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The Conservation Equations for Multicomponent Gas Mixtures in Arbitrary Coordinate Systems

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THE CONSERVATION equations for multicomponent reacting gas mixtures are generally given only in Cartesian or orthogonal curvilinear coordinate systems. Actually, the conservation equations are easily expressed in an arbitrary coordinate system. We present the general equations in tensor notation and then indicate the simplifications which arise for orthogonal curvilinear coordinates.

Let us consider a multicomponent gas mixture consisting of s different species which we identify by Greek subscripts. If Y_α is the mass fraction of species α, ρ is the density, v_i is the mass average velocity of the mixture, and $V_{\alpha i}$ is the diffusion velocity of species α, then the general equations for conservation of mass of component α, total mass, momentum, and energy may be written, respectively, as†

$$(\partial/\partial t)(\rho Y_\alpha) + (\rho Y_\alpha v^i)_{;i} + (\rho Y_\alpha V_\alpha{}^i)_{;i} = \omega_\alpha \tag{1}$$

$$(\partial\rho/\partial t) + (\rho v^i)_{;i} = 0 \tag{2}$$

$$\rho(\partial v_i/\partial t) + \rho v^j v_{i;j} = -P_i{}^j{}_{;j} + \rho \sum_{\alpha=1}^{s} Y_\alpha F_{\alpha i} \tag{3}$$

$$(\partial/\partial t)(\rho e) + (\rho e v^i)_{;i} = -Q^i{}_{;i} - P^{ij} v_{i;j} + \rho \sum_{\alpha=1}^{s} Y_\alpha V_\alpha{}^i F_{\alpha i} \tag{4}$$

Here ω_α is the mass rate of production of species α per unit volume by chemical reactions, P_{ij} represents the total stress tensor, and $F_{\alpha i}$ is the body force per unit mass acting on the component α. In Eq. (4) the quantity e represents the total internal energy of the mixture per unit mass, and Q_i denotes the total energy flux vector. English subscripts refer to covariant components, and superscripts identify contravariant components of the tensors.

In Eqs. (1) through (4) use is made of the summation convention for repeated English indices. The semicolon represents covariant differentiation with respect to the coordinates whose indices follow it. The covariant derivative of a tensor $A_{ij}{}^k$, for example, is given by

$$A_{ij}{}^k{}_{;l} = (\partial A_{ij}{}^k/\partial x^l) - A_{rj}{}^k \left\{ {r \atop i\,l} \right\} - A_{ir}{}^k \left\{ {r \atop j\,l} \right\} + A_{ij}{}^r \left\{ {k \atop r\,l} \right\} \tag{5}$$

where the Christoffel symbol of the second kind is defined by the relation

$$\left\{ {k \atop i\,j} \right\} = (1/2) g^{kl} [(\partial g_{il}/\partial x^j) + (\partial g_{jl}/\partial x^i) - (\partial g_{ij}/\partial x^l)] \tag{6}$$

In Eq. (6) the quantity g_{ij} is the metric tensor which defines the coordinate system by means of the expression for the invariant infinitesimal distance,

$$ds^2 = g_{ij} dx^i dx^j \tag{7}$$

In an orthogonal curvilinear coordinate system the metric tensor is diagonal and we can define the quantities $h_i = \partial s/\partial x^i$ by the equation

$$g_{ij} = \begin{bmatrix} (h_1)^2 & 0 & 0 \\ 0 & (h_2)^2 & 0 \\ 0 & 0 & (h_3)^2 \end{bmatrix} \tag{8}$$

It then becomes convenient to redefine a tensor in such a way that all of its components are of the same physical dimensions. This can be accomplished by dividing each covariant component i of the tensor by h_i and multiplying each contravariant component i by h_i. The new velocities u_i and $U_{\alpha i}$, body forces $f_{\alpha i}$, energy flux vector q_i, and stress tensor p_{ij} are therefore defined by the equations

$$\left. \begin{aligned} v_i &= h_i u_i \qquad [v^i = (1/h_i)\, u_i] \\ V_{\alpha i} &= h_i U_{\alpha i} \\ F_{\alpha i} &= h_i f_{\alpha i} \\ Q_i &= h_i q_i \\ P_{ij} &= h_i h_j p_{ij} \end{aligned} \right\} \tag{9}$$

The summation convention does not apply here nor in the following discussion because of the change in notation. The distinction between covariance and contravariance disappears in this formulation and we shall use subscripts for all indices.

