partial h}{\partial \hat{x}^1})(\frac{\partial h}{\partial s}) & (\frac{\partial h}{\partial \hat{x}^2})(\frac{\partial h}{\partial s}) & (\frac{\partial h}{\partial s})^2 \end{bmatrix}, \tag{5-7c}$$

$$\hat{\gamma} = \left|\hat{\gamma}_{jk}\right| = \frac{1}{m^4}\left(\partial h / \partial s\right)^2. \tag{5-7d}$$

With above relations, one can rewrite the governing momentum equation, Equation 5-1, into the horizontal and vertical components of the curvilinear coordinates as (Byun, 1999a):

$$\frac{\partial \hat{\mathbf{V}}_s}{\partial t} + (\hat{\mathbf{V}}_s \bullet \nabla_s)\hat{\mathbf{V}}_s + \hat{v}^3 \frac{\partial \hat{\mathbf{V}}_s}{\partial s} + f\hat{\tau}_3 \times \hat{\mathbf{V}}_s$$
$$+ m^2(\frac{1}{\rho}\nabla_s p + \nabla_s \Phi) - m^2\left(\frac{\partial s}{\partial z}\right)(\frac{1}{\rho}\frac{\partial p}{\partial s} + \frac{\partial \Phi}{\partial s})\nabla_s h = \hat{\mathbf{F}}_s \tag{5-8}$$

$$\frac{\partial \hat{v}^3}{\partial t} + (\hat{\mathbf{V}}_s \bullet \nabla_s)\hat{v}^3 + \hat{v}^3 \frac{\partial \hat{v}^3}{\partial s} + \hat{v}^k \hat{v}^j \frac{\partial^2 h}{\partial \hat{x}^k \partial \hat{x}^j}\left(\frac{\partial s}{\partial z}\right)$$
$$- m^2 \frac{\partial s}{\partial z}(\frac{1}{\rho}\nabla_s p + \nabla_s \Phi) \bullet \nabla_s h + \left|\nabla_z s\right|^2 (\frac{1}{\rho}\frac{\partial p}{\partial s} + \frac{\partial \Phi}{\partial s}) = \hat{F}_3 \tag{5-9}$$

where $\hat{\mathbf{V}}_s = \hat{v}^1\mathbf{i} + \hat{v}^2\mathbf{j}$, $\Phi(\hat{x}^1, \hat{x}^2, \hat{x}^3, \hat{t}) = gz$ represents the geopotential height, $\hat{\mathbf{F}}_s$ is the horizontal forcing vector, $\hat{\tau}_3$ is the vertical tangential basis vector and $\hat{F}_3$ is the forcing term in the momentum equation for $\hat{x}^3$ direction.

An alternative equation for the Cartesian vertical velocity component is given as:

$$\frac{\partial(\rho J_s w)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\rho J_s w \mathbf{V}_z}{m} \right) + \frac{\partial(\rho J_s w \hat{v}^3)}{\partial s}$$

$$+\rho J_s \left(\frac{m}{\rho} \frac{\partial p}{\partial s} + \frac{\partial \Phi}{\partial s} \right) \left(\frac{\partial s}{\partial z} \right) = \rho J_s \left(F_3 + \frac{w Q_\rho}{\rho} \right) \qquad (5\text{-}9')$$

where $\mathbf{V}_z = U\mathbf{i} + V\mathbf{j} = (\hat{v}^1 / m)\mathbf{i} + (\hat{v}^2 / m)\mathbf{j}$ is the horizontal wind vector represented in the Cartesian coordinate system, w is the vertical velocity component, J_s is the Jacobian for vertical coordinate transformation ($J_s = \left| \frac{\partial h}{\partial s} \right| = \frac{1}{g} \left| \frac{\partial \Phi}{\partial s} \right| = m^2 \sqrt{\hat{\gamma}}$), and F_3 is forcing term for the w-component. Note that the contravariant vertical velocity component is related to the Cartesian vertical velocity as:

$$\hat{v}^3 = \frac{ds}{dt} = \frac{\partial s}{\partial t} + \mathbf{V}_z \bullet \nabla_z s + w \left(\frac{\partial s}{\partial z} \right) = \frac{\partial s}{\partial t} + (-\frac{1}{g} \hat{\mathbf{V}}_s \bullet \nabla_s \Phi + w) \left(\frac{\partial s}{\partial z} \right), \qquad (5\text{-}10)$$

where $\nabla_z = \hat{\mathbf{i}} \partial / \partial x|_{z=const} + \hat{\mathbf{j}} \partial / \partial y|_{z=const}$.

The conservation equations for air density, entropy density, and tracer concentrations are found to be:

$$\frac{\partial(\rho J_s)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\rho J_s \hat{\mathbf{V}}_s}{m^2} \right) + \frac{\partial(\rho J_s \hat{v}^3)}{\partial s} = J_s Q_\rho \qquad (5\text{-}11)$$

$$\frac{\partial(\zeta J_s)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\zeta J_s \hat{\mathbf{V}}_s}{m^2} \right) + \frac{\partial(\zeta J_s \hat{v}^3)}{\partial s} = J_s Q_\zeta \qquad (5\text{-}12)$$

$$\frac{\partial(\varphi_i J_s)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{\varphi_i J_s \hat{\mathbf{V}}_s}{m^2} \right) + \frac{\partial(\varphi_i J_s \hat{v}^3)}{\partial s} = J_s Q_{\varphi_i} \qquad (5\text{-}13)$$

5.1.2 Assumptions of Atmospheric Dynamics

In this subsection, several popular assumptions used in meteorological models are reviewed. Here, the dynamic and thermodynamic assumptions are discussed separately because they have been applied as independent approximations in many atmospheric models. However, readers should be aware of the inseparable nature of the dynamics and thermodynamics of the atmosphere. This study focuses on the impact of basic assumptions of the mass conservation issues and limits of applications in air quality applications.

5.1.2.1 Boussinesq Approximation

The crux of the Boussinesq approximation is that variation in density is important only when it is combined as a factor with the acceleration of gravity. Originally, it was applied for studying shallow convection or boundary layer dynamics. Descriptions of the Boussinesq approximation can be found in the literature (e.g., Arya, 1988; Pielke, 1984; Stull, 1988; and Thunis and Bornstein, 1996). Although the Boussinesq approximation was originally developed for incompressible fluid, Dutton and Fichtl (1969) expanded the concept for anelastic deep convection applications. The results of the approximation lead to the following simplifications of the equations of motions in the planetary boundary layer (PBL):

(1) Flows can be treated essentially as solenoidal either in velocity field (incompressible) or in momentum field (anelastic).

(2) The equation of state for the fluctuating component is simplified because the ratio of fluctuating density to total density can be approximated by the ratio of temperature fluctuation to the reference temperature.

(3) Molecular properties including diffusivity are constant. These approximations are often used in air quality modeling to simplify the equations of motions and trace gas conservation equations. The effect of the Boussinesq approximation on mass continuity is in the limitation of the flow characteristics, such as incompressible or anelastic. For multiscale atmospheric studies, this approximation may be used only in the parameterization of the surface fluxes where the density can be treated essentially independent of height.

5.1.2.2 Nondivergent Flow Field Assumption

Essentially, this is an assumption about flow characteristics. The basis of this assumption is purely dynamic although an incompressible assumption leads to the nondivergent flow approximation. *A priori*, there is no connection with atmospheric thermodynamics. Therefore this assumption does not provide any information about the state variables, such as density, temperature, and pressure fields. For atmospheric applications, this approximation should be viewed as a result of the incompressible atmosphere assumption linked through the continuity equation of air. Because of the characteristics that the nondivergent velocity field can be expressed as the curl of a vector stream function, the field is also called solenoidal. Implications of this assumption on mass conservation of trace species are presented below in the description of the incompressible atmosphere assumption. In the generalized coordinate system, the nondivergent flow field is represented with following equation

$$\frac{1}{\sqrt{\hat{\gamma}}}\frac{\partial\left(\sqrt{\hat{\gamma}}\hat{v}^j\right)}{\partial\hat{x}^j} = 0, \ j = 1,2,3 \tag{5-14}$$

This is somewhat different from the meteorological nondivergent flow field assumption in the Cartesian coordinate system, $\nabla \bullet \mathbf{V} = 0$. In the generalized meteorological coordinate system, Equation 14 can be rewritten as

$$\frac{\partial \hat{v}^j}{\partial \hat{x}^j} - 2m\hat{v}^j \frac{\partial m}{\partial \hat{x}^j} + \hat{v}^j \frac{\partial \ln J_s}{\partial \hat{x}^j} = 0 \tag{5-14'}$$

The two additional terms represent essentially the effects of the map projection and the gradient of the vertical Jacobian on the divergence of wind. For a small domain and for a coordinate whose vertical Jacobian is constant with respect to height (e.g., σ_z-coordinate), Equation 14' becomes identical to the nondivergent wind flow assumption used in a meteorological model. When the vertical Jacobian is a function of air density, the dependency of the wind on the density distribution cannot be ignored.

5.1.2.3 Incompressible Atmosphere Assumption

This is an assumption about the thermodynamic characteristics of air. The equation of state describes how density is affected by the changes in pressure and temperature fields. The incompressibility of air can be assumed (Batchelor, 1967) if:

$$\left| \frac{1}{\rho} \frac{d\rho}{dt} \right| << \frac{U}{L}, \tag{5-15}$$

where U and L are the velocity and length scales, respectively, of the atmospheric motion.

As proposed in Byun (1999a), one can choose the density and the entropy as the two independent parameters of state. The total derivative of pressure with respect to time can be expressed as:

$$\frac{dp}{dt} = \left(\frac{\partial p}{\partial \rho} \right) \frac{d\rho}{dt} + \left(\frac{\partial p}{\partial \zeta} \right) \frac{d\zeta}{dt} \tag{5-16}$$

Then, Equation 5-15 becomes the relation:

$$\frac{1}{\rho c_{sound}^2} \left| \frac{dp}{dt} - \left(\frac{\partial p}{\partial \zeta} \right) \frac{d\zeta}{dt} \right| << \frac{U}{L}, \tag{5-17}$$

where c_{sound} is the speed of sound in the atmosphere, i.e., $c_{sound} = \sqrt{|\partial \rho / \partial p|}$. Batchelor (1967) stated that for Equation 5-17 to be satisfied, not only the difference between the two terms in the left hand side of Equation 5-17, but also the magnitude of each term should be small. When the condition

$$\left| \frac{1}{\rho c_{sound}^2} \frac{dp}{dt} \right| << \frac{U}{L} \tag{5-18}$$

is satisfied, the change in the density of a material element due to pressure variations are negligible, that is, the fluid is behaving as if it were incompressible. By expanding the term $\frac{dp}{dt}$

in an Eulerian expression one can show that in order for the atmosphere to be treated as incompressible, the following conditions must be satisfied:

$$\frac{U^2}{c_{sound}^2} << 1; \qquad \frac{U_p^{\ 2}}{c_{sound}^2} << 1; \qquad \frac{gL}{c_{sound}^2} << 1, \tag{5-19}$$

where U_p is the phase speed of dominant atmospheric waves. The first condition states that the movement of air should have a Mach number much smaller than one, say 10%; the second condition states that energy-carrying waves should not propagate as fast as 10% of the speed of sound; and the last condition limits the vertical extent of motion to less than about one kilometer. Similarly, Dutton and Fichtl (1969) showed that the nondivergent wind relation is generally applicable up to half a kilometer above ground level through a scale analysis of the continuity equation. Because of these limitations, a meteorological model with incompressible flow approximation may not be suitable for multiscale air quality simulations that require descriptions of atmospheric motions over a wide range of temporal and spatial scales. The second condition:

$$\left| \frac{1}{\rho c_{sound}^2} \left(\frac{\partial p}{\partial \zeta} \right) \frac{d\zeta}{dt} \right| << \frac{U}{L} \tag{5-20}$$

means that variation of entropy due to internal heating or due to molecular conduction of heat into the element must be small. For adiabatic or pseudo-adiabatic atmosphere, Equation 5-20 is usually satisfied.

