Continuum Derivation of the Conservation Equations

The equations for conservation of mass, momentum, and energy for a one-component continuum are well known and are derived in standard treatises on fluid mechanics [1]–[3]. On the other hand, the conservation equations for reacting, multicomponent gas mixtures are generally obtained as the equations of change for the summational invariants arising in the solution of the Boltzmann equation (see Appendix D and [4] and [5]). One of several exceptions to the last statement is the analysis of von Kármán [6], whose results are quoted in [7] and are extended in a more recent publication [8] to a point where the equivalence of the continuum-theory and kinetic-theory results becomes apparent [9]. This appendix is based on material in [8].

The objective is to derive the conservation laws for multicomponent, reacting gas mixtures. To this end we invent a physical model consistent with continuum theory. The model involves the idea of a multicomponent continuum composed of coexistent continua, each obeying the laws of dynamics and thermodynamics, a notion which was first introduced by Stefan in 1871.* For an $N$-component gas mixture we presume the existence of $N$ distinct continua within any arbitrary volume, continuum $K$ corresponding to the chemical species $K$. The terms continuum $K$, species $K$ and component

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* We arrive at the model of simultaneous coexistent continua as the logical transcription to continuum theory of the fact that the entire volume is accessible to all of the different molecules in a gas mixture.
C.1. Definitions and Basic Mathematical Relations

$K$ will be used interchangeably, it being understood that each of these phrases refers to continuum $K$ of the coexistent continua so long as we are following the derivation of conservation laws from continuum theory. It is apparent that each space point in the multicomponent continuum has $N$ velocities $v^K_i (K = 1, 2, \ldots, N)$, one velocity for each of the coexistent continua.

Section C.1 contains relevant definitions and basic mathematical relations, which will be used in subsequent sections. In Sections C.2, C.3, and C.4 we treat, respectively, the equations for conservation of mass, momentum and energy. The results are shown to be equivalent to the relations obtained from the kinetic theory of nonuniform gas mixtures in Section C.5.

C.1. DEFINITIONS AND BASIC MATHEMATICAL RELATIONS

The multicomponent continuum is considered to be defined in regions of space, every point in a region being an interior point of the region. All properties of the $N$ continua, including the velocities $v^K_i (K = 1, 2, \ldots, N)$, are assumed to be described by functions continuously differentiably in all variables within the region. This statement will be said to define continuous flow for the multicomponent continuum.

The conservation equations for continuous flow of species $K$ will be derived by using the idea of a control volume $\tau^K(t)$ enclosed by its control surface $\sigma^K(t)$ and lying wholly within a region occupied by the continuum; here $t$ denotes the time. In this appendix only, the notation of Cartesian tensors will be used.* Let $x_i (i = 1, 2, 3)$ denote the Cartesian coordinates of a point in space. In Cartesian tensor notation, the divergence theorem for any scalar function belonging to the $K$th continuum $\alpha^K(x_i, t)$, becomes

$$\int_{\sigma^K} \alpha^K n^K_\sigma d\sigma = \int_{\tau^K} \alpha^K_i d\tau, \quad (1)$$

where $n^K_\sigma$ denotes the outward normal to the surface $\sigma^K$ and $\alpha^K_i$ represents the gradient of the scalar $\alpha^K$. For any vector function belonging to the $K$th continuum, $u^K_i(x_i, t)$, we have

$$\int_{\sigma^K} u^K_i n^K_\sigma d\sigma = \int_{\tau^K} u^K_i d\tau, \quad (2)$$

with $u^K_i$ denoting the divergence of the vector $u^K_i$.

* Repeated subscript indices imply summation over all allowed values of the indices. The practical necessity of employing cartesian tensor notation here forces us to adopt a notation differing in some other respects from that employed elsewhere in the book (for example, the use of superscript $K$ to identify species).
Consider that some property of the \( K \)th continuum has a density (per unit volume) equal to \( \alpha^K(x_i, t) \), and let \( A^K(t) \) be the amount of this property contained within the control volume \( \tau^K \). Thus

\[
A^K(t) = \int_{\tau^K} \alpha^K(x_i, t) \, d\tau.
\]

(3)

For example, if \( \alpha^K = \rho^K \) = the density of mass of species \( K \), then \( A^K \) is the total mass of species \( K \) contained within \( \tau^K \). The property \( \alpha^K \) has a density per unit mass of mixture equal to \( \beta^K(x_i, t) \), where

\[
\alpha^K = \rho \beta^K,
\]

(4)

with \( \rho = \sum_{K=1}^{N} \rho^K \) representing the density of mass for the fluid mixture.

