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 \( Y_\alpha \) is the mass fraction of species \( \alpha \), \( \rho \) is the density, \( V_\alpha \) is the mass average velocity of the mixture, and \( V_{\alpha i} \) is the diffusion velocity of species \( \alpha \), then the general equations for conservation of mass of component \( \alpha \), total mass, momentum, and energy may be written, respectively, as:

\[
\begin{align*}
\frac{\partial}{\partial t} (\rho Y_\alpha) + \nabla \cdot (\rho V_\alpha Y_\alpha) & = 0 \\
\frac{\partial}{\partial t} \rho V_\alpha + \nabla \cdot (\rho V_{\alpha i} V_i) & = 0 \\
\frac{\partial}{\partial t} \rho e + \nabla \cdot (\rho c_v T V_\alpha) + \nabla \cdot (\rho V_{\alpha i} V_i) & = 0
\end{align*}
\]

Here \( \rho \) is the mass rate of production of species \( \alpha \). The semicolon represents covariant differentiation with respect to the coordinates whose indices follow it. The covariant derivative of a tensor \( A_\alpha^i \), for example, is given by

\[
A_\alpha^i = \frac{\partial A_\alpha^i}{\partial x^j} - \Gamma^j_{ik} A_\alpha^k \]

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

\[
[\Gamma^j_{ik}] = \frac{1}{2} g^{jk} \left( \frac{\partial g_{ik}}{\partial x^j} + \frac{\partial g_{ij}}{\partial x^k} - \frac{\partial g_{jk}}{\partial x^i} \right)
\]

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,

\[
ds^2 = g_{ij} dx^i dx^j
\]

It 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 \( \dot{u}_\alpha \) and \( U_{\alpha i} \), body forces \( f_{\alpha i} \), energy flux vector \( q_\alpha \), and stress tensor \( \rho_{ij} \) are therefore defined by the equations

\[
\begin{align*}
\dot{u}_\alpha &= h_i u_i \\
V_{\alpha i} &= \frac{h_i}{h_j} V_{\alpha j} \\
f_{\alpha i} &= h_i f_{\alpha j} \\
Q_\alpha &= h_i Q_i \\
\rho_{ij} &= h_i h_j \rho_{ij}
\end{align*}
\]

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

\[
[\Gamma^j_{ik}] = (\delta_{ik}/h_k) (\partial h_k/\partial x_j) + (\delta_{ij}/h_i) (\partial h_i/\partial x_k) - (h_i h_j/h_k) (\partial h_k/\partial x_i)
\]

is valid. Here \( \delta_{ij} \) 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:

\[
\begin{align*}
\frac{\partial}{\partial t} (\rho Y_\alpha) + \sum_i [(1/h_i) (\partial/\partial x_i) (\rho V_{\alpha i} (u_i + U_{ai})) + \rho V_{\alpha i} (u_i + U_{ai})] \sum_j (1/h_j h_i) (\partial h_j/\partial x_i) &= 0 \\
\frac{\partial}{\partial t} (\rho V_\alpha) + \sum_i [(1/h_i) (\partial/\partial x_i) (\rho u_i + \rho u_i)] \sum_j (1/h_j h_i) (\partial h_j/\partial x_i) &= 0 \\
\frac{\partial}{\partial t} (\rho e) + \sum_i [(1/h_i) (\partial e/\partial x_i) (\rho u_i + q_i) + (\rho u_i + q_i)] \sum_j (1/h_j h_i) (\partial h_j/\partial x_i) &= 0
\end{align*}
\]

\[
\begin{align*}
\frac{\partial}{\partial t} (\rho e) + \sum_i [(1/h_i) (\partial e/\partial x_i) (\rho u_i + q_i) + (\rho u_i + q_i)] \sum_j (1/h_j h_i) (\partial h_j/\partial x_i) &= 0 \\
- \sum_i \frac{(p_{ij}/h_i)}{(\partial h_i/\partial x_i)} + [(p_{ij}/h_i) - (p_{ij}/h_i)] (u_i/h_i) (\partial h_i/\partial x_i) + \rho \sum_{a=1}^s (Y_a U_{a\alpha i}) + \rho \sum_{a=1}^s (Y_a U_{a\alpha i})
\end{align*}
\]

In Eqs. (3) and (4), 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).