Basically, an incompressible atmosphere assumption is a shallow-water approximation for an adiabatic atmosphere. With the incompressibility assumption, the distinction between the continuity equation and its advective form becomes blurred. Consequently, concentrations in the form of either density or mixing ratio are often used indiscriminately in atmospheric diffusion equations. As presented above, the incompressible atmosphere assumption is a very restrictive approximation that disassociates linkage between the thermodynamics and dynamics of atmospheric motions. The incompressible atmosphere approximation simplifies the continuity equation of the air to the nondivergent wind component relation regardless of the type of vertical coordinates used. Compared with this, the atmosphere described with the hydrostatic pressure coordinate is not necessarily incompressible even for the hydrostatic atmosphere. Because the vertical layer is defined by the pressure surface, the hydrostatic approximation applied with the hydrostatic pressure coordinate system limits only the vertical propagation of sound waves and the atmosphere is not totally incompressible.

One might expect that as long as the wind field satisfies the nondivergent flow approximation, an air quality model would satisfy the pollutant species mass conservation. In the following, it is shown that this expectation is correct only when the air density field is perfectly mass consistent. As will be shown later in Equation 5-24, the trace species mass conservation is affected by the air density error term Q_ρ irrespective of whether or not the wind field is solenoidal. The implication is that a nondivergent wind field does not guarantee the mass conservation of pollutant species as long as there is inconsistency in air density and wind fields. It is not a surprising statement, but in general this fact has not been actively addressed in air quality modeling studies. Because the nondivergent relation simply disassociates density and wind fields, it cannot be used to estimate the mass consistency error in the meteorological data set. On the other hand, the diagnostic relations applicable for the family of hydrostatic pressure coordinates based on total air density maintain the consistency in wind and air density fields.

5.1.2.4 Anelastic Atmosphere Assumption

Another popular limiting approximation applied in meteorological modeling is the anelastic assumption. It simplifies the continuity equation as a diagnostic relation for the momentum ($\rho_o \mathbf{V}$, where ρ_o is density of reference atmosphere) components as follows:

$$\nabla_s \bullet (\sqrt{\hat{\gamma}} \rho_o \hat{\mathbf{V}}_s) + \frac{\partial}{\partial s} (\sqrt{\hat{\gamma}} \rho_o \hat{v}^3) = 0 \tag{5-21}$$

Ogura and Phillips (1962) and Dutton and Fitchl (1969) found that for deep atmospheric convection, if the characteristic vertical scale of motions is smaller than the atmospheric scale height, the anelastic assumption is satisfied. For shallow convection, the Boussinesq approximation allows us to treat the fluid as incompressible; for deep convection, the approximate continuity equation requires the momentum field to be solenoidal, and the expansion or contraction of parcels moving in the vertical is taken into account. Lipps and Hemler (1982) also performed a scale analysis to propose a set of approximate equations of motion which are anelastic when the time scale is larger than the inverse of Brunt-Väisäla frequency. The anelastic approximation leads to a divergent wind field, i.e.:

$$\nabla_s \bullet (\sqrt{\hat{\gamma}} \hat{\mathbf{V}}_s) + \frac{\partial (\sqrt{\hat{\gamma}} \hat{v}^3)}{\partial s} = -\sqrt{\hat{\gamma}} (\hat{\mathbf{V}}_s \bullet \nabla_s \ln \rho_o + \hat{v}^3 \frac{\partial}{\partial s} \ln \rho_o) \tag{5-22}$$

Usually, the right hand side of Equation 5-22 does not vanish. Like the nondivergent wind field approximation, this assumption provides a diagnostic relation among wind components although it cannot be used to estimate the inconsistency in the total air density, ρ, and wind field data provided by a meteorological model. However, unlike the incompressible atmosphere assumption, the pressure, temperature and wind fields are not completely independent with the anelastic assumption. The distribution of pressure must be such that the wind fields predicted by the momentum equations continue to satisfy the anelastic relation (Gal-Chen and Somerville, 1975). For this reason, most anelastic meteorological models solve for the elliptic equation for the pressure that is derived from Equation 5-22. Refer to Nance and Durran (1994) for a recent review on the accuracy of anelastic meteorological modeling systems.

For air quality application, the anelastic approximation still requires use of a full continuity equation for the perturbation density component. However, most anelastic meteorological models do not solve for the perturbation air density directly. Therefore, one needs to infer it from other thermodynamic fields. Also, because the trace gas concentration depends on the total density of air, not on just the reference density, it does not simplify the pollutant continuity equation and the concentration distribution represented in density units cannot be interchanged with trace species mixing ratio.

5.1.2.5 Hydrostatic Atmosphere Approximation

Perhaps one of the most popular assumptions of atmospheric dynamics used in meteorological models is the hydrostatic approximation. In the case of a hydrostatic atmosphere, the acceleration and the frictional force terms in the *z*-direction of the earth-tangential Cartesian coordinates are considered negligible. In earlier days of atmospheric modeling, the hydrostatic approximation was usually applied with the pressure coordinate. It is well known that the hydrostatic pressure coordinate applied to a hydrostatic atmosphere has a special property that simplifies the continuity equation into a solenoidal form and provides a diagnostic equation for the vertical velocity component. On the other hand, the geometric height coordinate was not used extensively for studying a hydrostatic atmosphere. Recently, Ooyama (1990) and DeMaria (1995) have presented a diagnostic vertical velocity equation. Extending this, a general diagnostic equation for the vertical velocity component can be obtained with the hydrostatic approximation for a coordinate whose Jacobian is independent of time (Byun, 1999a):

$$\frac{\partial}{\partial s}\left(\tilde{\rho}c_{sound}^2\frac{\partial\hat{v}^3}{\partial s}\right) = -sign(\frac{\partial s}{\partial z})g\left[m^2\nabla_s\bullet\left(\frac{J_s\tilde{\rho}\hat{\mathbf{V}}_s}{m^2}\right) - J_sQ_\rho\right]$$

$$+\frac{\partial}{\partial s}\left[(\frac{\partial p}{\partial\tilde{\rho}}Q_\rho + \frac{\partial p}{\partial\zeta}Q_\zeta) - m^2\tilde{\rho}c_{sound}^2\nabla_s\bullet\left(\frac{\hat{\mathbf{V}}_s}{m^2}\right) - \hat{\mathbf{V}}_s\bullet\nabla_s p\right] \quad (5\text{-}23)$$

The diagnostic Equation 5-23 can be used to maintain mass consistency in meteorological data for air quality simulations.

It is worthwhile to note that the hydrostatic or nonhydrostatic atmospheric description, which is a characterization of the vertical motion, is rather independent from either the compressible/incompressible atmosphere or the anelastic atmosphere assumption, which is an approximation of the mass continuity equation. Choices of the assumptions from the two distinct groups have been used to simplify atmospheric motions, although some of the combinations, such as compressible but hydrostatic atmosphere, are rarely used in atmospheric studies.

5.2 Choice of Vertical Coordinate System for Air Quality Modeling

Figure 5-1 provides a pedigree of vertical coordinates used in many atmospheric models. Definitions of the coordinates are provided in Tables 5-1, 5-2 and 5-3. The hierarchy of classification is: (1) temporal dependency of coordinates, (2) base physical characteristic of coordinate variables, and (3) method of topography treatments. Application assumptions, such as hydrostatic or nonhydrostatic atmosphere approximations, are not part of the classification criteria. Isentropic coordinates are not included here because they are not suitable for the regional and urban scale air quality simulation due to their inherent difficulties representing planetary boundary layer (PBL) structure. For larger-scale simulations, an isentropic coordinate system can serve as an interesting alternative (Arakawa et al., 1992). Also, there are new developments of hybrid coordinates that combine isentropic coordinates with other coordinates to mitigate the problem.

Many different types of vertical coordinates have been used for various meteorological simulations. For example, the geometric height is used to study boundary layer phenomenon because of its obvious advantage of relating near surface measurements with modeled results. Pressure coordinates are natural choices for atmospheric studies because many upper atmospheric measurements are made on pressure surfaces. Because most radiosonde measurements are based on hydrostatic pressure, one may prefer use of the pressure coordinate to study cloud dynamics. This idea of using the most appropriate vertical coordinate for describing a physical process is referred to as a generic coordinate concept (Byun et al., 1995). Several different generic coordinates can be used in a CTM for describing different atmospheric processes while the underlying model structure should be based on a specific coordinate consistent with the preprocessor meteorological model. The Models-3 Community Multiscale Air Quality (CMAQ) modeling system allows users to choose a specific coordinate without having to exchange science process modules (i.e., subroutines with physical parameterizations for describing atmospheric processes) which are written in their generic coordinates. The coordinate transformation is performed implicitly through the use of Jacobian within CMAQ.

Byun (1999a) discusses key science issues related to using a particular vertical coordinate for air quality simulations. They include a governing set of equations for atmospheric dynamics and thermodynamics, the vertical component of the Jacobian, the form of continuity equation for air, the height of a model layer (expressed in terms of geopotential height), and other special characteristics of a vertical coordinate for either hydrostatic or nonhydrostatic atmosphere applications. Tables 5-1, 5-2 and 5-3 summarize properties of the popular time-independent vertical coordinates (e.g., terrain-influenced height and the reference hydrostatic pressure coordinate systems) and the time-dependent terrain-influenced coordinate systems, respectively.

Not only the assumptions on atmospheric dynamics, but also the choice of coordinate can affect the characteristics of atmospheric simulations. For the time-independent vertical coordinates (z, p_o, *sigma-z*, *sigma-p_o*), the vertical Jacobians are also time-independent. Especially with the hydrostatic assumption, one can obtain a diagnostic equation for the vertical velocity component , which includes soundwaves together with meteorological signals. Further assumptions on flow characteristics, such as anelastic approximation, provide a simpler diagnostic equation for the nonsolenoidal air flow. For such cases, with or without the anelastic approximation, one can maintain trace species mass conservation in a CTM by using the vertical velocity field estimated from the diagnostic relation. The scheme works whether the horizontal wind components, temperature, and density field data are directly provided from a meteorological model or interpolated from hourly data at the transport time step. This suggests that the mass error can be estimated with the diagnostic relations that originate from one of the governing equations of the preprocessor meteorological models. For a nonhydrostatic atmosphere, which does not have a special diagnostic relation for time independent coordinates, one should rely on the methods described below to account for the mass consistency errors.