The derivative \( dA^K/dt \) is defined to mean the time rate of change of \( A^K \) as the volume \( \tau^K \) and its surface \( \sigma^K \) move with the flow of species \( K \). Consider that equation (3) holds at a time \( t_0 \); at time \( t_0 + \Delta t \) the particles in \( \tau^K \) at \( x_i \) will have been displaced to new positions \( x'_i \) and will be contained within some new volume \( \tau^K(t_0 + \Delta t) = \tau'^K \) enclosed by a surface \( \sigma^K(t_0 + \Delta t) = \sigma'^K \); in general \( \tau^K \) and \( \sigma^K \) are different from \( \tau'^K \) and \( \sigma'^K \). Therefore,

\[
A^K(t_0 + \Delta t) = \int_{\tau'^K} \alpha^K(x'_i, t_0 + \Delta t) \, d\tau
\]

and

\[
\left( \frac{dA^K}{dt} \right)_{t=t_0} = \lim_{\Delta t \to 0} \left\{ \frac{1}{\Delta t} \left[ \int_{\tau^K} \alpha^K(x'_i, t_0 + \Delta t) \, d\tau - \int_{\tau^K} \alpha^K(x_i, t_0) \, d\tau \right] \right\}. \quad (5)
\]

It is demonstrated in Section C.6 that equation (5) is equivalent to the relation

\[
\frac{dA^K}{dt} = \int_{\tau^K} \left[ \frac{\partial \alpha^K}{\partial t} + (\alpha^K v_i^K)_{,i} \right] \, d\tau. \quad (6)
\]

Hence, using the divergence theorem given in equation (2), it is found that

\[
\frac{dA^K}{dt} = \int_{\tau^K} \frac{\partial \alpha^K}{\partial t} \, d\tau + \int_{\sigma^K} \alpha^K v_i^K n_i \, d\sigma. \quad (7)
\]

Equation (7) expresses the idea that the time rate of change of \( A^K \) in a flow, for an arbitrary volume \( \tau^K \) bounded by a surface \( \sigma^K \), is equal to the stationary rate of change of \( A^K \) in the interior of \( \tau^K \) plus the rate of change of \( A^K \) due to the movement of \( \tau^K \) and \( \sigma^K \).

Equation (6) may be rewritten in the equivalent form

\[
\frac{d}{dt} \left( \int_{\tau^K} \rho \beta^K \, d\tau \right) = \int_{\tau^K} \left[ \frac{\partial (\rho \beta^K)}{\partial t} + (\rho \beta^K v_i^K)_{,i} \right] \, d\tau. \quad (8)
\]
The overall transport equation for the multicomponent continuum is then obtained by summing over components, a procedure which is in accord with the idea of independent coexistent continua. We choose at the arbitrary time \( t \) all of the control volumes \( \tau^K \) to be coexistent, that is, \( \tau^K = \tau \) for all \( K \). We henceforth refer to a volume \( \tau \) thus defined as being of the multicomponent continuum at time \( t \). After summation, equation (8) becomes

\[
\sum_{K} \left( \frac{d}{dt} \int_{\tau^K} \rho \beta^K d\tau \right)_{\tau^K = \tau} = \int_{\tau^K} \left[ \frac{\partial}{\partial t} \left( \sum_{K} \rho \beta^K \right) + \sum_{K} (\rho \beta^K v^K_i) \right] d\tau.
\]  

C.2. CONTINUITY EQUATIONS

Denote by \( w^K \) the net production of mass of species \( K \) per unit volume per unit time. Since mass is neither created nor destroyed by chemical reactions but only converted from one species to another, it follows that

\[
\sum_{K} w^K = 0.
\]  

The conservation of the mass of species \( K \) in an arbitrary volume \( \tau^K \) is expressed by the equation

\[
\frac{d}{dt} \left( \int_{\tau^K} \rho Y^K d\tau \right) = \int_{\tau^K} w^K d\tau,
\]  

where \( Y^K \) is the mass or weight fraction of species \( K \) (that is, \( \rho^K = \rho Y^K \), and \( Y^K \) equals the mass of species \( K \) in unit mass of mixture). Let \( \beta^K = Y^K \) in equation (8); then equation (11) becomes

\[
\int_{\tau^K} \left[ \frac{\partial (\rho Y^K)}{\partial t} + (\rho Y^K v^K_i) \right] d\tau = 0,
\]  

and, since \( \tau^K \) is arbitrary,

\[
w^K = \frac{\partial (\rho Y^K)}{\partial t} + (\rho Y^K v^K_i).
\]  