By substituting Eq. (8) into Eq. (6) we find that, in orthogonal curvilinear coordinates, the relation

$$\left\{ {k \atop i\,j} \right\} = (\delta_{ik}/h_k)(\partial h_k/\partial x_j) + (\delta_{jk}/h_k)(\partial h_k/\partial x_i) - (h_i \delta_{ij}/h_k^2)(\partial h_i/\partial x_k) \tag{10}$$

is valid. Here δ_{ij} denotes the Kronecker delta. If Eqs. (9) and (10) are used in Eqs. (1) through (4), then the following simplified forms for the conservation equations are obtained:

$$(\partial/\partial t)(\rho Y_\alpha) + \sum_i \Big\{ (1/h_i)(\partial/\partial x_i)[\rho Y_\alpha (u_i + U_{\alpha i})] + [\rho Y_\alpha (u_i + U_{\alpha i})] \sum_{j \neq i} (1/h_j h_i)(\partial h_j/\partial x_i) \Big\} = \omega_\alpha \tag{11}$$

$$(\partial \rho/\partial t) + \sum_i [(1/h_i)(\partial/\partial x_i)(\rho u_i) + \rho u_i \sum_{j\neq i} (1/h_j h_i)(\partial h_j/\partial x_i)] = 0 \tag{12}$$

$$\begin{aligned} \rho(\partial u_i/\partial t) + \sum_j \rho u_j \{ (1/h_j)(\partial u_i/\partial x_j) + (1/h_i h_j)[u_i(\partial h_i/\partial x_j) - u_j(\partial h_j/\partial x_i)] \} = \\ - \sum_j \Big\{ (1/h_j)(\partial p_{ij}/\partial x_j) + p_{ij}(1/h_i h_j)[(\partial h_i/\partial x_j) - (h_i/h_j)(\partial h_j/\partial x_j) + \sum_k (h_i/h_k)(\partial h_k/\partial x_j)] - \\ p_{jj}(1/h_i h_j)(\partial h_j/\partial x_i) \Big\} + \rho \sum_{\alpha=1}^{s} Y_\alpha f_{\alpha i} \end{aligned} \tag{13}$$

$$\begin{aligned} (\partial/\partial t)(\rho e) + \sum_i [(1/h_i)(\partial/\partial x_i)(\rho e u_i + q_i) + (\rho e u_i + q_i) \sum_{j \neq i} (1/h_j h_i)(\partial h_j/\partial x_i)] = \\ - \sum_{i,j} \{ (p_{ij}/h_j)(\partial u_i/\partial x_j) + [(p_{jj}/h_j) - (p_{ij}/h_i)](u_i/h_j)(\partial h_i/\partial x_j) \} + \rho \sum_{\alpha=1}^{s} \Big(Y_\alpha \sum_i U_{\alpha i} f_{\alpha i} \Big) \end{aligned} \tag{14}$$

In Eqs. (13) and (14), use has been made of the symmetry of the pressure tensor p_{ij}. The derivation of Eqs. (11) through (14) for orthogonal curvilinear coordinates illustrates the method of application of the general conservation equations given in Eqs. (1) through (4).

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† For a discussion of the reasoning by which Eqs. (1) through (4) can be derived, see, for example, P. G. Bergmann, *Introduction to the Theory of Relativity*, Prentice-Hall, New York, 1942.