For time dependent coordinates, the vertical Jacobians are also time dependent. In general, this makes it more difficult to derive a diagnostic relation from the continuity equation. However, for a coordinate with the Jacobian-weighted air density independent of height, a diagnostic equation for the vertical velocity is available when appropriate top and bottom boundary conditions are used. Vertical layers defined with this type of vertical coordinate are considered as material surfaces because mass continuity can be satisfied in a diagnostic fashion. Air particles are not expected to cross material surfaces during the advection process. An atmospheric model based on this type of coordinate may not have a mass consistency problem except for numerical reasons. The dynamic pressure coordinates based on true air density belong to this category, which includes such coordinates as π -coordinate, σ_π-coordinate, and the η -coordinate defined in conjunction with σ_π (See Table 5-3). A meteorological model using one of these coordinates will conserve mass within the limits of numerical errors expected from finite differencing and computer precision. For these coordinates, one can apply the same mass conservation procedure for both hydrostatic and nonhydrostatic cases. Note that the diagnostic relations obtained by appropriate choices of coordinates and assumptions on atmospheric dynamics allow estimation of the density error term in the continuity equation. This information can be used to reconstruct mass-consistent air density and wind fields that ensure mass conservation of pollutant species in air quality models.

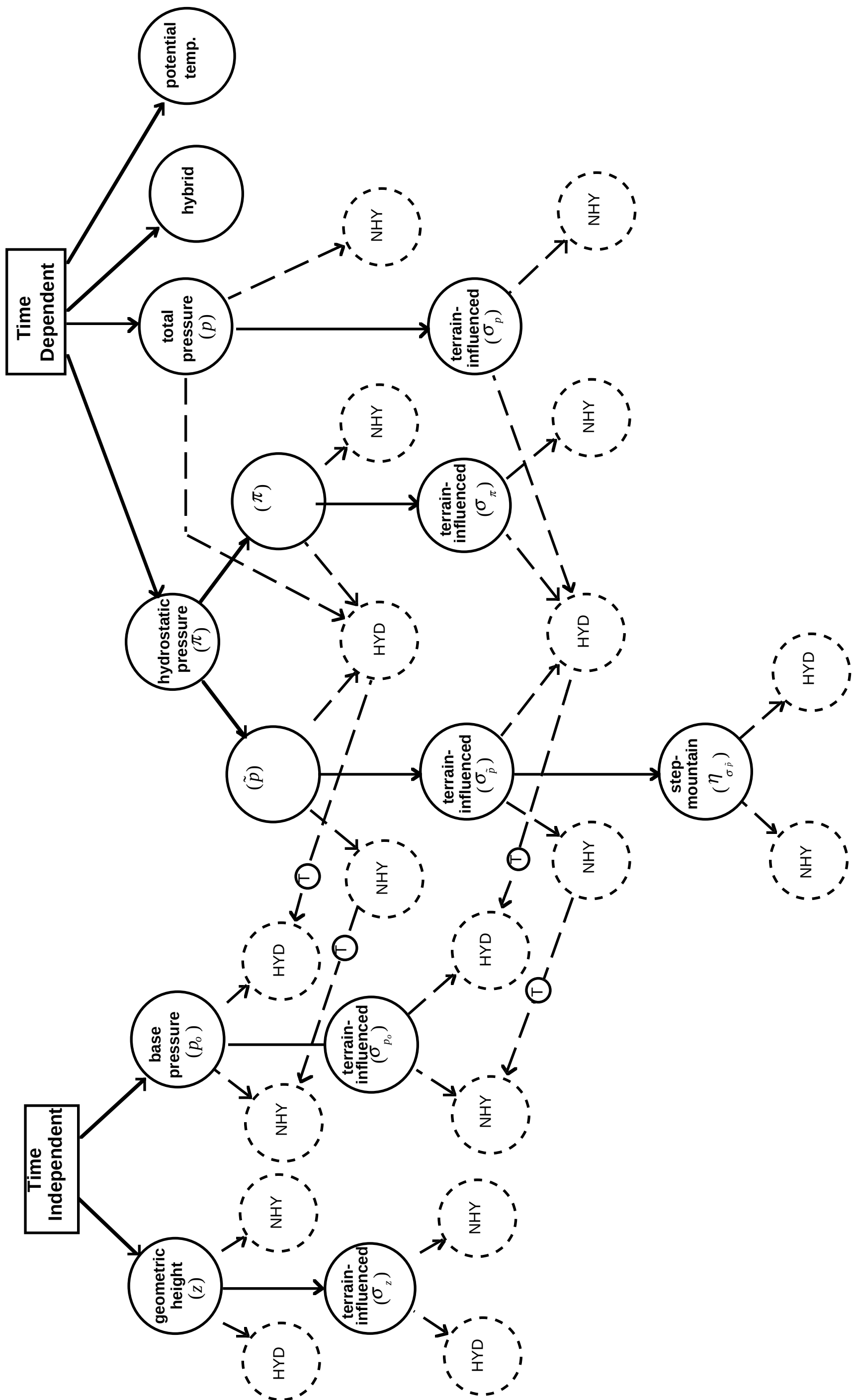

Figure 5-1. Pedigree of meteorological vertical coordinates. The encircled T symbol represents that the associated coordinates are identical when temporal dependency is ignored. Dashed-circles show that all the coordinates can be used for hydrostatic (HYD) and nonhydrostatic (NHY) application, regardless of the dynamic characteristics of the variables used to define vertical coordinates.

Table 5-1. Summary of Characteristics of the Geometric Height and Pressure Coordinate Systems. [Note: HYD and NHY stand for hydrostatic and nonhydrostatic applications, respectively. D( ) and P( ) symbols are assigned for diagnostic and prognostic formulas with equation numbers. ρ_o and $\tilde{\rho}$ are the reference and dynamic (time-dependent) hydrostatic pressure, respectively.]

Coordinate	vertical velocity	Vertical Jacobian	Geopotential height
geometric height (z)	NHY: w with P(5-9) or P(5-9') HYD: D(5-23)	$J_z=1$ constant in $(\hat{x}^1,\hat{x}^2,\hat{x}^3,t)$	$\Phi = gz$
reference hydrostatic pressure (p_o) $\frac{\partial p_o}{\partial z} = -\rho_o(z)g$	NHY: P(5-9) or P(5-9') HYD: D(5-23)	$J_{p_o} = (\rho_o g)^{-1}$ constant in $(\hat{x}^1,\hat{x}^2,t)$	$\Phi = \Phi_{sfc} - \int_{p_{osfc}}^{p_o} \frac{dp_o'}{\rho_o}$
dynamic hydrostatic pressure (π), $\frac{\partial \pi}{\partial z} = -\rho(x,y,z,t)g$	$\hat{v}^3 = \dot{\pi} = -\int_{\pi_T}^{\pi} [m^2 \nabla_{\pi'} \bullet \left(\frac{\hat{\mathbf{V}}_\pi}{m^2}\right) - \frac{Q_\rho}{\rho}] d\pi'$ for both NHY & HYD	$J_\pi = (\rho g)^{-1}$ but, $\rho J_\pi = 1/g$ constant in $(\hat{x}^1,\hat{x}^2,\hat{x}^3,t)$	$\Phi = \Phi_{sfc} - \int_{\pi_{sfc}}^{\pi} \frac{d\pi'}{\rho}$
large-scale hydrostatic pressure $(\tilde{p})$, $\frac{\partial \tilde{p}}{\partial z} = -\tilde{\rho}(x,y,z,t)g$	NHY: P(5-9) or P(5-9') for perturbation component HYD: $\hat{v}^3 = \dot{\tilde{p}} = -\int_{\tilde{p}_T}^{\tilde{p}} [m^2 \nabla_{\tilde{p}} \bullet \left(\frac{\hat{\mathbf{V}}_{\tilde{p}}}{m^2}\right) - \frac{Q_\rho}{\tilde{\rho}}] d\tilde{p}$	$J_{\tilde{p}} = (\tilde{\rho} g)^{-1}$	$\Phi = \Phi_{sfc} - \int_{\tilde{p}_{sfc}}^{\tilde{p}} \frac{d\tilde{p}'}{\tilde{\rho}}$

Table 5-2. Summary of Time Independent Terrain-influenced Height and Reference Hydrostatic Pressure Coordinate Systems. [Note: D( ) and P( ) symbols are assigned for diagnostic and prognostic formulas with equation numbers, respectively, and '$\neq f(\,)$' represents that the parameter is not dependent on the argument.]

Coordinate	Application	Vertical Momentum	Vertical Jacobian	Geopotential height
normalized geometric height (σ_z) $\sigma_z = \frac{z - z_{sfc}}{H - z_{sfc}}$	hydrostatic	D(5-23)	$J_{\sigma_z} = H - z_{sfc}$ $\neq f(\hat{x}^3, t)$	$\Phi = gz =$ $g[z_{sfc} + \sigma_z (H - z_{sfc})]$
	generalized hydrostatic	P(5-9) or, P(5-9') with Eq.(5-10)		
	non-hydrostatic			
terrain-influenced reference pressure (σ_{p_o}) $\sigma_{po} = \frac{p_o - p_T}{p_o(z_{sfc}) - p_T}$	hydrostatic	D(5-23)	$J_{\sigma_{Po}} = \frac{p_o^*}{\rho_o(\hat{x}^3) g}$ $\neq f(t)$, $p_o^* = p_o(z_{sfc}) - p_T$	$\Phi = \Phi_{sfc} - \int_{\sigma_{Posfc}}^{\sigma_{po}} \frac{p_o^*}{\rho_o} d\sigma_{po}'$
	non-hydrostatic	P(5-9) or, P(5-9') with Eq.(5-10) for perturbation component		

Table 5-3. Summary of Characteristics of the Time Dependent Terrain-influenced Coordinate Systems.