Now let \( v^K_i \), the flow velocity for species \( K \), be represented as

\[
v^K_i = v'_i + \dot{v}^K_i,
\]  

where

\[
v'_i = \sum_{K} Y^K v^K_i.
\]  

The summation in equation (14) is extended over all \( N \) distinct chemical components. Thus \( v'_i \) is the mass-weighted average velocity of the fluid mixture, and \( V^K_i \) is said to denote the diffusion velocity of species \( K \). Since

\[
\sum_{K} Y^K = 1,
\]
it follows from equations (13) and (14) that
\[ \sum_{k} Y^k V^k_i = 0. \] (16)

Introducing equation (13) into equation (12) leads to the following equation for continuity of species \( K \):
\[ w^k = \frac{D}{Dt} (\rho Y^k) + \rho Y^k v'_i, + (\rho Y^k V^k_i),. \] (17)

where
\[ \frac{D}{Dt} (\cdot) = \frac{\partial}{\partial t} (\cdot) + v'_i (\cdot),. \] (18)

is the Euler total time derivative following the mass-weighted average motion of the multicomponent continuum. Summing equation (17) over all distinct components, in view of equations (10), (15), and (16), leads to the overall continuity equation
\[ \frac{D\rho}{Dt} + \rho v'_i, = 0. \] (19)

Equation (19) is evidently also the correct form of the continuity equation for a one-component system.

We may now transform equation (9) by using equations (18) and (19) to obtain a form which is useful for the derivation of the differential equations expressing conservation of momentum and energy:
\[ \sum_{k} \left( \frac{d}{dt} \int_{r^k} \rho \beta^k d\tau \right)_{r^k = \tau} = \int_{\tau} \left[ \frac{D\rho}{Dt} + \left( \rho \sum_{k} \beta^k V^k_i \right) \right] d\tau, \] (20)

where
\[ \beta = \sum_{k} \beta^k. \]

C.3. MOMENTUM EQUATION

For an arbitrary volume \( \tau \) of the multicomponent continuum, the total rate of change of linear momentum in the \( j \)th coordinate direction must equal the sum of the following: (1) the surface integral of the stress vector \( \sum_{k} \sigma^k_{ij} n_i \), where \( \sigma^k_{ij} \) equals* the component in the direction \( x_j \) of the stress vector acting on that face of an elemental parallelepiped of species \( K \) which has an

* The species vectors \( \sigma^k_{ij} n_i \) and \( \rho f^j \) represent the sums of all forces which act upon species \( K \) and which move with the velocity of species \( K \) in the mixture. These definitions are used in Section C.5 to identify our results with the results obtained from kinetic theory.
outward normal in the direction $x_i$; (2) the volume integral of the total vector body force $\sum_K \rho^K f^K_j$ acting on unit volume of mixture, where $f^K_j$ is the vector body force per unit mass of species $K$; and (3) the volume integral of the total rate of generation of momentum in unit volume through production of species. Let the rate of generation of momentum in unit volume for species $K$ be $w^K m^K_j$, where $m^K_j$ is the average momentum of the generated mass of species $K$ per unit mass of species $K$. We postulate that, overall, linear momentum is neither created nor destroyed by chemical reactions; the consequent conservation principle states that the total rate of generation of linear momentum per unit volume by chemical production of species is zero:

$$\sum_K w^K m^K_j = 0. \quad (21)$$

The total rate of change of linear momentum is then expressed mathematically by

$$\sum_K \left( \frac{d}{dt} \int_{\tau_K} \rho Y^K v^K_j d\tau \right)_{\tau_K = \tau} = \int_{\tau} \sum_K \sigma^K_{ij} n_i d\sigma + \int_{\tau} \sum_K \rho^K f^K_j d\tau. \quad (22)$$

In view of the divergence theorem, equation (1), and the transport relation given in equation (20), with

$$\beta^K = Y^K v^K_j, \quad \beta = v_j,$$

equation (22) becomes

$$\int_{\tau} \left[ \rho \frac{Dv_j}{Dt} + \left( \rho \sum_K Y^K v^K_j V^K_j \right)_{ij} \right] d\tau = \int_{\tau} \sum_K \left( \sigma^K_{ij,i} + \rho^K f^K_j \right) d\tau. \quad (23)$$

We now define $\sigma^K_{ij}$, the diffusion stress tensor, as

$$\sigma^K_{ij} = \rho \sum_K Y^K V^K_i V^K_j \quad (24)$$

and $f_j$, the vector body force per unit mass of mixture, as

$$f_j = \sum_K f^K_j Y^K. \quad (25)$$

Since $\tau$ is arbitrary, equation (23) then leads to an expression for overall conservation of momentum, namely,

$$\rho \frac{Dv_j}{Dt} = \rho \frac{\partial v_j}{\partial t} + \rho v_j v_{ji,i} + \sum_K \sigma^K_{ij,i} + \sigma^K_{ij,i} + \rho f_j. \quad (26)$$

If we define $\sigma_{ij}$ as

$$\sigma_{ij} = \sum_K \sigma^K_{ij} + \sigma^K_{ij}, \quad (27)$$

then equation (26) is reduced to the well-known form of the momentum equation for one-component systems. Therefore, $\sigma_{ij}$ is the stress tensor and
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\( \rho f_j \) is the body force acting on an elemental parallelepiped which is moving with the mass-weighted average velocity \( v'_j \). Furthermore, we can express \( \sigma_{ij} \) as a sum of partial stress tensors \( \sigma_{ij}^{*,K} \)

\[
\sigma_{ij} \equiv \sum_K \sigma_{ij}^{*,K}, \tag{28}
\]

where, from equations (24) and (27)

\[
\sigma_{ij}^{*,K} \equiv \sigma_{ij}^K - \rho Y_i^KV_j^KV_j. \tag{29}
\]

Each stress tensor can then always be expressed as the sum of a mean pressure tensor, a viscous stress tensor, and a viscous diffusion-stress tensor; thus,

\[
\sigma_{ij}^{*,K} \equiv -p^K \delta_{ij} + \tau_{ij}^{V,K} + \tau_{ij}^{D,K}, \tag{29}
\]

where

\[
p^K \equiv -\frac{1}{3} \sigma_{ii}^{*,K},
\]

and

\[
\sigma_{ij} \equiv -p \delta_{ij} + \tau_{ij}^{V} + \tau_{ij}^{D}, \tag{30}
\]

where

\[
p \equiv -\frac{1}{3} \sigma_{ii}.
\]

The total pressure \( p \) is the sum of the partial pressures \( p^K \) for the different species, that is,

\[
p = \sum_K p^K, \tag{31}
\]

and so, in view of equation (28), it follows now that

\[
\tau_{ij}^{V} = \sum_K \tau_{ij}^{V,K}, \tag{32}
\]

\[
\tau_{ij}^{D} = \sum_K \tau_{ij}^{D,K}. \tag{33}
\]

The equations of von Kármán [6], [7] are obtained by using equation (30) in equation (26), namely,

\[
\rho \frac{Dv'_j}{Dt} = -p_{,j} + (\tau_{ij}^{V} + \tau_{ij}^{D})_{,i} + \rho f_j. \tag{34}
\]

C.4. ENERGY EQUATION

For an arbitrary volume \( \tau \) of the multicomponent continuum, the first law of thermodynamics states that

\[
\text{Rate of increase of (internal plus kinetic) energy} = \text{rate at which work is done on} \ \tau \ (\text{by body forces plus surface stresses}) + \text{rate of inward transport of heat by radiation, thermal conduction, and other transport process through the surface} \ \sigma \ \text{enclosing} \ \tau + \text{rate of generation of energy through production of species within} \ \tau + \text{rate at which work is done on material produced within} \ \tau.
\]
Let $u^K$ denote the absolute internal energy of species $K$ per unit mass of species $K$ and let $u$ denote the absolute internal energy per unit mass of mixture. Then

$$u = \sum_K Y^K u^K. \quad (35)$$

The kinetic energy of species $K$ per unit mass of species $K$ is $\frac{1}{2}v_j^K v_j^K$. The total rate at which work is done on $\tau$ by surface stresses and body forces is represented as the superposition of the rate of work done on the individual continua by their own surface stresses and body forces.