<table>
<tr><th>Coordinate</th><th>Application</th><th>Vertical Momentum</th><th>Vertical Jacobian</th><th>Geopotential height</th></tr>
<tr><td rowspan="2">terrain-influenced hydrostatic pressure (σ_π)
$\sigma_\pi = \frac{\pi - \pi_T}{\pi_{sfc} - \pi_T}$</td><td>hydrostatic</td><td rowspan="2">$\pi^* \dot{\sigma}_\pi \Big|_{\sigma_{\pi T}}^{\sigma_\pi}$
$= \int_{\sigma_{\pi T}}^{\sigma_\pi} [\pi^* \frac{Q_\rho}{\rho} - m^2 \nabla_{\sigma_\pi} \bullet \frac{\pi^* \hat{\mathbf{V}}_{\sigma_\pi}}{m^2}] \, d\sigma'_\pi$
$-(\sigma_\pi - \sigma_{\pi T}) \frac{\partial \pi^*}{\partial t}$</td><td>$\tilde{\rho} J_{\sigma_{\tilde{p}}} = \frac{\tilde{p}^*}{g}$
$\neq f(\hat{x}^3)$</td><td>$\Phi = \Phi_{sfc} - \int_{\sigma_{\tilde{p}sfc}}^{\sigma_{\tilde{p}}} \frac{\tilde{p}^*}{\tilde{\rho}} d\sigma_{\tilde{p}}'$</td></tr>
<tr><td>non-hydrostatic</td><td>$\pi^* = \pi_{sfc} - \pi_T$
$\rho J_{\sigma_\pi} = \frac{\pi^*}{g}$
$\neq f(\hat{x}^3)$</td><td>$\Phi = \Phi_{sfc} - \int_{\sigma_{\pi sfc}}^{\sigma_\pi} \frac{\pi^*}{\tilde{\rho}} d\sigma_\pi'$</td></tr>
<tr><td>terrain-influenced large-scale hydrostatic pressure $(\sigma_{\tilde{p}})$</td><td>non-hydrostatic</td><td>P(5-9) or, P(5-9') with Eq.(5-10) for perturbation component when $\tilde{p}$ and $\tilde{\rho}$ given</td><td>$\tilde{\rho} J_{\sigma_{\tilde{p}}} = \frac{\tilde{p}^*}{g}$
$\neq f(\hat{x}^3)$</td><td>$\Phi = \Phi_{sfc} - \int_{\sigma_{\tilde{p}sfc}}^{\sigma_{\tilde{p}}} \frac{\tilde{p}^*}{\tilde{\rho}} d\sigma_{\tilde{p}}'$</td></tr>
<tr><td rowspan="2">step-mountain eta (η) with
σ_π,
$\eta = \sigma_\pi \eta_{sfc}$,
$\eta_{sfc} = \frac{p_o(z_{sfc}) - p_T}{p_o(0) - p_T}$</td><td>hydrostatic</td><td rowspan="2">$\frac{\partial \pi^*}{\partial t} = \frac{1}{\eta_{sfc}} \int_0^{\eta_{sfc}} [\pi^* \frac{Q_\rho}{\rho} - m^2 \eta_{sfc} \nabla_\eta \bullet \frac{\pi^* \hat{\mathbf{V}}_\eta}{m^2 \eta_{sfc}}] \, d\eta'$

$\pi^* \dot{\eta} \Big|_0^\eta = -\eta \frac{\partial \pi^*}{\partial t} +$
$\int_0^\eta [\pi^* \frac{Q_\rho}{\rho} - m^2 \eta_{sfc} \nabla_\eta \bullet \frac{\pi^* \hat{\mathbf{V}}_\eta}{m^2 \eta_{sfc}}] \, d\eta'$</td><td>$J_\eta = \frac{\tilde{p}^*}{\tilde{\rho} g \eta_{sfc}}$
$\tilde{\rho} J_\eta \neq$
$f(\hat{x}^3)$</td><td>$\Phi = \Phi_{sfc} - \int_{\eta_{sfc}}^{\eta} \frac{\tilde{p}^*}{\tilde{\rho} \eta_{sfc}} d\eta'$</td></tr>
<tr><td>non-hydrostatic</td><td>$J_\eta = \frac{\pi^*}{\rho g \eta_{sfc}}$
$\rho J_\eta \neq$
$f(\hat{x}^3)$</td><td>$\Phi = \Phi_{sfc} - \int_{\eta_{sfc}}^{\eta} \frac{\pi^*}{\rho \eta_{sfc}} d\eta'$</td></tr>
<tr><td>step-mountain ETA $(\eta_{\sigma_{\tilde{p}}})$ with $\sigma_{\tilde{p}}$,
$\eta_{\sigma_{\tilde{p}}} = \sigma_{\tilde{p}} \eta_{sfc}$</td><td>non-hydrostatic</td><td>P(5-9) or, P(5-9') with Eq.(5-10) for perturbation component when $\dot{\eta}_{\sigma_{\tilde{p}}}$, $\tilde{\rho}$ provided</td><td>$J_\eta = \frac{\tilde{p}^*}{\tilde{\rho} g \eta_{sfc}}$</td><td>$\Phi = \Phi_{sfc} - \int_{\eta_{sfc}}^{\eta} \frac{\tilde{p}^*}{\tilde{\rho} \eta_{sfc}} d\eta'$</td></tr>
</table>

5.3 Coupling of Meteorology and Air Quality

Characteristics of air quality model simulations are heavily dependent on the quality of the meteorological data. Meteorological data for air quality can be provided either by diagnostic models, which analyze observations at surface sites and upper air soundings, or by dynamic models with or without four-dimensional data assimilation (FDDA). Readers are referred to Seaman (1999) for a state-of-science review on this topic. In the next section a dynamic modeling with FDDA approach, which is used in the Models-3 CMAQ system, is described.

5.3.1 Meteorological Data for Air Quality Modeling

Meteorological simulations are applied to drive a CTM for solving atmospheric diffusion equations for trace species. For regional scale simulations, whose problem size is continental scale or somewhat smaller, hydrostatic meteorological models have been used, usually with FDDA. For small scale simulations where topographic effects are important, nonhydrostatic or compressible atmospheric models are used. These differences in the assumptions used for atmospheric characterization affect air quality simulations greatly.

Meteorological data can be supplied by running dynamic models prognostically, or with the archived reanalysis data routinely available as a part of numerical weather forecasting for air quality simulations (Schulze and Turner, 1998). Currently, GCIP (GEWAX Continental-scale International Project) provides an archive of the Eta model reanalysis of surface and upper air fields at 48 km resolution (Leese, 1993; Kalany et al., 1996). Based on the success of GCIP, the National Center for Environmental Prediction (NCEP), NOAA, is planning to archive regional reanalysis at a higher resolution. Similarly, the Mesoscale Analysis and Prediction System/Rapid Update Cycle (MAPS/RUC) of the Forecast Systems Laboratory (FSL), NOAA, produces accurate and timely analyses and short-term forecasts at 40-60 km resolutions (Benjamin et al., 1995, 1998). The output data are archived at 1-3 hour intervals on 25-34 levels. These alternative data sources are promising because of the wealth of observation data used for the reanalysis and the availability of long-term meteorological characterization data suitable for seasonal or annual assessment studies.

5.3.2 Off-line and On-line Modeling Paradigms

Air quality models are run many times to understand the effects of emissions control strategies on the pollutant concentrations using the same meteorological data. A non-coupled prognostic model with FDDA can provide adequate meteorological data needed for such operational use. This is the so-called off-line mode air quality simulation. However, a successful air quality simulation requires that the key parameters in meteorological data be consistent. For example, to ensure the mass conservation of trace species, the density and velocity component should satisfy the continuity equation accurately. Details of this issue will be discussed below.

If air quality is solved as a part of the meteorology modeling, this data consistency problem would be much less apparent. Dynamic and thermodynamic descriptions of operational meteorological models should be self-consistent, and necessary meteorological parameters are readily available at the finite time steps needed for the air quality process modules during the numerical integration. The ultimate goal within atmospheric community is the development of a fully integrated meteorological-chemical model (Seaman, 1995). This is the so-called on-line mode air quality simulation. There have been a few successful examples of integrating meteorology and atmospheric chemistry algorithms into a single computer program (e.g., Vogel et al., 1995). For certain research purposes, such as studying two-way interactions of radiation processes, the on-line modeling approach is needed. However, the conventional on-line modeling approach, where chemistry-transport code is imbedded in one system, exhibits many operational difficulties. For example, in addition to tremendously increasing the computer resource requirements, differences in model dynamics and code structures hinder development and maintenance of a fully coupled meteorological/chemical/emissions modeling system for use in routine air quality management.

Figure 5-2 shows structures of the on-line and off-line air quality modeling systems, respectively, commonly used at present time. Table 5-4 compares a few characteristics of on-line and off-line modeling paradigms. Each method has associated pros and cons. Therefore, in the future versions of the Models-3 CMAQ system, we intend to realize both on-line and off-line modes of operations through the use of an advanced input/output (I/O) applications programming interface (API) (Coats, 1996). Figure 5-3 provides a schematic diagram of the implementation idea. A proof-of-concept research effort using MM5 and a prototype version of CMAQ is underway (Xiu et al., 1998). However, to accomplish the goals of multiscale on-line/off-line modeling with one system, a full adaptation of the one-atmosphere concept is needed.

Development of the fully coupled chemistry-transport model to a meteorological modeling system requires a fundamental rethinking of the atmospheric modeling approach in general. Some of the suggested requirements for a next generation mesoscale meteorological model that can be used as a host of the on-line/off-line modeling paradigms are:

- **Scaleable dynamics and thermodynamics:** Use fully compressible form of governing set of equations and a flexible coordinate system that can deal with multiscale dynamics.

- **Unified governing set of equations:** Not only the weather forecasting, dynamics and thermodynamics research but also the air quality studies should rely on the same general governing set of equations describing the atmosphere.

- **Cell-based mass conservation:** As opposed to the simple conservation of domain total mass, cell-based conservation of the scalar (conserving) quantities is needed. Use of proper state variables, such as density and entropy, instead of pressure and temperature, and representation of governing equations in the conservation form rather than in the advective form are recommended.

- **State-of-the-art data assimilation method:** Not only the surface measurements and upper air soundings, but also other observation data obtained through the remote sensing and other in situ means must be included for the data assimilation.

- **Multiscale physics descriptions:** It has been known that certain parameterizations of physical processes, including clouds, used in present weather forecasting models are scale dependent. General parameterization schemes capable of dealing with a wide spectrum of spatial and temporal scales are needed.

The Weather Research & Forecasting (WRF) Modeling System (Dudhia et al., 1998), which is under development by scientists at NCAR and NOAA, could meet most of the above requirements. Therefore, the WRF modeling system has the potential to be the future meteorological model of the Models–3 CMAQ system to provide the multiscale on-line/off-line air quality modeling capability simultaneously.

	Off-line Modeling	**On-line Modeling**
Dynamic Consistency	• Need sophisticated interface processors • Need careful treatment of meteorology data in AQM	• Easier to accomplish, but must have proper governing equations. • Meteorology data available as computed
Process Interactions	• No two-way interactions between meteorology and air quality	• Two-way interaction • Small error in meteorological data will cause large problem in air quality simulation (positive feedback problem).
System Characteristics	• Systems maintained at different institutions • Modular at system level. Different algorithms can be mixed and tested • Large and diverse user base • Community Involvement	• Proprietary ownership • Expensive in terms of computer resource need (memory and CPU) • Unnecessary repeat of computations for control strategy study • Low flexibility • Limited user base • Legacy complex code, which hinders new development
Application Characteristics	• Easy to test new science concept • Efficient for emissions control study • Good for independent air quality process study	• Difficult to isolate individual effects • Excellent for studying feedback of met. and air quality