For the mass $w^K$ of species $K$, which is generated by chemical reaction in unit volume per unit time, the sum of (1) the internal and kinetic energy carried by this mass, and (2) the work done on this mass in unit time, is $w^K(\eta^K + \frac{1}{2}m_j^K m_j^K)$, where $\eta^K$ is the average specific enthalpy of generated mass of species $K$. We postulate that, overall, energy is redistributed among various states but is neither created nor destroyed by chemical reaction; the consequent conservation principle states that the total rate of generation of (absolute enthalpy plus kinetic energy) per unit volume by chemical production of species is zero:

$$\sum_K w^K(\eta^K + \frac{1}{2}m_j^K m_j^K) = 0. \quad (36)$$

The analytical expression of the first law of thermodynamics, subject to the fundamental postulates of independence and conservation, is therefore

$$\sum_K \left[ \frac{d}{dt} \int_{\partial x_k} \rho Y^K(u^K + \frac{1}{2}v_j^K v_j^K) \, d\tau \right]_{x=x_0} = \sum_K \left[ \int_{\sigma} \sigma^K_{ij} n_i v_j^K \, d\sigma + \int_{\tau} \rho^K f^K v_j^K \, d\tau \right] - \int_{\sigma} \sum_K q_j^K v_j \, d\sigma. \quad (37)$$

Here $q_j^K$ is the heat flux vector for species $K$, taken as positive for outward heat transport. Equation (37) can be transformed by the use of equation (20) with

$$\beta^K = Y^K u^K + \frac{1}{2} Y^K v_j^K v_j^K$$

and

$$\beta = u + \frac{1}{2}v_j v_j + \frac{1}{2} \sum_K Y^K v_i^K v_j^K. \quad (38)$$

Since $\tau$ is arbitrary, the following differential equation for overall conservation of energy then results:

$$\rho \frac{D}{Dt} \left( u + \frac{1}{2}v_j v_j \right) + \frac{1}{2} \rho \frac{D}{Dt} \left( \sum_K Y^K v_i^K v_j^K \right) + \left[ \rho \sum_K (Y^K u^K v_i^K + \frac{1}{2} Y^K v_j^K v_j^K) \right]_i = \rho \sum_K Y^K f^K v_j^K + \sum_K (\sigma^K_{ij} v_j^K) \, d\tau - \sum_K q_j^K v_j. \quad (39)$$

* The quantity $\eta^K$ should not be confused with the total (average) specific enthalpy of species $K$, which is denoted by $h^K$, as in equation (40).
Let $h^K$ denote the absolute specific enthalpy of species $K$, which is defined as

$$Y^K h^K = Y^K u^K + \frac{p^K}{\rho}.$$  \hspace{1cm} (40)

The absolute specific enthalpy of the mixture is then $h = \sum_K Y^K h^K = u + p/\rho$. The total heat-flux vector is defined as

$$q_j = \sum_K q_j^K.$$  \hspace{1cm} (41)

In view of the definitions given by equations (29), (30), (40), and (41), equation (39) can be written in a desired form:

$$\rho \frac{D}{Dt} \left( u + \frac{1}{2}v_j v'_j \right) + \left( \rho \sum_K Y^K h^K V^K_f \right)_{,j}$$
$$= \rho f_j v'_j - (pv'_j),_j$$
$$+ \left[ (\tau_{ij}^V + \tau_{ij}^p) v'_j \right]_i - q_j,_{,j}$$
$$+ \rho \sum_K Y^K f^K_j V^K_f + \sum_K \left[ (\tau_{ij}^{V^K} + \tau_{ij}^{p^K}) V^K_f \right]_i$$
$$+ \frac{1}{2} \left( \rho \sum_K Y^K V^K_v V^K_v V^K_f \right)_{,i} - \rho \frac{D}{Dt} \left( \frac{1}{2} \sum_K Y^K V^K_v V^K_f \right).$$  \hspace{1cm} (42)

C.5. COMPARISON BETWEEN THE CONSERVATION LAWS DERIVED FOR INDEPENDENT COEXISTENT CONTINUA AND THE KINETIC-THEORY RESULTS FOR MULTICOMPONENT GAS MIXTURES

In order to show that the model of independent, coexistent continua represents correctly a real mixture of gases composed of different chemical species, we must compare the results obtained from this model with those of the kinetic theory of nonuniform gas mixtures (see Appendix D). Quantities such as the density $\rho$, the mass-weighted average velocity $v'_j$, and the body force $f_j$ have obviously analogous meanings in both the kinetic theory and the coexistent-continua model. On the other hand, the precise kinetic-theory meaning of terms such as the stress tensor $\sigma_{ij}^V$, the absolute internal energy per unit mass $u^K$, and the heat-flux vector $q^K_f$ is not immediately apparent. In view of the known success of continuum theory for one-component systems, we shall identify the continuum-theory properties $\sigma_{ij}^V$, $u^K$ and $q^K_f$ for species $K$ with their kinetic-theory counterparts. The proof then involves a comparison of the conservation equations obtained from multi-component-continuum theory (replacing continuum properties for each species by their kinetic-theory definitions) with the conservation equations
obtained from the kinetic theory of nonuniform gas mixtures. For readers not familiar with the kinetic-theory approach, to obtain a more complete understanding of this section it is advisable to read Appendix D first.

C.5.1. Definitions of kinetic theory

Let $c_{jK}^m$ be the velocity of a particular molecule $m$ of species $K$, and let $V_{jK}^m$ be the velocity of this molecule in excess of the velocity $v_j^K$ which is identified in kinetic theory as the mean of velocity of all molecules of species $K$. Then

$$c_{jK}^m = v_j^K + V_{jK}^m = v_j^K + V_{jK}^m,$$

$$\langle c_{jK}^m \rangle = v_j^K \quad \text{and} \quad \langle V_{jK}^m \rangle = 0,$$

where the angle brackets indicate an average over all molecules of species $K$ taken with respect to a distribution function appropriate for the mixture.

From kinetic theory, the following definitions* for the properties of species $K$ in the mixture are obtained:

$$\sigma_{ij}^K \equiv -\rho^K \langle V_{iK}^m V_{jK}^m \rangle,$$

$$u^K \equiv \frac{1}{2} \rho^K \langle (\frac{1}{2} V_{iK}^m V_{iK}^m + i_{K}^m) V_{jK}^m \rangle + i^K,$$

$$q_j^K \equiv \rho^K \langle (\frac{1}{2} V_{iK}^m V_{iK}^m + i_{K}^m) V_{jK}^m \rangle$$

$$\equiv \rho^K \langle (\frac{1}{2} V_{iK}^m V_{iK}^m + i_{K}^m) V_{jK}^m \rangle.$$

In equations (44) and (45), $u^K$, $m$, the total internal energy per unit mass of a molecule of species $K$, is expressed as the sum of $\frac{1}{2} V_{iK}^m V_{iK}^m$, the molecular translatory kinetic energy per unit mass, and $i_{K}^m$, the contribution of additional internal energy terms (rotational, vibrational, etc.) per unit mass. We have then defined $u^K \equiv \langle u^K \rangle$ and $i^K \equiv \langle i^K \rangle$.

The corresponding definitions in the kinetic theory for the properties of the gas mixture will be denoted here by the superscript $T$; these are† the mixture stress tensor $\sigma_{ij}^T$, where

$$\sigma_{ij}^T \equiv -\sum_k \rho^K \langle (V_{iK}^m + V_{jK}^m)(V_{jK}^m + V_{jK}^m) \rangle$$

$$\equiv -\sum_k \rho^K \langle V_{iK}^m V_{jK}^m \rangle - \sum_k \rho^K V_{iK}^m V_{jK}^m,$$

the internal energy per unit mass of mixture $u^T$, where

$$\rho u^T \equiv \sum_k \left[ \frac{1}{2} \rho^K \langle V_{jK}^m + V_{jK}^m \rangle + \rho^K \langle V_{jK}^m + V_{jK}^m \rangle \right]$$

$$\equiv \frac{1}{2} \sum_k \rho^K \langle V_{jK}^m V_{jK}^m \rangle + \frac{1}{2} \sum_k \rho^K V_{jK}^m V_{jK}^m + \sum_k \rho^K i^K.$$

* See, for example, equations (18), (23), (24), (25), and (28) in Section D.2.
† See, for example, equations (21), (27), and (29) in Section D.2.
and the heat-flux vector for the mixture $q^T_j$, where

$$ q^T_j = \sum_K \rho^K \langle \frac{1}{2} (V_i V_i^K + V_i^K V_i^K + i^K m_j) (V_j V_j^K + V_j^K V_j^K) \rangle $$

$$ = \sum_K \rho^K \left\{ \frac{1}{2} \langle V_i V_i^K V_j V_j^K + \frac{1}{2} V_i^K V_j^K \rangle \right\} $$

$$ + V_i \langle V_i V_i^K V_j V_j^K \rangle + \frac{1}{2} V_i^K V_j^K V_j^K + \langle i^K m_j V_j^K \rangle + \langle i^K V_j V_j^K \rangle. \quad (48) $$