Table 5-4. Comparison of On-line and Off-line Modeling Paradigms

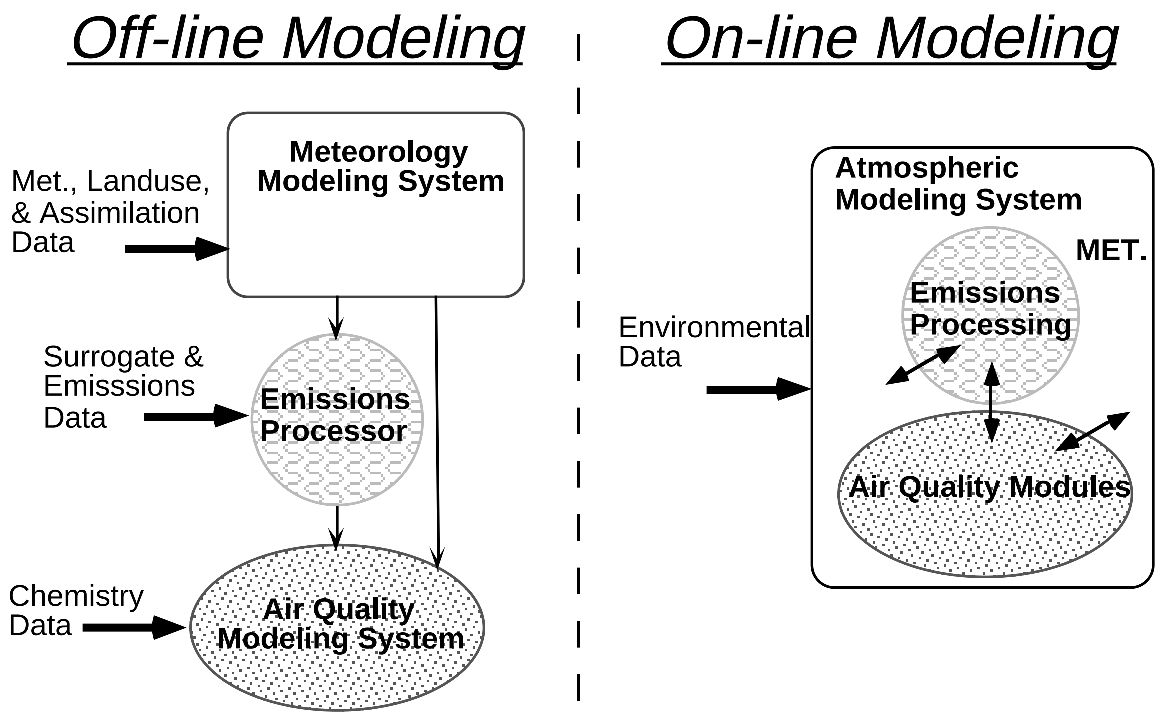

Figure 5-2. Current On-line and Off-line Air Quality Modeling Paradigms

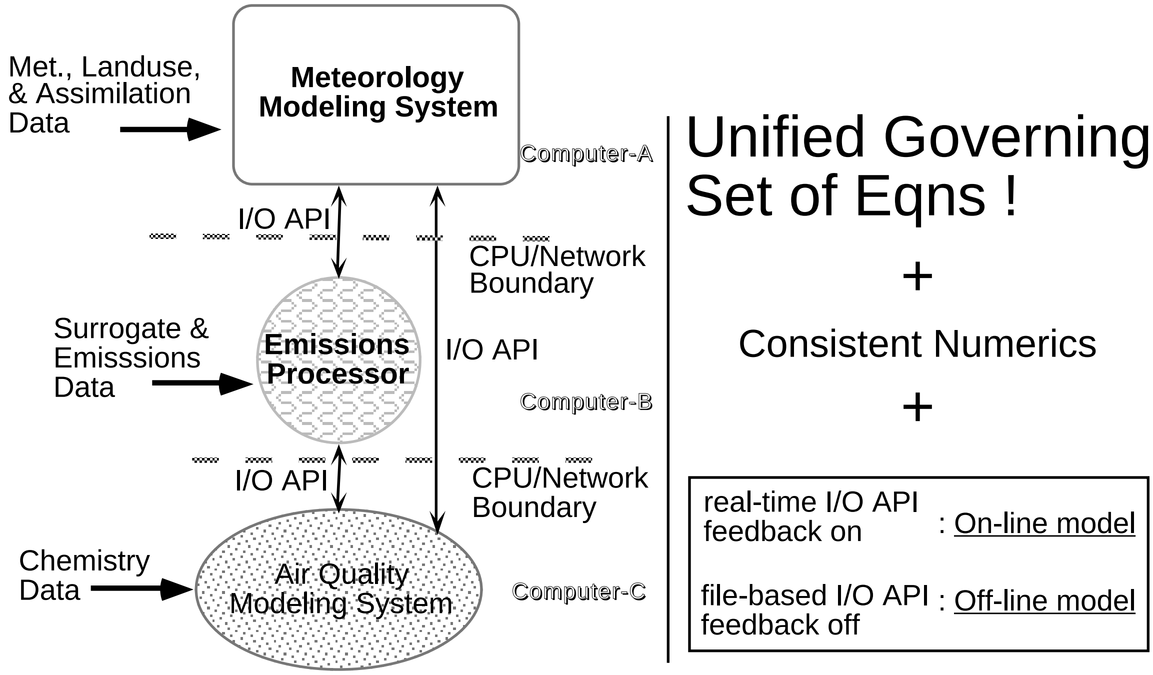

Figure 5-3. Proposed One-atmosphere Air Quality Modeling Paradigms. Double arrowhead lines represent possibility of two-way coupling. The coupling of independent modeling components is accomplished through the I/O API linking the cooperating executables.

5.4 Mass Conservation

For air quality simulations, mass conservation is the most important physical constraint. This is because it is unrealistic to have injection of primary pollutant mass through any other means than a real source emission process, and also because the little perturbations in the mass of both primary and secondary pollutants will jeopardize the correct simulation of reactions among trace species. Therefore, conserving mass of a passive primary trace species is a necessary property of an air quality model.

5.4.1 Mass Consistency in Meteorological Data

The main objective of many meteorological models has been to predict synoptic or mesoscale weather phenomena. Therefore, major design considerations are focused on such issues important for energy conservation, resolving a spectrum of different wavelengths, and energy cascade under nonlinear wave-wave interactions. Conservation of mass is not usually emphasized as the other constraints listed. Also, the predictive quantities are generally thermodynamic parameters, such as temperature and pressure. The conservation equation for air density is rarely solved directly in meteorological models because of little operational use of air density for weather forecasting and no direct measurements to compare. Usually it is estimated from the equation for the state of ideal gas or from a hydrostatic relation when hydrostatic assumptions are made. Even the predictive equations for the moisture variables are often written in an advective form rather than a continuity equation form. On the other hand, air quality simulation relies mostly on the continuity equation. The success of a simulation is heavily dependent on the consistency of density and wind data (i.e., how well they satisfy the continuity equation).

The mass inconsistency in density and wind fields from a meteorological model is most likely caused by one or more of the following reasons:

1. Many meteorological models do not use the proposed ideal set of governing equations. A continuity equation for air is not used as one of the prognostic equations and air density is usually a diagnostic parameter in meteorological models.

2. The prognostic equation for temperature is often used to represent thermodynamics of the atmosphere. It is well known that temperature is not a good conserving parameter.

3. Removal of hydrometeors due to condensation or sublimation may subtract and add mass and heat to the moist atmosphere making the system nonadiabatic (thermodynamically irreversible) and not mass-conserving.

4. Numerical schemes used in meteorological models are designed to conserve energy, entropy, rather than the mass of air.

5. The FDDA and overall assimilation process, including the effects of Newtonian forcing terms in the momentum and temperature equations, may cause inadvertent modification of the energy balance and subsequent perturbation of air density resulting in mass conservation problems.

6. Heat, moisture and momentum flux exchanges at the surface-atmosphere interface may affect the air density distribution. Usually this effect is not significant as it is often neglected with the Boussinesq approximation.

7. Flux exchanges at the nesting boundaries for nested runs affect mass balance.

8. Energy and mass balance characteristics of cloud modules used influence air and moisture density fields.

9. Data output time steps are too large to capture the dynamic variations in the meteorological models. If temporally averaged data are provided from the meteorology model this problem can be minimized (Scamarock, 1998).

5.4.2 Techniques for Mass Conservation in Air Quality Models

As presented in Byun (1999b), species mixing ratios (c_i / ρ) is a useful conserved quantity for photochemical Eulerian air quality modeling, in particular. In limited area atmospheric modeling like an urban or a regional scale simulation, the total air mass in the simulation domain is subject to the inflow conditions determined by large synoptic scale weather systems. In this situation, the conservation of pollutant mass in the modeling domain can be difficult unless the density and wind fields are perfectly mass consistent. When the mass inconsistency in the meteorological fields is expected, the conservation equation for mixing ratio must be used as a necessary condition to ensure exact conservation of pollutant mass. This is accomplished by replacing the right-hand-side term of Equation 5-11 with $Q_{c_i} = c_i \frac{Q_\rho}{\rho}$. Then, the conservation equation for pollutant species is rewritten as:

$$\frac{\partial(c_i J_s)}{\partial t} + m^2 \nabla_s \bullet \left(\frac{c_i J_s \hat{\mathbf{V}}_s}{m^2} \right) + \frac{\partial(c_i J_s \hat{v}^3)}{\partial s} = c_i J_s \frac{Q_\rho}{\rho} \tag{5-24}$$

This adjustment alone is not sufficient to conserve pollutant mass when the density error term is not small. Equation 5-24 shows that the correction term has the same form as a first-order chemical reaction whose reaction rate is determined by the normalized air density error term. Table 7-5 in Chapter 7 in this document summarizes correction methods discussed in Byun (1999b). Among these, the method based on the two-step procedure (i.e., solving the *lhs* of Equation 5-24 first followed by the mass correction step solving for *rhs*) is expected to be the most accurate:

$$(c_i J_s)^{cor} = \frac{(c_i J_s)^T}{(\rho J_s)^T} (\rho J_s)^{\text{int}}, \tag{5-25}$$

where superscripts *cor*, *int*, and *T* represent corrected, transported (advected), and interpolated quantities, respectively. It should be noted that J_s in Equation 5-25 must not be canceled out even for a coordinate with time independent J_s because the spatial variation of the Jacobian must be taken into account for the numerical advection. In the event the total air mass in the computational domain fluctuates, this correction procedure would affect air quality predictions. In general, the air quality prediction can be as good as the density prediction of the meteorological model. However, considering the nonlinear interactions of trace species in the chemical production/loss calculations, one could expect serious effects on air quality simulations when the quality of meteorology data is in doubt.

Byun (1999b) also provides an alternative method to deal with the mass inconsistency in meteorological data through the modification of wind field, while keeping the density field intact, before solving the species conservation equation. Assuming a modified wind field exists that eliminates the source term in the continuity equation for air, the relationship between the original and modified wind components is given as:

$$\hat{\mathbf{V}}_s^M = \hat{\mathbf{V}}_s + \frac{1}{2\alpha_1^2} \nabla_s \lambda \tag{5-26a}$$

$$\hat{v}^{3M} = \hat{v}^3 + \frac{1}{2\alpha_3^2} \frac{\partial \lambda}{\partial s} \tag{5-26b}$$

where λ is the Lagrangian multiplier to be determined and α_1 and α_3 are the weights for the horizontal and vertical wind components. λ must satisfy the Poisson equation

$$m^2\nabla_s \bullet \left[\frac{\rho J_s}{2\alpha_1^2 m^2}\nabla_s\lambda\right] + \frac{\partial}{\partial s}[\frac{\rho J_s}{2\alpha_3^2}\frac{\partial\lambda}{\partial s}] = J_s Q_\rho, \tag{5-27}$$

with the associated boundary conditions:

$\lambda = 0$ for flow-through boundaries; and

$\partial\lambda / \partial s = 0$ for impenetrable boundaries (i.e., at the topographic surface).