When use is made of equations (43), (44), and (45) in equations (46), (47), and (48), the following identities are obtained between the properties $\sigma_{ij}^T$, $\rho u^T$, and $q^T_j$ of the gas mixture and the properties $\sigma_{ij}^K$, $\rho^K u^K$ and $q^K_j$ of the individual species:

$$ \sigma_{ij}^T = \sum_K \sigma_{ij}^K - \sum_K \rho^K V_i^K V_j^K, \quad (49) $$

$$ \rho u^T = \sum_K \rho^K u^K + \frac{1}{2} \sum_K \rho^K V_i^K V_j^K, \quad (50) $$

$$ q^T_j = \sum_K q^T_j - \sum_K \sigma_{ij}^K V_i^K + \sum_K \rho^K u^K V_j^K + \frac{1}{2} \sum_K \rho^K V_i^K V_j^K V_j^K. \quad (51) $$

In each of the above relations, the property for the mixture is equal to the sum, over all species, of the corresponding property for the components plus various diffusion terms. The diffusion terms arise because the reference coordinate system for species $K$ is taken to move with velocity $v_j^K + V_j^K$, which is the mass-weighted average velocity for molecules in species $K$ alone; the reference coordinate system for the mixture on the other hand is taken to move with velocity $v_j$, which is the mass-weighted average velocity for all molecules in the mixture. The latter is a natural coordinate system in that it is consistent with equations (19) and (34).

Derivations of conservation equations from the viewpoint of kinetic theory usually do not exhibit explicitly the diffusion terms, such as diffusion stresses, that appear on the right-hand sides of equations (49), (50), and (51), since it is unnecessary to introduce quantities such as $\sigma_{ij}^K$ specifically in these derivations. Kinetic-theory developments work directly with the left-hand sides of equations (49), (50), and (51). Transport coefficients (Appendix E) are defined only in terms of these kinetic-theory quantities because prescriptions for calculating the individual continua transports, $\sigma_{ij}^K$ and $q^K_j$, are unduly complex. Moreover, measurement of diffusion stresses is feasible only by direct measurement of diffusion velocities, followed by use of equation (24). Therefore, it has not been fruitful to study the diffusion terms which, in a sense, may be viewed as artifacts of the continuum approach.

**C.5.2. Comparison of conservation equations**

The conservation equation for species $K$, as given by equation (17), is readily seen to be identical with the corresponding relation in the kinetic
theory for multicomponent gas mixtures if \( w^K \) is the net mass rate of production of species \( K \) per unit volume by chemical reaction.\(^*\) Explicit evaluation of \( w^K \) requires the introduction of the laws of chemical kinetics.\(^†\)

The expression for overall conservation of momentum, equation (26), is also identical with the corresponding relation in the kinetic theory,\(^‡\) since a comparison of equations (27) and (49) shows that \( \sigma_{ij} \equiv \sigma_{ij}^T \).

To demonstrate the equivalence of the energy conservation equations, rewrite equation (39) in the form

\[
\rho \frac{D}{Dt} \left[ \sum_K \left( Y^K u^K + \frac{1}{2} Y^K V^K u^K \right) + \frac{1}{2} v'_j v'_j \right] + \left( \rho \sum_K Y^K u^K V^K \right)_{,j} = \rho f_j v'_j + \rho \sum_K Y^K f^K V^K_{,j} + \left( v'_j \sum_K \sigma^K_{ij} \right)_{,i} + \sum_K \left( \sigma^K_{ij} V^K_{,j} \right)_{,i} - \sum_K q^K_{j,j} - \left( \rho v'_j \sum_K Y^K V^K_{,j} V^K_{,i} \right)_{,i} - \frac{1}{2} \left( \rho \sum_K Y^K V^K_{,j} V^K_{,i} \right)_{,i}. \tag{52}
\]

Replacing \( \sum_K \sigma^K_{ij} \), \( \sum_K Y^K u^K \) and \( \sum_K q^K_{j,j} \) by their kinetic-theory equivalents, as given by equations (49), (50), and (51), reduces equation (52) to

\[
\rho \frac{D}{Dt} \left[ u^T + \frac{1}{2} v'_j v'_j \right] = \rho f_j v'_j + \rho \sum_K Y^K f^K V^K_{,j} - q^K_{j,j} + \left( \sigma^K_{ij} v'_j \right)_{,i}. \tag{53}
\]

Multiplying the momentum conservation equations by \( v'_j \) and contracting produces the scalar equation

\[
\frac{1}{2} \rho \frac{D}{Dt} (v'_j v'_j) = \sigma^K_{ij, i} v'_j + \rho f_j v'_j. \tag{54}
\]

With this relation and equation (19), equation (53) can be placed in a form which is identical with the usual form of the result obtained from kinetic theory,\(^§\) namely,

\[
\rho \frac{D}{Dt} (u^T) = \rho \sum_K Y^K f^K V^K_{,j} - q^K_{j,j} + \sigma^K_{ij} v'_j_{,i}. \tag{55}
\]

### C.6. PROOF OF EQUATION (6)

In order to prove equation (6), it is more convenient to work from equation (3) than from the limiting relation given in equation (5) and also to introduce the Lagrangian representation [10]. For any continuum \( K \), let the three parameters \( a^K_{ij} \) identify the individual point particles of continuum \( K \); for

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\(^*\) See, for example, equation (D-39).

\(^†\) See Appendix B or Chapter 1.

\(^‡\) See, for example, equation (D-35).

\(^§\) See, for example, equation (D-37).
Continuum Derivation of the Conservation Equations

Definiteness, suppose that \( a^K_i \) are the spatial coordinates of the particles of continuum \( K \) at some fixed time \( t_0 \). The spatial coordinates \( x_i \) for any particle \( a^K_j \) at any time \( t, t \geq t_0 \), are then assumed to be given by the functions \( x^K_i(a^K_j, t) \) which are taken to be single-valued and at least twice continuously differentiable with respect to each of their variables:

\[
x_i = x^K_i(a^K_j, t), \quad t \geq t_0,
\]

and \( a^K_j = x^K_i(a^K_j, t_0) \). The transformations are assumed to be one-to-one, so that the inverse transformations \( a^K_j(x_j, t) \) also exist and are twice continuously differentiable. The flow velocities, or "particle velocities," for continuum \( K \), \( v^K_i(a^K_j, t) \), are then defined as

\[
v^K_i(a^K_j, t) \equiv \frac{\partial x^K_i}{\partial t} = v_i^K(x_j, t),
\]

where the \( v^K_i \) are defined by the inverse transformation. Similarly, the Jacobian of equation (56) is given as \( \Delta^K \) or \( \Delta^K \):

\[
\Delta^K(a^K_j, t) \equiv \det \left( \frac{\partial x^K_i}{\partial a^K_j} \right) = \Delta^K(x_j, t).
\]

If the integral of equation (3) is changed with the use of equation (56) to an integration at time \( t = t_0 \) over the volume \( \tau^K_0 \), then

\[
A^K(t) = \int_{\tau^K_0} \alpha^K(a^K_j, t) \Delta^K d\tau^K_0.
\]

The definition of the time derivative given in equation (5) is therefore equivalent to

\[
\frac{dA^K}{dt} = \int_{\tau^K_0} \left( \frac{\partial \alpha^K}{\partial t} + \alpha^K \frac{\partial \Delta^K}{\partial t} \right) d\tau^K_0.
\]

But it is readily shown that

\[
\frac{\partial \Delta^K}{\partial t} \equiv \frac{\partial v^K_i}{\partial x_i} \Delta^K = v^K_i \Delta^K
\]

and, therefore, equation (59) may be written as

\[
\frac{dA^K}{dt} = \int_{\tau^K_0} \left( \frac{\partial \alpha^K}{\partial t} + v^K_i \alpha^K \right) \Delta^K d\tau^K_0.
\]

Transformation of equation (60) to spatial coordinates leads to equation (6).

* In this section only, an asterisk on any function indicates that its variables are \( a_i, t \); functions without asterisks have the independent variables \( x_i, t \).

† See [10], equation (7.07).
REFERENCES

1. L. Prandtl, Essentials of Fluid Dynamics, Glasgow: Blackie and Sons, Ltd., 1952, Chapter II.