The modified wind components are subject to the same top and bottom boundary conditions imposed by the given coordinate system and dynamic assumptions.

The main difference in the two proposed correction methods, correction after advection versus correction of wind fields before advection, is practically philosophical. Should we process a CTM using meteorological data as supplied, then correct possible errors in the species concentrations, or should we modify the velocity field to be mass consistent before the computation of trace gas concentrations in the CTM? The answer to this question lies in whether the air quality modeling need is satisfied with simple mixing ratio conservation with the adjustment process or not. In case the source-receptor relation is important, it is preferable to maintain the linearity of transport process using the mass-consistent wind components, which have been modified at the expense of truthfulness of meteorological fields. In practice, a combination of both methods is needed. The mass consistency error in the meteorological data must be corrected before air quality simulations with the wind-field adjustment method and the mixing ratio correction method Equation 5-25 should be applied to compensate the numerical differences in advection processes between meteorological and air quality models.

5.4.3 Temporal Interpolation of Meteorological Data

Byun (1999b) discusses a mass-conservative temporal interpolation method to complement the mass inconsistency correction. Temporal interpolations of density and velocity data are often required in a CTM because the meteorological model output has a coarser temporal resolution than the transport time step (which is usually the synchronization time step for a CTM using a fractional time-step method).

The Jacobian and density at a time $t_\alpha = (1-\alpha)t_n + \alpha t_{n+1}$ between the two consecutive output time steps, t_n and t_{n+1}, are interpolated with linearity assumed:

$$(J_s)_\alpha = (1-\alpha)(J_s)_n + \alpha(J_s)_{n+1} \tag{5-28a}$$

$$(\rho J_s)_\alpha = (1-\alpha)(\rho J_s)_n + \alpha(\rho J_s)_{n+1} \tag{5-28b}$$

where $0 \le \alpha \le 1$. It is obvious that the functional form of the Jacobian (which depends on a vertical coordinate) changes the characteristic of density interpolation. The premise used here is that the Jacobian is a fundamental quantity that determines the coordinate system. When the Jacobian is interpolated to define the vertical layers through linear interpolation, all other components involved in the mass conservation equation need to be interpolated accordingly. Wind components multiplied with the Jacobian-weighted density are interpolated linearly:

$$(\rho J_s \hat{\mathbf{V}}_s)_\alpha = (1-\alpha)(\rho J_s \hat{\mathbf{V}}_s)_n + \alpha(\rho J_s \hat{\mathbf{V}}_s)_{n+1} \tag{5-29a}$$

$$(\rho J_s \hat{v}^3)_\alpha = (1-\alpha)(\rho J_s \hat{v}^3)_n + \alpha(\rho J_s \hat{v}^3)_{n+1} \tag{5-29b}$$

and interpolated wind components are derived with:

$$(\hat{\mathbf{V}}_s)_\alpha = \frac{(\rho J_s \hat{\mathbf{V}}_s)_\alpha}{(\rho J_s)_\alpha} \tag{5-30a}$$

$$(\hat{v}^3)_\alpha = \frac{(\rho J_s \hat{v}^3)_\alpha}{(\rho J_s)_\alpha} \tag{5-30b}$$

However, the proposed scheme, Equation 5-28b, has a problem in such cases where the finite difference value of (ρJ_s) cannot approximate the linear interpolation of the time rate change of the quantity, $\frac{\partial(\rho J_s)}{\partial t}$, adequately. Usually, this tendency term is not available with the meteorological data. However, when the tendency is available or can be estimated with the diagnostic relations for certain meteorological coordinate systems, a different interpolation rule must be sought. Because the tendency term, not (ρJ_s) itself, is a component of the continuity equation, linear interpolation of the tendency may be more appropriate. Then, (ρJ_s) at the interpolation time step must be estimated in such a way that satisfies the continuity as well as the tendency term (Byun 1999b).

5.5 Conclusion

In this chapter I attempted to bridge the information gap between dynamic meteorologists and air quality modelers and to promote the proper use of meteorological information in air quality modeling studies. It highlights the importance of dynamic consistency in meteorological and air quality modeling systems. The effects of the common assumptions used for the atmospheric study on the mass conservation for trace species have been reviewed. Although meteorological data provided by operational meteorological models are usually self-consistent, air quality modelers need to evaluate the data for exact consistency before they can be used in air quality simulation. Minor adjustment of the meteorological data may be needed to assure mass conservation of trace gas species in CTMs. Also, characteristics of vertical coordinates have been discussed. Certain coordinates provide diagnostic relations that can be used to maintain mass consistency in meteorological fields. When meteorological data are needed at sub-output time steps within CTM, the interpolation of the data should be done in such a way that the mass conservation and consistency in the thermodynamic variables are not compromised.

In addition, the on-line and off-line modeling concepts are discussed to provide design guidance for fully integrated meteorological-chemical models. To realize the noble goal of implementing the one-atmosphere modeling system, both the multi-pollutant chemistry and multiscale physics capability in meteorology are needed. The following are the features that make the CMAQ air quality model a suitable key component of an one-atmosphere modeling system:

- Flexible chemistry representations through a mechanism reader;
- Comprehensive list of atmospheric processes that are implemented;
- Modular coding structure and versatile data handling method;
- Capability to handle multiscale dynamics and thermodynamics;
- Fully compressible governing set of equations in generalized coordinates; and
- Robust mixing ratio conservation scheme, even with mass inconsistent meteorology data.

At present, we are encouraged by the efforts of the WRF meteorology model development groups that focus on issues such as choice of coordinates, grid staggering method, state variables in the governing equations (e.g., fully compressible), conservation properties (mass and energy) both in the model equations and numerics, modularity of code, data communication methods, and coding language. This entails continuous exchange of ideas between the Models-3 CMAQ and WRF modeling groups.

To achieve the true one-atmosphere modeling system, we must address multi-pollutant and multiscale processes that are typically broader than any one group (or institution) has expertise to address. The need is well summarized in Dennis (1998):

> Considering additional needs for emerging environmental problems such as coastal eutrophication and ecological damage issues related with cross-media purview, encompassing the one-atmosphere scope is needed. This means we have to work with a more complete one-atmosphere description to facilitate interactions within it as efficiently as broadly as possible. One potential answer is to foster a community modeling perspective and model system framework that is supported and used by a critical fraction of the scientific community.

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Appendix 5A. Tensor Primer and Derivation of the Continuity Equation in a Generalized Curvilinear Coordinate System

The Appendix 5A summarizes essential information needed for understanding the governing equations represented in tensor form. It includes tensor primer and derivation of the continuity equation in a generalized coordinate system. Readers are referred to classic references such as Dutton (1976), Defrise (1964), and Pielke (1984) for the details.

5A.1 Tensor Analysis in a Curvilinear Coordinate System

Cartesian coordinates are those curvilinear systems in which the positions of fluid elements are determined by their distance from intersecting planes. Although the Cartesian coordinates with orthogonal intersecting planes are specifically called rectangular, the adjective rectangular is often dropped. To represent formulations governing atmospheric phenomena in a coordinate system other than a rectangular Cartesian one, a tensor representation is often used. This generally involves determination of the unit vectors in the new system, determination of the components of a tensor with respect to theses unit vectors, and determination of the differential derivatives (e.g., divergence, curl, and gradient) of a tensor. All these quantities depend explicitly on the form of the new coordinate system and it is always convenient to express these quantities in a rectangular Cartesian coordinate system for comparison purposes.

In atmospheric modeling one is frequently led to adopt a curvilinear coordinate system other than the Cartesian coordinates depending on the problem under consideration. A general curvilinear coordinate system can be defined relative to a Cartesian system $\mathbf{x} = (x^1, x^2, x^3)$ represented by three families of curved surfaces

$$\hat{x}^i = \psi_i(x^1, x^2, x^3, t),\ i = 1,2,3 \qquad \text{(5A-1)}$$

Here, the symbols with carat (^) are used to denote a transformed curvilinear system. In vector form, it is given as:

$$\hat{\mathbf{x}} = \boldsymbol{\psi}(\mathbf{x}, t). \qquad \text{(5A-2)}$$

When the curvilinear system ψ is at rest relative to the rectangular Cartesian system, i.e., independent of time, $\hat{x}^i = \psi_i(x^1, x^2, x^3)$, then the system is called a Euclidean system. Here we assume that components of vector $\hat{\mathbf{x}}$, $(\hat{x}^1, \hat{x}^2, \hat{x}^3)$, are three independent, single-valued, and differentiable scalar point functions such that to every point of some region $\hat{\Re}$ of three-dimensional Euclidean space, there is a corresponding unique triple of values (x^1, x^2, x^3) in the Cartesian space $\Re$. In other words, the function ψ prescribes one and only one value of $\boldsymbol{x}$ and is such that the three coordinates are independent of each other. Also, we assume continuity of the function ψ. Then the new coordinates $\hat{\mathbf{x}}$ are called curvilinear and the surfaces $\hat{x}^1 = \psi_1 =$ constant, $\hat{x}^2 = \psi_2 =$ constant, $\hat{x}^3 = \psi_3 =$ constant are called coordinate surfaces. The curvilinear coordinates $(\hat{x}^1, \hat{x}^2, \hat{x}^3)$ should be independent, single-valued, and differentiable. As shown in

Figure 5A-1, the vector $\overrightarrow{OP}$ pointing a parcel of air enclosed by the boundary $\partial\Omega$ can be represented either in Cartesian or Euclidean curvilinear coordinate systems.

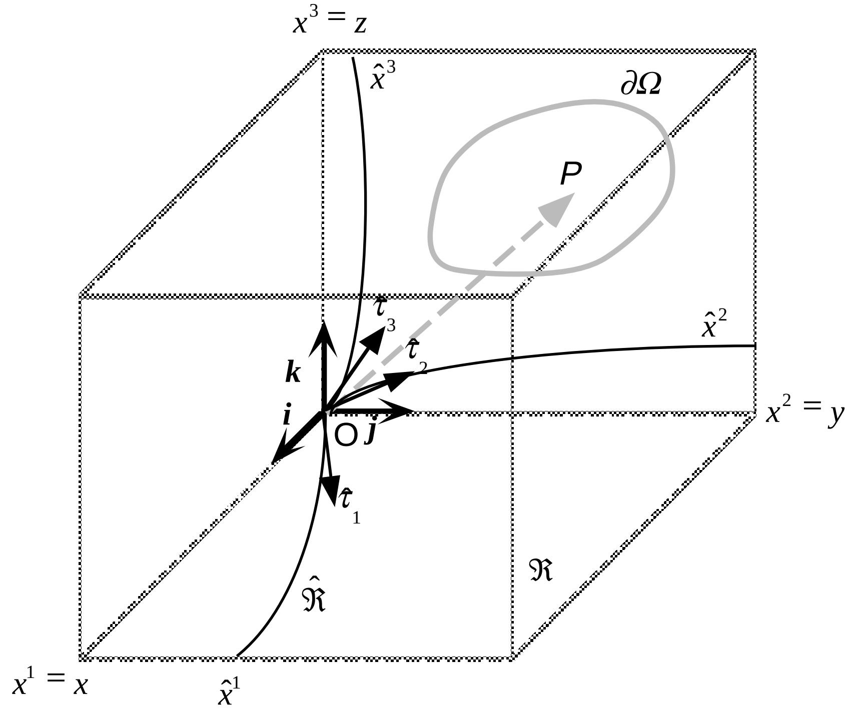

Figure 5A-1. Coordinates of the Cartesian and Curvilinear Coordinates. $\Re$ and $\hat{\Re}$ represent Cartesian and Euclidean spaces, respectively.

Note that the transformation involves with not only the spatial variables but also time as an independent variable. We need a tensor calculus in the four variables of space-time with regard to the coordinate transformations. Defrise (1964) used the term ‘world tensor’ to distinguish it from the time independent Euclidean tensor.

5A.2 Basis Vectors

In a rectangular coordinate system, directions of the basis vectors are constant in space. However, in a general curvilinear coordinates, directions of the basis vectors will vary from point to point and no one set of directions can be regarded as more natural than any other for the directions of base vectors to define the local base vectors. Usually, an upper index denotes contravariant, and a lower index denotes covariant tensors, respectively.

With the coordinates defined by Equation 5A-2, the chain rule provides the two expansions:

$$d\mathbf{x} = \frac{\partial \mathbf{x}}{\partial \hat{x}^j} d\hat{x}^j \tag{5A-3}$$

$$d\hat{x}^i = \frac{\partial \hat{x}^i}{\partial x^j} dx^j = (\nabla \hat{x}^i) \bullet d\mathbf{x} \qquad (5A\text{-}4)$$

Here, the Einstein summation convention (i.e., the repeated indices on two quantities that are multiplied by each other are summed over) has been implied. The symbol (•) represents the inner product. An inner product of two vectors yields a scalar that is invariant of the coordinate system. An inner product of two tensors results in contraction of the rank in the resulting tensor.

From Equations 5A-3 and 5A-4, we can form two distinct sets of basis vectors. One is the tangential vectors:

$$\hat{\boldsymbol{\tau}}_i = \frac{\partial \mathbf{x}}{\partial \hat{x}^j} \qquad (5A\text{-}5)$$

that reveals the variation of the position vector as it traces out a curve in which $\hat{x}^j$ varies and the other two coordinates are constant. Hence $\hat{\boldsymbol{\tau}}_i$ is tangent to the curve along which only $\hat{x}^j$ varies. The other set of basis vectors is the normal vectors of the surfaces where $\hat{x}^i$ = constant:

$$\hat{\boldsymbol{\eta}}^i = \nabla \hat{x}^i \qquad (5A\text{-}6)$$

While there could be many choices, the tangential ($\hat{\boldsymbol{\tau}}_i$) and normal ($\hat{\boldsymbol{\eta}}^j$) vectors are considered as a natural choice for the local basis vectors for the curvilinear coordinate system. Using Equations 5A-5 and 5A-6, one can show that:

$$\hat{\tau}_i \otimes \hat{\eta}^j = \delta_i^j = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \qquad (5A\text{-}7)$$

where δ_i^j is the Kronecker delta and the symbol $\otimes$ represents the outer product. Outer product of two tensors with rank r_1 and r_2 yields a tensor with rank (r_1+r_2).

A curvilinear system is not orthogonal when not all the off-diagonal components of $\hat{\eta}^i \otimes \hat{\eta}^j$ and $\hat{\tau}_i \otimes \hat{\tau}_j$ vanish. The orthogonal curvilinear coordinate system is often used for interesting engineering problems that can be described with simple geometric orthogonal coordinates, such as spherical, cylindrical coordinate systems. Usually, meteorological coordinates are not orthogonal and therefore, the vector calculus specific for the orthogonal curvilinear coordinates must not be used.

5A.3 Distance and Metric Tensor in a Curvilinear Coordinate System

The differential element of distance *ds* can be expressed in terms of the curvilinear coordinates as:

$$(ds)^2 = dx_i dx^i = \frac{\partial x^i}{\partial \hat{x}^j} d\hat{x}^j \frac{\partial x^i}{\partial \hat{x}^k} d\hat{x}^k = \frac{\partial x^i}{\partial \hat{x}^j}\frac{\partial x^i}{\partial \hat{x}^k} d\hat{x}^j d\hat{x}^k = \hat{\gamma}_{jk} d\hat{x}^j d\hat{x}^k \qquad (5A\text{-}8)$$

$$\hat{\gamma}_{jk} = \frac{\partial x^i}{\partial \hat{x}^j}\frac{\partial x^i}{\partial \hat{x}^k} = \hat{\boldsymbol{\tau}}_j \otimes \hat{\boldsymbol{\tau}}_k \tag{5A-9}$$

Because of its obvious role in the measurement of distance, the quantity $\hat{\gamma}^{ik}$ is called the metric tensor. It is a symmetric tensor. As such, it has an inverse matrix $\hat{\gamma}^{ik}$, which will satisfy following condition:

$$\hat{\gamma}^{ik} = \frac{\partial \hat{x}^i}{\partial x^l}\frac{\partial \hat{x}^k}{\partial x^l} = \hat{\boldsymbol{\eta}}^i \otimes \hat{\boldsymbol{\eta}}^k \tag{5A-10}$$

$$\hat{\gamma}_{ij}\hat{\gamma}^{ik} = \delta_j^k = \begin{cases} 1 & j = k \\ 0 & j \neq k \end{cases} \tag{5A-11}$$

The Levi-Cevita symbol ε used in Equation 5-1 is an antisymmetric tensor defined as

$$\varepsilon^{ijk} = \begin{cases} 0 & if \;\; i = j, \;\; j = k, \;\; or \;\; i = k \\ 1 & if \;\; i, j, k \;\; are \;\; an \;\; even \;\; permutation \;\; of \;\; 1,2,3 \\ -1 & if \;\; i, j, k \;\; are \;\; an \;\; odd \;\; permutation \;\; of \;\; 1,2,3 \end{cases} \tag{5A-12}$$

Using the Levi-Cevita symbol, the cross vector product $\mathbf{A} = \mathbf{B} \times \mathbf{C}$ can be written as $A^i = \varepsilon^{ijk} B_j C_k$.

One of the uses of the metric tensor and its inverse is for converting a covariant tensor to a contravariant tensor, and vice versa. Another important usage of the metric tensor is the estimation of the Jacobian determinant of the transformation, which is defined as:

$$J = \sqrt{\hat{\gamma}} = \sqrt{\det(\hat{\gamma}_{ij})} = \sqrt{[\det(\hat{\gamma}^{ij})]^{-1}} \tag{5A-13}$$

where $J = \left|\{J_x^{\hat{x}}\}\right| = \left|\frac{\partial(x_1, x_2, x_3)}{\partial(\hat{x}_1, \hat{x}_2, \hat{x}_3)}\right|$. Note that the Jacobian matrix and the metric tensor are related as:

$$\hat{\gamma}_{ij} = \{J_x^{\hat{x}}\}^T \{J_x^{\hat{x}}\} \tag{5A-14}$$

A necessary and sufficient condition that $(\hat{x}^1, \hat{x}^2, \hat{x}^3)$ be orthogonal at every point in $\Re$ is that the components of the metric tensor vanish for $i \neq j$.

5A.4 Covariant Tensor and Contravariant Tensor

In this section, the covariant and contravariant tensor concepts are presented using a vector, which is a simple form of a tensor (i.e., a tensor of rank one). A distance in a Euclidean space can be represented in two corresponding sets of tangential basis vectors:

$$ds = d\hat{x}^j \hat{\tau}_j = dx^l \tau_l \tag{5A-15}$$

where

$$\hat{\tau}_j = \frac{\partial x^l}{\partial \hat{x}^j} \tau_l \tag{5A-16}$$

Any vector that transforms similarly to the tangential basis vector $\hat{\boldsymbol{\tau}}_j$ is called as a covariant vector. On the other hand, when a vector transforms like the local normal basis vectors $\hat{\boldsymbol{\eta}}^i$, we call it a contravariant vector:

$$\hat{v}^k = \frac{\partial \hat{x}^k}{\partial x^j} v^j, \tag{5A-17}$$

where v^j is the components of **V** with respect to the normal base vectors.

Since a vector **A** is invariant between coordinate systems, we can express it using either contravariant components (i.e., with the tangential basis vectors) or covariant components (i.e., with the normal basis vectors):

$$\mathbf{A} = A_j \hat{\eta}^j = A^l \hat{\tau}_l \tag{5A-18}$$

Using Equation 5A-7, one can readily find the covariant and contravariant components with:

$$A_j = \mathbf{A} \bullet \hat{\tau}_j \tag{5A-19a}$$

$$A^i = \mathbf{A} \bullet \hat{\eta}^i \tag{5A-19b}$$

5A.5 Derivatives, Total Derivative, and Divergence in Euclidean Coordinate

Covariant derivative of a contravariant vector is defined as:

$$\hat{V}^i_{;k} = \frac{\partial \hat{V}^i}{\partial \hat{x}^k} + \hat{\Gamma}^i_{kj} \hat{V}^j, \quad \hat{\Gamma}^i_{kj} = \frac{\partial \hat{x}^i}{\partial x^l} \frac{\partial^2 x^l}{\partial \hat{x}^k \partial \hat{x}^j}. \tag{5A-20}$$

Similarly, covariant derivative of a covariant vector is defined as:

$$\tilde{A}_{i;k} = \frac{\partial \tilde{A}^i}{\partial \tilde{x}^k} - \tilde{\Gamma}^l_{ki} \tilde{A}^l, \quad \tilde{\Gamma}^l_{ki} = \frac{\partial \tilde{x}^l}{\partial x^r} \frac{\partial^2 x^r}{\partial \tilde{x}^k \partial \tilde{x}^i}. \tag{5A-21}$$

The Christoffel symbol $\hat{\Gamma}^i_{kj}$ is not a tensor but it is an important quantity relating the derivatives in the curvilinear coordinate system with those in the original Cartesian coordinate system. Its relation with the metric tensor is:

$$\hat{\Gamma}^i_{kj} = \frac{1}{2}\hat{\gamma}^{jl}\left(\frac{\partial \gamma_{il}}{\partial \hat{x}^k} + \frac{\partial \gamma_{kl}}{\partial \hat{x}^i} - \frac{\partial \gamma_{ik}}{\partial \hat{x}^l}\right) \tag{5A-22}$$

Divergence of a contravariant vector $\hat{\boldsymbol{W}}$, wind for example, can be expressed as:

$$\hat{W}^i_{;i} = \frac{\partial \hat{W}^i}{\partial \hat{x}^i} + \hat{\Gamma}^i_{ij}\hat{W}^j = \frac{\partial \hat{W}^i}{\partial \hat{x}^i} + \frac{\hat{W}^j}{\sqrt{\hat{\gamma}}}\frac{\partial \sqrt{\hat{\gamma}}}{\partial \hat{x}^j}$$

$$= \frac{1}{\sqrt{\hat{\gamma}}}\left\{\sqrt{\hat{\gamma}}\frac{\partial \hat{W}^i}{\partial \hat{x}^i} + \hat{W}^j\frac{\partial \sqrt{\hat{\gamma}}}{\partial \hat{x}^j}\right\} = \frac{1}{\sqrt{\hat{\gamma}}}\frac{\partial(\sqrt{\hat{\gamma}}\hat{W}^i)}{\partial \hat{x}^i} \tag{5A-23}$$

The total derivative of a covariant vector $\boldsymbol{A}$ is represented in a Cartesian coordinate as

$$\frac{d\mathbf{A}}{dt} = \frac{\partial \mathbf{A}}{\partial t} + \mathbf{v} \bullet \nabla \mathbf{A} = \frac{\partial A_i}{\partial t} + \hat{v}^j\frac{\partial A_i}{\partial \hat{x}^j} \tag{5A-24}$$

where $\mathbf{v} \bullet \nabla = v^l\frac{\partial}{\partial x^l} = \hat{v}^j\frac{\partial x^l}{\partial \hat{x}^j}\frac{\partial}{\partial x^l} = \hat{v}^j\frac{\partial}{\partial \hat{x}^j}$ was used. This expression is correct in any holonomic coordinate system where the covariant component A_i, metric tensor, velocity, and x^k all refer to the same system whether or not the coordinate system is time dependent.

5A.6 Continuity Equation in Generalized Curvilinear Coordinate System

Many practical coordinate systems used for atmospheric studies are time dependent. Consider the case when a volume element that confines the fluid moves with the fluid. Then, this is also the velocity of the fluid in the respective coordinate system. A direct conversion from the continuity equation expressed in a Cartesian coordinate system does not work because the divergence term should take into account for the time rate change of volume element as well the same for the time dependent curvilinear coordinates. In this situation, the Lie derivative concept (e.g., Bishop and Goldberg, 1968) becomes appropriate. A Lie derivative is obtained by differentiating a function with respect to the parameters along the moving frame of reference. Following Defrise (1964), one can show that a Lie derivative of a mass volume integral along the moving frame vanishes:

$$\mathcal{L}(\delta M) = 0 \tag{5A-25}$$

where $\delta M = \rho \delta V = \rho\sqrt{\hat{\gamma}}\delta\hat{V}$, $\delta V = \delta x^1 \delta x^2 \delta x^3$, and $\delta\hat{V} = \delta\hat{x}^1\delta\hat{x}^2\delta\hat{x}^3$. Therefore:

$$\delta\hat{V}\mathcal{L}(\rho\sqrt{\hat{\gamma}}) = \delta\hat{V}\left(\hat{v}^\mu\frac{\partial \rho\sqrt{\hat{\gamma}}}{\partial \hat{x}^\mu} + \rho\sqrt{\hat{\gamma}}\frac{\partial \hat{v}^\mu}{\partial \hat{x}^\mu}\right)$$

$$= \delta\hat{V}\frac{\partial(\rho\sqrt{\hat{\gamma}}\hat{v}^\mu)}{\partial \hat{x}^\mu} = 0 \tag{5A-26}$$

where, index μ = 1,4; $\hat{x}^4 = t$ and $\hat{v}^4 = 1$. Using the same notation convention, the contravariant velocity is defined as for the coordinates that moves with fluid:

$$\hat{v}^\mu = \frac{\partial \hat{x}^\mu}{\partial x^\alpha} v^\alpha;\ \alpha, \mu = 1,4 \tag{5A-27}$$

Note that one cannot derive the same result by directly replacing the divergence term in the continuity equation for a Cartesian coordinate system because the volume element is dependent on time as well.

Alternatively, one can obtain Equation 5A-26 by a method based on the finite derivative of a volume integral with the application of the Leibnitz rule. This method of derivation helps to visualize the meaning of terms in the equation more clearly than the procedure based on the Lie derivative. Volume integral in a Cartesian coordinates is defined as:

$$F = \iiint_{\partial\Omega} f(x^1, x^2, x^3) \delta V \tag{5A-28}$$

where *f* is a conservative quantity, such as density or total kinetic energy. Equation 5A-28 can be rewritten in the curvilinear coordinate as:

$$F = \iiint_{\partial\Omega} f(\hat{x}^1, \hat{x}^2, \hat{x}^3) \sqrt{\hat{\gamma}} \delta \hat{V} \tag{5A-29}$$

For example, if *f* =1:

$$F = \iiint_{\partial\Omega} \delta V = V_{\partial\Omega} = \iiint_{\partial\Omega} \sqrt{\hat{\gamma}} \delta \hat{V} = \sqrt{\hat{\gamma}} \hat{V}_{\partial\Omega} \tag{5A-30}$$

The meaning of the metric becomes very clear–it is a measure of volume correction for the transformed coordinates.

$$F = \iiint_{\partial\Omega} f(\hat{x}^1, \hat{x}^2, \hat{x}^3) \sqrt{\hat{\gamma}} \delta \hat{V} = \iiint_{\partial\Omega} h(\hat{x}^1, \hat{x}^2, \hat{x}^3) \delta \hat{x}^1 \delta \hat{x}^2 \delta \hat{x}^3 \tag{5A-31}$$

where $h(\hat{x}^1, \hat{x}^2, \hat{x}^3) = f(\hat{x}^1, \hat{x}^2, \hat{x}^3) \sqrt{\hat{\gamma}}$ was used.

Consider a time derivative following the control volume. Applying a three-dimensional version of Leibnitz rule for the time differential of the integral, we get:

$$\left. \frac{\delta F}{\delta t} \right|_{\substack{following \\ volume}} = \frac{\delta}{\delta t} \iiint_{\partial\Omega} h(\hat{x}^1, \hat{x}^2, \hat{x}^3) \delta \hat{x}^1 \delta \hat{x}^2 \delta \hat{x}^3$$

$$= \iiint_{\partial\Omega} \left(\frac{\partial h}{\partial t} \right)_{\hat{x}^1, \hat{x}^2, \hat{x}^3} \delta \hat{x}^1 \delta \hat{x}^2 \delta \hat{x}^3$$

$$+\int_{\hat{x}_a^2}^{\hat{x}_b^2}\int_{\hat{x}_a^3}^{\hat{x}_b^3}\left[h(\hat{x}_b^1,\hat{x}^2,\hat{x}^3)\frac{d\hat{x}_b^1}{dt}-h(\hat{x}_a^1,\hat{x}^2,\hat{x}^3)\frac{d\hat{x}_a^1}{dt}\right]\delta\hat{x}^3\delta\hat{x}^2$$

$$+\int_{\hat{x}_a^1}^{\hat{x}_b^1}\int_{\hat{x}_a^2}^{\hat{x}_b^2}\left[h(\hat{x}^1,\hat{x}^2,\hat{x}_b^3)\frac{d\hat{x}_b^3}{dt}-h(\hat{x}^1,\hat{x}^2,\hat{x}_a^3)\frac{d\hat{x}_a^3}{dt}\right]\delta\hat{x}^2\delta\hat{x}^1$$

$$+\int_{\hat{x}_a^3}^{\hat{x}_b^3}\int_{\hat{x}_a^1}^{\hat{x}_b^1}\left[h(\hat{x}^1,\hat{x}_b^2,\hat{x}^3)\frac{d\hat{x}_b^2}{dt}-h(\hat{x}^1,\hat{x}_a^2,\hat{x}^3)\frac{d\hat{x}_a^2}{dt}\right]\delta\hat{x}^1\delta\hat{x}^3 \tag{5A-32}$$

Then, using the following relation with the aid of Figure 5A-2:

$$\int_{\hat{x}_a^2}^{\hat{x}_b^2}\frac{\partial}{\partial\hat{x}^2}h\left(\left.\frac{d\hat{x}^2}{dt}\right|_{bd}\right)\delta\hat{x}^2 = h(\hat{x}_b^2)\frac{d\hat{x}_b^2}{dt}-h(\hat{x}_a^2)\frac{d\hat{x}_a^2}{dt} \tag{5A-33}$$

we obtain an integral equation:

$$\left.\frac{\delta F}{\delta t}\right|_{\substack{following\\volume}} = \iiint_{\partial\Omega}\left\{\frac{\partial h}{\partial t}+\frac{\partial}{\partial\hat{x}^1}\left(h\left.\frac{d\hat{x}^1}{dt}\right|_{bd}\right)+\frac{\partial}{\partial\hat{x}^2}\left(h\left.\frac{d\hat{x}^2}{dt}\right|_{bd}\right)+\frac{\partial}{\partial\hat{x}^3}\left(h\left.\frac{d\hat{x}^3}{dt}\right|_{bd}\right)\right\}\delta\hat{x}^1\delta\hat{x}^2\delta\hat{x}^3 \tag{5A-34}$$

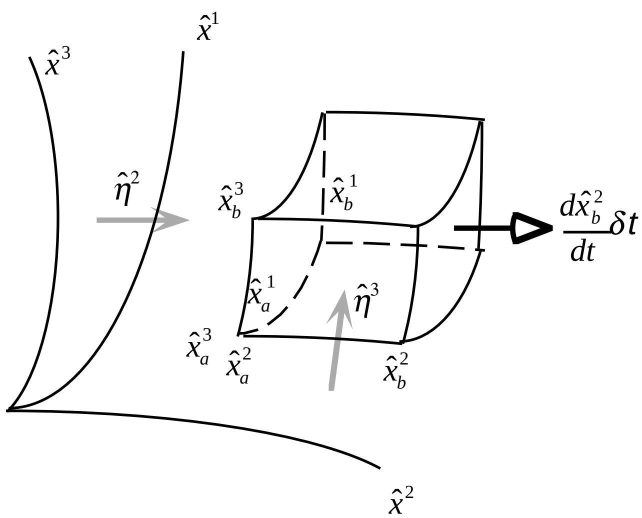

Figure 5A-2. Volume Element in a Curvilinear Coordinate System

When $f = \rho$ (density), then $F = \iiint_{\partial\Omega}\rho(x^1,x^2,x^3)\delta x^1\delta x^2\delta x^3 = M$ = mass of the volume element.

Therefore, the conservation law states:

$$\left.\frac{\delta F}{\delta t}\right|_{\substack{following\\volume}} = \left.\frac{\delta M}{\delta t}\right|_{\substack{following\\volume}} = 0 \qquad (5A\text{-}35)$$

Here, for example, $\left.\frac{d\hat{x}^2}{dt}\right|_{bd}$ is the velocity of the boundary of the volume element in the curvilinear coordinate $\hat{x}^2$. Because the volume element confines the fluid and moves with the fluid, this is velocity component of the fluid in the curvilinear coordinate $\hat{x}^2$. Then, we have

$$\iiint_{\partial\Omega}\left[\frac{\partial(\rho\sqrt{\hat{\gamma}})}{\partial t} + \frac{\partial(\rho\sqrt{\hat{\gamma}}\hat{v}^j)}{\partial \hat{x}^j}\right]\delta\hat{V} = 0 \qquad (5A\text{-}36)$$

Since above integral should be satisfied for an arbitrarily infinitesimal volume element, we obtain the continuity equation in differential equation form for the time-dependent curvilinear coordinate as follows:

$$\frac{\partial(\rho\sqrt{\hat{\gamma}})}{\partial t} + \frac{\partial(\rho\sqrt{\hat{\gamma}}\hat{v}^j)}{\partial \hat{x}^j} = 0 \qquad (5A\text{-}37)$$